



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:23 PM UTC

PDB ID : 3VGO / pdb\_00003vgo  
Title : Crystal structure of the N-terminal fragment of Cbl-b  
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Deposited on : 2011-08-18  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

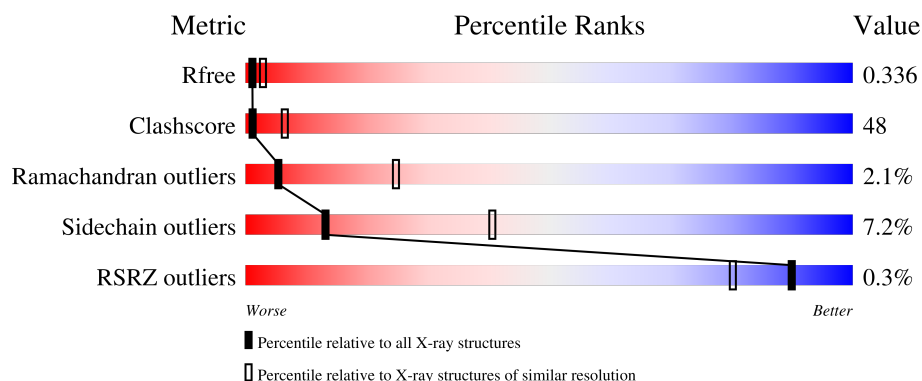
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 394    |                  |
| 1   | B     | 394    |                  |
| 1   | C     | 394    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6668 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 E3 ubiquitin-protein ligase CBL-B.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 287      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2196  | 1430 | 371 | 385 | 10 |         |         |       |
| 1   | B     | 294      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2252  | 1465 | 384 | 393 | 10 |         |         |       |
| 1   | C     | 292      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2220  | 1450 | 370 | 391 | 9  |         |         |       |

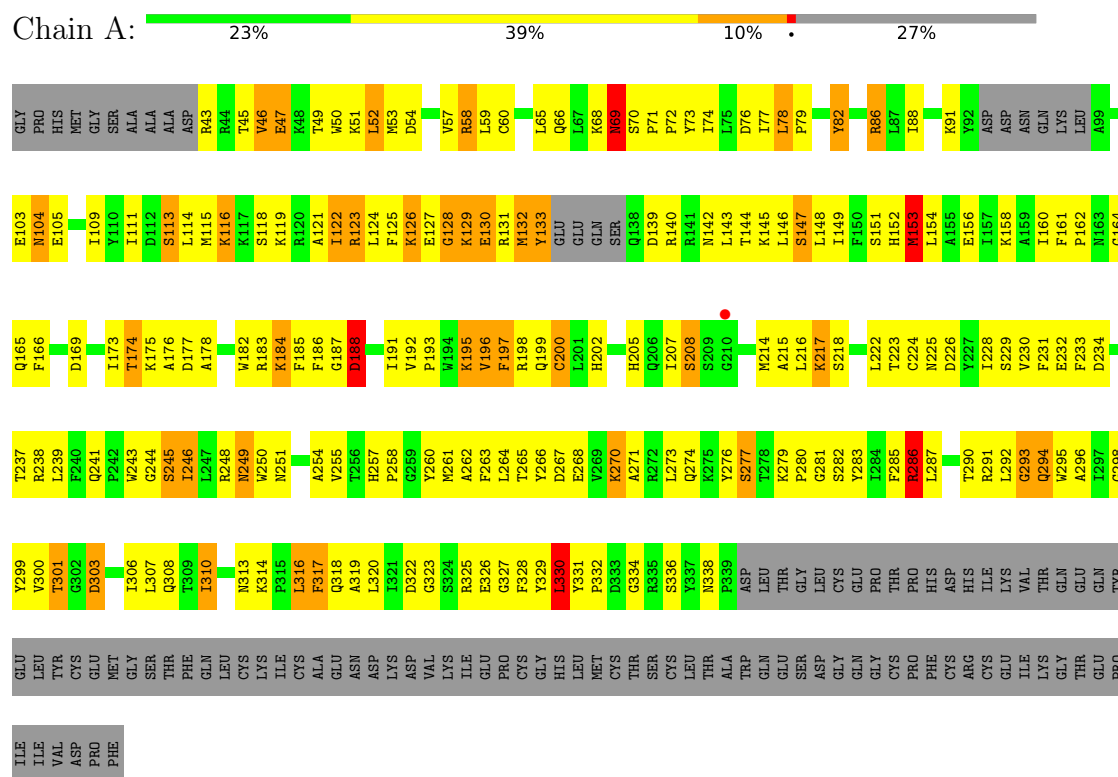
There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 33      | GLY      | -      | expression tag | UNP Q13191 |
| A     | 34      | PRO      | -      | expression tag | UNP Q13191 |
| A     | 35      | HIS      | -      | expression tag | UNP Q13191 |
| A     | 36      | MET      | -      | expression tag | UNP Q13191 |
| A     | 37      | GLY      | -      | expression tag | UNP Q13191 |
| A     | 38      | SER      | -      | expression tag | UNP Q13191 |
| B     | 33      | GLY      | -      | expression tag | UNP Q13191 |
| B     | 34      | PRO      | -      | expression tag | UNP Q13191 |
| B     | 35      | HIS      | -      | expression tag | UNP Q13191 |
| B     | 36      | MET      | -      | expression tag | UNP Q13191 |
| B     | 37      | GLY      | -      | expression tag | UNP Q13191 |
| B     | 38      | SER      | -      | expression tag | UNP Q13191 |
| C     | 33      | GLY      | -      | expression tag | UNP Q13191 |
| C     | 34      | PRO      | -      | expression tag | UNP Q13191 |
| C     | 35      | HIS      | -      | expression tag | UNP Q13191 |
| C     | 36      | MET      | -      | expression tag | UNP Q13191 |
| C     | 37      | GLY      | -      | expression tag | UNP Q13191 |
| C     | 38      | SER      | -      | expression tag | UNP Q13191 |

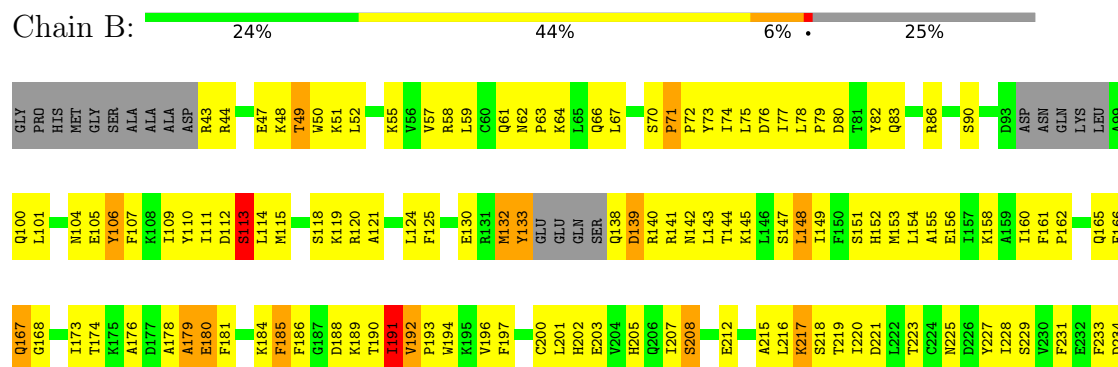
### 3 Residue-property plots

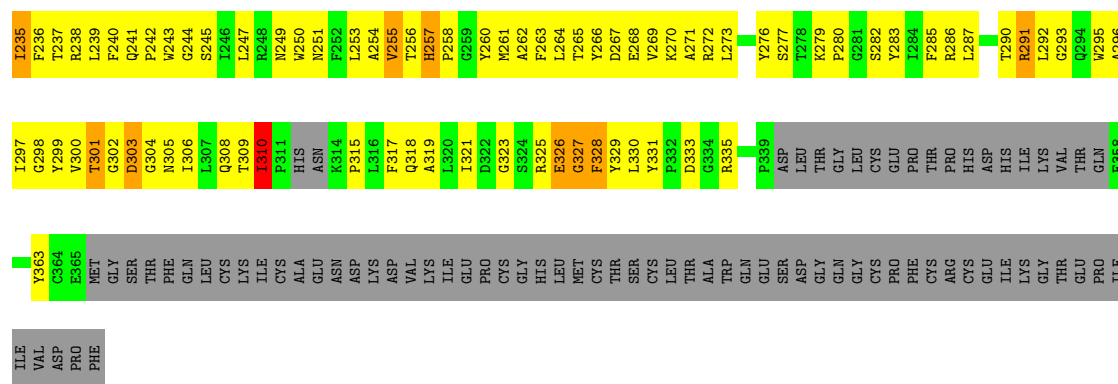
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: E3 ubiquitin-protein ligase CBL-B

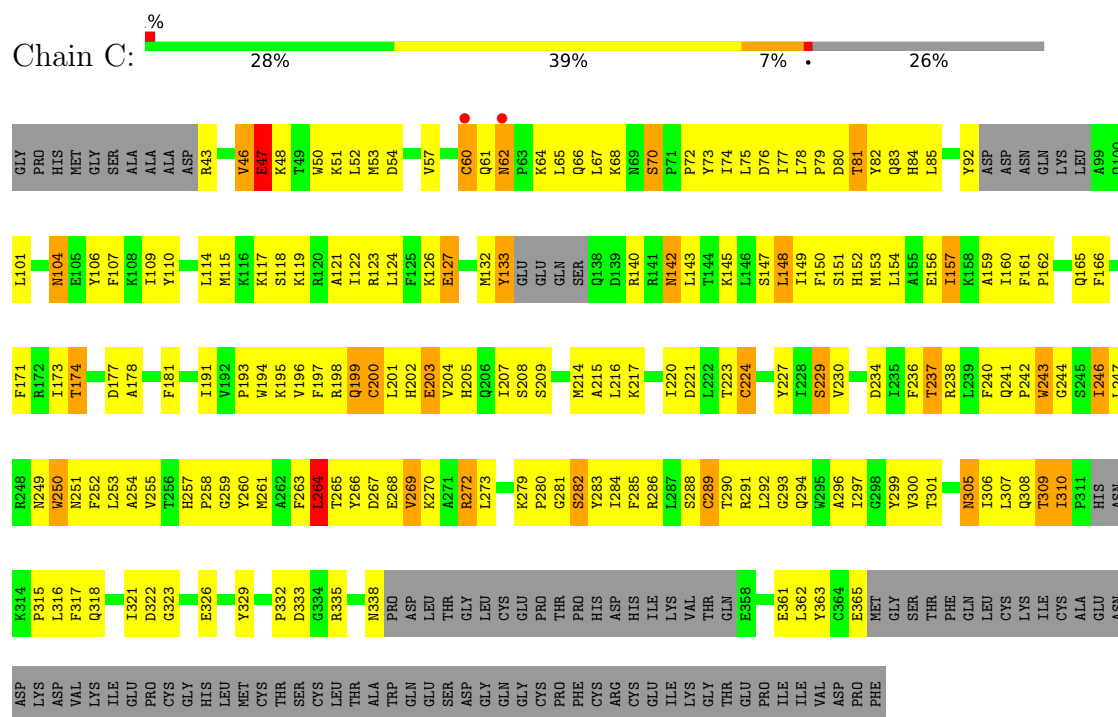


#### • Molecule 1: E3 ubiquitin-protein ligase CBL-B





• Molecule 1: E3 ubiquitin-protein ligase CBL-B



## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 31                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 98.88Å 98.88Å 105.18Å<br>90.00° 90.00° 120.00°                 | Depositor        |
| Resolution (Å)                                                          | 42.82 – 3.10<br>42.82 – 3.10                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.3 (42.82-3.10)<br>97.3 (42.82-3.10)                         | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                           | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.73 (at 3.01Å)                                                | Xtriage          |
| Refinement program                                                      | CNS                                                            | Depositor        |
| R, $R_{free}$                                                           | 0.270 , 0.328<br>0.272 , 0.336                                 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1909 reflections (8.28%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.1                                                           | Xtriage          |
| Anisotropy                                                              | 0.036                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 69.4                                                    | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$    | Xtriage          |
| Estimated twinning fraction                                             | 0.074 for -h,-k,l<br>0.074 for h,-h-k,-l<br>0.477 for -k,-h,-l | Xtriage          |
| Reported twinning fraction                                              | 0.500 for H, K, L<br>0.500 for h+k,-k,-l                       | Depositor        |
| Outliers                                                                | 0 of 23046 reflections                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                           | EDS              |
| Total number of atoms                                                   | 6668                                                           | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 52.0                                                           | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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     | 0.90         | 3/2253 (0.1%) | 1.40        | 30/3063 (1.0%) |
| 1   | B     | 0.89         | 4/2308 (0.2%) | 1.29        | 30/3133 (1.0%) |
| 1   | C     | 0.77         | 2/2275 (0.1%) | 1.25        | 23/3091 (0.7%) |
| All | All   | 0.85         | 9/6836 (0.1%) | 1.32        | 83/9287 (0.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 68  | LYS  | CA-CB | 7.53  | 1.62        | 1.52     |
| 1   | B     | 132 | MET  | SD-CE | 6.47  | 1.95        | 1.79     |
| 1   | A     | 69  | ASN  | CA-CB | 6.35  | 1.64        | 1.53     |
| 1   | B     | 70  | SER  | CA-C  | 6.23  | 1.59        | 1.52     |
| 1   | B     | 191 | ILE  | CA-CB | 5.93  | 1.62        | 1.54     |
| 1   | A     | 313 | ASN  | CA-CB | 5.62  | 1.57        | 1.53     |
| 1   | B     | 310 | ILE  | CA-CB | 5.48  | 1.61        | 1.54     |
| 1   | C     | 309 | THR  | CA-C  | -5.38 | 1.46        | 1.52     |
| 1   | C     | 157 | ILE  | CA-CB | -5.25 | 1.48        | 1.54     |

All (83) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 100 | GLN  | N-CA-C | -11.53 | 98.73       | 111.07   |
| 1   | A     | 47  | GLU  | N-CA-C | -11.45 | 98.54       | 111.82   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 70  | SER  | N-CA-C  | -11.09 | 90.07       | 109.48   |
| 1   | B     | 185 | PHE  | N-CA-C  | 10.78  | 122.60      | 111.07   |
| 1   | B     | 180 | GLU  | N-CA-C  | -10.03 | 100.04      | 110.97   |
| 1   | C     | 119 | LYS  | N-CA-C  | 9.43   | 121.55      | 111.28   |
| 1   | A     | 217 | LYS  | N-CA-C  | -9.33  | 101.09      | 111.07   |
| 1   | A     | 128 | GLY  | N-CA-C  | 9.09   | 123.92      | 112.83   |
| 1   | A     | 116 | LYS  | N-CA-C  | -8.97  | 100.35      | 111.11   |
| 1   | A     | 314 | LYS  | N-CA-C  | -8.71  | 96.98       | 110.14   |
| 1   | C     | 269 | VAL  | N-CA-C  | -8.62  | 102.15      | 110.42   |
| 1   | A     | 129 | LYS  | CB-CA-C | -8.56  | 106.70      | 116.54   |
| 1   | C     | 47  | GLU  | N-CA-C  | -8.42  | 102.11      | 111.28   |
| 1   | A     | 316 | LEU  | N-CA-C  | -8.30  | 102.17      | 111.14   |
| 1   | B     | 255 | VAL  | N-CA-C  | 8.26   | 119.52      | 111.67   |
| 1   | A     | 303 | ASP  | N-CA-C  | -8.25  | 103.00      | 113.72   |
| 1   | A     | 274 | GLN  | N-CA-C  | -8.11  | 103.17      | 113.23   |
| 1   | C     | 250 | TRP  | N-CA-C  | 7.35   | 119.29      | 111.28   |
| 1   | B     | 120 | ARG  | N-CA-C  | -7.26  | 103.30      | 111.07   |
| 1   | B     | 167 | GLN  | N-CA-C  | -7.23  | 102.75      | 112.94   |
| 1   | B     | 208 | SER  | N-CA-C  | 7.20   | 120.04      | 111.33   |
| 1   | C     | 117 | LYS  | N-CA-C  | -6.88  | 103.86      | 111.36   |
| 1   | A     | 188 | ASP  | N-CA-C  | 6.82   | 119.55      | 111.71   |
| 1   | B     | 302 | GLY  | N-CA-C  | -6.77  | 106.88      | 114.40   |
| 1   | C     | 62  | ASN  | CA-C-N  | 6.72   | 126.23      | 119.24   |
| 1   | C     | 62  | ASN  | C-N-CA  | 6.72   | 126.23      | 119.24   |
| 1   | C     | 289 | CYS  | N-CA-C  | -6.71  | 103.77      | 112.23   |
| 1   | B     | 90  | SER  | N-CA-C  | -6.62  | 103.99      | 111.14   |
| 1   | C     | 209 | SER  | N-CA-C  | 6.62   | 118.26      | 108.60   |
| 1   | C     | 132 | MET  | N-CA-C  | 6.58   | 120.41      | 112.38   |
| 1   | A     | 86  | ARG  | N-CA-C  | -6.48  | 103.72      | 111.69   |
| 1   | B     | 109 | ILE  | N-CA-C  | 6.42   | 117.21      | 110.72   |
| 1   | B     | 235 | ILE  | N-CA-C  | -6.42  | 104.90      | 110.74   |
| 1   | B     | 179 | ALA  | N-CA-C  | -6.37  | 104.38      | 111.71   |
| 1   | A     | 118 | SER  | N-CA-C  | 6.36   | 118.74      | 111.11   |
| 1   | C     | 309 | THR  | N-CA-C  | -6.34  | 99.69       | 109.52   |
| 1   | A     | 91  | LYS  | N-CA-C  | 6.32   | 118.97      | 111.33   |
| 1   | C     | 305 | ASN  | N-CA-C  | 6.29   | 118.90      | 110.35   |
| 1   | B     | 188 | ASP  | N-CA-C  | 6.15   | 120.33      | 112.34   |
| 1   | C     | 261 | MET  | N-CA-C  | 6.10   | 120.59      | 112.30   |
| 1   | B     | 106 | TYR  | N-CA-C  | -6.08  | 104.73      | 111.36   |
| 1   | B     | 71  | PRO  | C-N-CD  | 6.03   | 133.87      | 120.60   |
| 1   | C     | 203 | GLU  | N-CA-C  | -6.01  | 105.05      | 112.38   |
| 1   | A     | 277 | SER  | N-CA-C  | -5.89  | 104.04      | 111.11   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 111 | ILE  | N-CA-C  | -5.87 | 104.79      | 110.72   |
| 1   | A     | 293 | GLY  | N-CA-C  | -5.82 | 107.22      | 115.43   |
| 1   | B     | 70  | SER  | CB-CA-C | 5.78  | 117.87      | 109.20   |
| 1   | B     | 165 | GLN  | N-CA-C  | 5.77  | 118.34      | 110.55   |
| 1   | A     | 281 | GLY  | N-CA-C  | -5.70 | 107.48      | 113.58   |
| 1   | C     | 152 | HIS  | N-CA-C  | 5.69  | 117.49      | 111.28   |
| 1   | A     | 104 | ASN  | N-CA-C  | -5.69 | 101.76      | 110.30   |
| 1   | B     | 328 | PHE  | N-CA-C  | -5.64 | 106.94      | 113.88   |
| 1   | C     | 194 | TRP  | N-CA-C  | 5.63  | 117.28      | 111.03   |
| 1   | C     | 122 | ILE  | N-CA-C  | -5.58 | 104.89      | 110.30   |
| 1   | C     | 199 | GLN  | N-CA-C  | -5.55 | 105.14      | 111.07   |
| 1   | A     | 208 | SER  | N-CA-C  | 5.53  | 122.57      | 110.80   |
| 1   | B     | 113 | SER  | N-CA-C  | -5.49 | 105.21      | 111.14   |
| 1   | B     | 139 | ASP  | N-CA-C  | -5.49 | 104.94      | 111.69   |
| 1   | A     | 294 | GLN  | N-CA-C  | 5.49  | 118.03      | 108.76   |
| 1   | A     | 153 | MET  | N-CA-C  | -5.42 | 105.48      | 111.71   |
| 1   | B     | 257 | HIS  | CA-C-N  | 5.36  | 125.05      | 119.64   |
| 1   | B     | 257 | HIS  | C-N-CA  | 5.36  | 125.05      | 119.64   |
| 1   | B     | 49  | THR  | N-CA-C  | -5.34 | 104.70      | 111.11   |
| 1   | B     | 297 | ILE  | N-CA-C  | 5.31  | 115.51      | 107.75   |
| 1   | A     | 270 | LYS  | N-CA-C  | -5.31 | 104.54      | 111.02   |
| 1   | A     | 301 | THR  | N-CA-C  | 5.31  | 118.38      | 110.52   |
| 1   | A     | 144 | THR  | N-CA-C  | 5.26  | 117.02      | 111.28   |
| 1   | A     | 286 | ARG  | N-CA-C  | 5.26  | 116.80      | 108.96   |
| 1   | C     | 264 | LEU  | N-CA-C  | 5.22  | 116.08      | 108.14   |
| 1   | B     | 62  | ASN  | CA-C-N  | 5.22  | 126.36      | 119.84   |
| 1   | B     | 62  | ASN  | C-N-CA  | 5.22  | 126.36      | 119.84   |
| 1   | B     | 277 | SER  | N-CA-C  | -5.22 | 106.92      | 113.28   |
| 1   | B     | 303 | ASP  | N-CA-C  | -5.21 | 106.76      | 113.02   |
| 1   | C     | 293 | GLY  | N-CA-C  | -5.17 | 108.70      | 115.47   |
| 1   | A     | 254 | ALA  | N-CA-C  | 5.13  | 119.11      | 113.21   |
| 1   | C     | 237 | THR  | N-CA-C  | 5.13  | 116.87      | 111.28   |
| 1   | C     | 81  | THR  | N-CA-C  | -5.11 | 105.40      | 110.97   |
| 1   | B     | 217 | LYS  | N-CA-C  | -5.09 | 105.17      | 111.33   |
| 1   | C     | 282 | SER  | N-CA-C  | -5.07 | 103.25      | 110.35   |
| 1   | A     | 174 | THR  | N-CA-C  | 5.06  | 117.20      | 111.02   |
| 1   | B     | 327 | GLY  | N-CA-C  | 5.04  | 123.59      | 114.46   |
| 1   | A     | 122 | ILE  | N-CA-C  | -5.02 | 105.43      | 110.30   |
| 1   | A     | 330 | LEU  | N-CA-C  | 5.01  | 120.92      | 114.56   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 82  | TYR  | Sidechain |
| 1   | C     | 133 | TYR  | Sidechain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2196  | 0        | 2035     | 211     | 0            |
| 1   | B     | 2252  | 0        | 2084     | 227     | 0            |
| 1   | C     | 2220  | 0        | 2045     | 181     | 0            |
| All | All   | 6668  | 0        | 6164     | 619     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (619) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:77:ILE:HG23  | 1:C:154:LEU:HD22 | 1.22                     | 1.14              |
| 1:C:174:THR:HG21 | 1:C:238:ARG:HD3  | 1.29                     | 1.10              |
| 1:A:263:PHE:O    | 1:A:264:LEU:HD12 | 1.49                     | 1.10              |
| 1:B:193:PRO:HG2  | 1:B:196:VAL:HB   | 1.40                     | 1.03              |
| 1:A:52:LEU:HD21  | 1:A:119:LYS:HG2  | 1.41                     | 1.01              |
| 1:B:156:GLU:O    | 1:B:160:ILE:HG12 | 1.60                     | 1.01              |
| 1:A:290:THR:O    | 1:A:291:ARG:HG3  | 1.61                     | 1.01              |
| 1:C:263:PHE:O    | 1:C:264:LEU:HD12 | 1.59                     | 1.00              |
| 1:A:174:THR:HG21 | 1:A:238:ARG:HD3  | 1.44                     | 0.99              |
| 1:B:142:ASN:O    | 1:B:145:LYS:HB3  | 1.62                     | 0.98              |
| 1:B:173:ILE:HB   | 1:B:179:ALA:HB2  | 1.48                     | 0.96              |
| 1:A:49:THR:HA    | 1:A:115:MET:SD   | 2.07                     | 0.94              |
| 1:B:265:THR:HG22 | 1:B:267:ASP:H    | 1.28                     | 0.94              |
| 1:C:201:LEU:O    | 1:C:205:HIS:N    | 2.03                     | 0.92              |
| 1:A:280:PRO:HB3  | 1:A:301:THR:O    | 1.71                     | 0.90              |
| 1:B:282:SER:HA   | 1:B:331:TYR:O    | 1.71                     | 0.90              |
| 1:B:72:PRO:HB2   | 1:B:77:ILE:HD11  | 1.54                     | 0.89              |
| 1:B:48:LYS:O     | 1:B:52:LEU:HD13  | 1.73                     | 0.87              |
| 1:A:60:CYS:SG    | 1:A:74:ILE:HD13  | 2.15                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:295:TRP:O    | 1:B:310:ILE:HG22 | 1.74                     | 0.86              |
| 1:A:318:GLN:HG3  | 1:A:322:ASP:OD2  | 1.74                     | 0.86              |
| 1:C:153:MET:HG2  | 1:C:223:THR:HG22 | 1.55                     | 0.86              |
| 1:B:263:PHE:O    | 1:B:264:LEU:HD12 | 1.75                     | 0.86              |
| 1:C:241:GLN:HG3  | 1:C:315:PRO:HB3  | 1.57                     | 0.86              |
| 1:A:299:TYR:CE1  | 1:A:307:LEU:HB2  | 2.11                     | 0.85              |
| 1:A:121:ALA:O    | 1:A:124:LEU:HB3  | 1.78                     | 0.84              |
| 1:C:269:VAL:HG21 | 1:C:286:ARG:HE   | 1.43                     | 0.84              |
| 1:B:245:SER:O    | 1:B:249:ASN:ND2  | 2.10                     | 0.84              |
| 1:C:174:THR:CG2  | 1:C:238:ARG:HD3  | 2.09                     | 0.83              |
| 1:B:315:PRO:HG3  | 1:B:317:PHE:CE1  | 2.14                     | 0.83              |
| 1:A:52:LEU:HD21  | 1:A:119:LYS:CG   | 2.09                     | 0.82              |
| 1:A:76:ASP:C     | 1:A:79:PRO:HD2   | 2.05                     | 0.82              |
| 1:A:49:THR:CA    | 1:A:115:MET:SD   | 2.69                     | 0.81              |
| 1:A:185:PHE:CD1  | 1:A:200:CYS:HB3  | 2.16                     | 0.80              |
| 1:A:156:GLU:O    | 1:A:160:ILE:HG12 | 1.81                     | 0.80              |
| 1:A:332:PRO:HD3  | 1:A:338:ASN:HD22 | 1.47                     | 0.80              |
| 1:B:138:GLN:OE1  | 1:B:141:ARG:HD2  | 1.83                     | 0.79              |
| 1:A:285:PHE:CE1  | 1:A:316:LEU:HD21 | 2.18                     | 0.79              |
| 1:C:156:GLU:O    | 1:C:160:ILE:HG12 | 1.84                     | 0.78              |
| 1:A:195:LYS:HD2  | 1:A:196:VAL:N    | 1.99                     | 0.78              |
| 1:C:205:HIS:HE1  | 1:C:244:GLY:O    | 1.66                     | 0.77              |
| 1:A:49:THR:CB    | 1:A:115:MET:SD   | 2.72                     | 0.77              |
| 1:B:296:ALA:HB1  | 1:B:308:GLN:HE21 | 1.49                     | 0.77              |
| 1:B:101:LEU:HD11 | 1:B:107:PHE:CE1  | 2.20                     | 0.77              |
| 1:A:299:TYR:OH   | 1:A:307:LEU:HD12 | 1.85                     | 0.77              |
| 1:C:77:ILE:HD13  | 1:C:151:SER:HA   | 1.67                     | 0.77              |
| 1:B:286:ARG:HH21 | 1:B:308:GLN:HE22 | 1.30                     | 0.76              |
| 1:B:185:PHE:CD1  | 1:B:200:CYS:HB3  | 2.20                     | 0.76              |
| 1:B:193:PRO:HG2  | 1:B:196:VAL:CB   | 2.14                     | 0.76              |
| 1:C:72:PRO:HG2   | 1:C:147:SER:HB3  | 1.68                     | 0.76              |
| 1:A:192:VAL:HG22 | 1:A:228:ILE:O    | 1.86                     | 0.76              |
| 1:B:162:PRO:CG   | 1:B:167:GLN:HG3  | 2.17                     | 0.75              |
| 1:A:185:PHE:CE1  | 1:A:200:CYS:HB3  | 2.22                     | 0.75              |
| 1:C:250:TRP:O    | 1:C:255:VAL:HG23 | 1.87                     | 0.75              |
| 1:A:325:ARG:C    | 1:A:327:GLY:H    | 1.94                     | 0.75              |
| 1:C:299:TYR:CE1  | 1:C:307:LEU:HB2  | 2.21                     | 0.75              |
| 1:A:174:THR:HG22 | 1:A:175:LYS:HD2  | 1.67                     | 0.75              |
| 1:C:280:PRO:HB3  | 1:C:301:THR:O    | 1.87                     | 0.75              |
| 1:A:178:ALA:HB2  | 1:A:237:THR:HG21 | 1.70                     | 0.74              |
| 1:B:191:ILE:HA   | 1:B:229:SER:HA   | 1.70                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:142:ASN:ND2  | 1:C:145:LYS:HD2  | 2.02                     | 0.74              |
| 1:A:175:LYS:O    | 1:A:178:ALA:HB3  | 1.87                     | 0.74              |
| 1:C:109:ILE:HG21 | 1:C:191:ILE:HD13 | 1.70                     | 0.74              |
| 1:B:72:PRO:HB2   | 1:B:77:ILE:CD1   | 2.18                     | 0.74              |
| 1:A:76:ASP:O     | 1:A:79:PRO:HD2   | 1.87                     | 0.73              |
| 1:A:258:PRO:HG2  | 1:A:332:PRO:HB2  | 1.69                     | 0.73              |
| 1:A:162:PRO:HD2  | 1:A:165:GLN:O    | 1.89                     | 0.73              |
| 1:A:273:LEU:O    | 1:A:306:ILE:HD11 | 1.88                     | 0.73              |
| 1:C:60:CYS:HB3   | 1:C:75:LEU:HD21  | 1.71                     | 0.73              |
| 1:B:132:MET:HB2  | 1:B:133:TYR:CE1  | 2.23                     | 0.73              |
| 1:B:160:ILE:HD11 | 1:B:231:PHE:HB2  | 1.71                     | 0.73              |
| 1:B:286:ARG:NH2  | 1:B:308:GLN:HE22 | 1.87                     | 0.72              |
| 1:A:261:MET:O    | 1:A:264:LEU:HD13 | 1.88                     | 0.72              |
| 1:A:178:ALA:CB   | 1:A:237:THR:HG21 | 2.19                     | 0.72              |
| 1:B:205:HIS:HE1  | 1:B:244:GLY:O    | 1.72                     | 0.72              |
| 1:B:335:ARG:HG3  | 1:B:335:ARG:HH11 | 1.54                     | 0.72              |
| 1:A:260:TYR:CZ   | 1:A:262:ALA:HA   | 2.25                     | 0.72              |
| 1:B:145:LYS:O    | 1:B:149:ILE:HG13 | 1.89                     | 0.71              |
| 1:B:234:ASP:O    | 1:B:238:ARG:HG3  | 1.89                     | 0.71              |
| 1:A:43:ARG:O     | 1:A:47:GLU:HG2   | 1.90                     | 0.71              |
| 1:B:296:ALA:HA   | 1:B:310:ILE:CG2  | 2.20                     | 0.71              |
| 1:A:160:ILE:HG22 | 1:A:166:PHE:CE1  | 2.26                     | 0.71              |
| 1:B:296:ALA:HB1  | 1:B:308:GLN:NE2  | 2.04                     | 0.71              |
| 1:C:332:PRO:HD3  | 1:C:338:ASN:HD22 | 1.56                     | 0.71              |
| 1:A:152:HIS:CD2  | 1:A:292:LEU:HD21 | 2.26                     | 0.70              |
| 1:B:300:VAL:HA   | 1:B:305:ASN:O    | 1.91                     | 0.70              |
| 1:C:216:LEU:HD11 | 1:C:220:ILE:HD11 | 1.73                     | 0.70              |
| 1:A:123:ARG:O    | 1:A:127:GLU:HG2  | 1.90                     | 0.70              |
| 1:B:242:PRO:HD3  | 1:B:317:PHE:HE1  | 1.55                     | 0.70              |
| 1:B:326:GLU:HA   | 1:B:326:GLU:OE1  | 1.90                     | 0.70              |
| 1:C:191:ILE:HG12 | 1:C:227:TYR:HD2  | 1.57                     | 0.70              |
| 1:B:72:PRO:HG2   | 1:B:147:SER:HB3  | 1.73                     | 0.69              |
| 1:A:301:THR:C    | 1:A:303:ASP:H    | 1.99                     | 0.68              |
| 1:B:216:LEU:HD11 | 1:B:236:PHE:CZ   | 2.28                     | 0.68              |
| 1:A:327:GLY:HA2  | 1:A:330:LEU:HD21 | 1.73                     | 0.68              |
| 1:A:285:PHE:CZ   | 1:A:316:LEU:HD21 | 2.29                     | 0.68              |
| 1:B:104:ASN:HB3  | 1:B:107:PHE:HB2  | 1.76                     | 0.68              |
| 1:B:202:HIS:CD2  | 1:B:207:ILE:H    | 2.12                     | 0.68              |
| 1:B:43:ARG:O     | 1:B:47:GLU:HG2   | 1.94                     | 0.67              |
| 1:B:217:LYS:NZ   | 1:B:221:ASP:OD2  | 2.27                     | 0.67              |
| 1:C:193:PRO:HG2  | 1:C:196:VAL:HB   | 1.74                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:64:LYS:O     | 1:B:66:GLN:HG3   | 1.94                     | 0.67              |
| 1:B:301:THR:O    | 1:B:304:GLY:N    | 2.23                     | 0.67              |
| 1:B:326:GLU:HB3  | 1:B:328:PHE:CE2  | 2.30                     | 0.67              |
| 1:B:194:TRP:HE3  | 1:B:228:ILE:HD11 | 1.60                     | 0.67              |
| 1:A:316:LEU:HG   | 1:A:320:LEU:HD11 | 1.75                     | 0.67              |
| 1:C:161:PHE:HA   | 1:C:165:GLN:O    | 1.95                     | 0.66              |
| 1:B:202:HIS:HD2  | 1:B:207:ILE:H    | 1.43                     | 0.66              |
| 1:C:43:ARG:O     | 1:C:47:GLU:HG2   | 1.96                     | 0.66              |
| 1:C:288:SER:O    | 1:C:292:LEU:HD23 | 1.95                     | 0.66              |
| 1:C:332:PRO:HD3  | 1:C:338:ASN:HB2  | 1.77                     | 0.66              |
| 1:A:113:SER:OG   | 1:A:225:ASN:HB3  | 1.95                     | 0.66              |
| 1:A:148:LEU:O    | 1:A:151:SER:HB3  | 1.95                     | 0.66              |
| 1:C:361:GLU:HG3  | 1:C:362:LEU:N    | 2.10                     | 0.66              |
| 1:B:181:PHE:CG   | 1:B:243:TRP:CH2  | 2.84                     | 0.66              |
| 1:A:54:ASP:O     | 1:A:58:ARG:HB2   | 1.96                     | 0.66              |
| 1:A:257:HIS:CD2  | 1:A:258:PRO:HD2  | 2.31                     | 0.65              |
| 1:B:57:VAL:HG13  | 1:B:75:LEU:CD2   | 2.27                     | 0.65              |
| 1:B:242:PRO:HD3  | 1:B:317:PHE:CE1  | 2.31                     | 0.65              |
| 1:C:43:ARG:O     | 1:C:46:VAL:HG22  | 1.97                     | 0.65              |
| 1:C:332:PRO:CD   | 1:C:338:ASN:HB2  | 2.27                     | 0.65              |
| 1:A:151:SER:O    | 1:A:154:LEU:HB3  | 1.97                     | 0.65              |
| 1:C:289:CYS:HA   | 1:C:292:LEU:CD2  | 2.26                     | 0.65              |
| 1:B:261:MET:O    | 1:B:262:ALA:HB3  | 1.95                     | 0.65              |
| 1:A:145:LYS:O    | 1:A:149:ILE:HG13 | 1.96                     | 0.65              |
| 1:B:315:PRO:CG   | 1:B:317:PHE:CE1  | 2.79                     | 0.65              |
| 1:C:148:LEU:O    | 1:C:151:SER:HB3  | 1.97                     | 0.65              |
| 1:C:280:PRO:HA   | 1:C:300:VAL:HB   | 1.80                     | 0.64              |
| 1:B:241:GLN:CG   | 1:B:315:PRO:HB3  | 2.27                     | 0.64              |
| 1:C:283:TYR:OH   | 1:C:338:ASN:ND2  | 2.30                     | 0.64              |
| 1:B:138:GLN:CD   | 1:B:141:ARG:HD2  | 2.22                     | 0.64              |
| 1:C:301:THR:OG1  | 1:C:305:ASN:HB2  | 1.97                     | 0.64              |
| 1:B:130:GLU:HA   | 1:B:133:TYR:CE2  | 2.33                     | 0.64              |
| 1:B:216:LEU:HD11 | 1:B:236:PHE:HZ   | 1.62                     | 0.64              |
| 1:B:265:THR:HG22 | 1:B:267:ASP:N    | 2.09                     | 0.63              |
| 1:C:253:LEU:HD22 | 1:C:316:LEU:HD23 | 1.79                     | 0.63              |
| 1:A:160:ILE:HG22 | 1:A:166:PHE:HE1  | 1.61                     | 0.63              |
| 1:B:161:PHE:CZ   | 1:B:166:PHE:HD1  | 2.17                     | 0.63              |
| 1:B:173:ILE:HB   | 1:B:179:ALA:CB   | 2.26                     | 0.63              |
| 1:A:332:PRO:HD3  | 1:A:338:ASN:HB2  | 1.79                     | 0.62              |
| 1:B:101:LEU:HD11 | 1:B:107:PHE:CD1  | 2.34                     | 0.62              |
| 1:B:49:THR:CB    | 1:B:115:MET:SD   | 2.87                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:265:THR:HG22 | 1:A:267:ASP:H    | 1.63                     | 0.62              |
| 1:A:323:GLY:HA3  | 1:A:329:TYR:CE2  | 2.35                     | 0.62              |
| 1:C:202:HIS:HD2  | 1:C:207:ILE:H    | 1.48                     | 0.62              |
| 1:B:296:ALA:HA   | 1:B:310:ILE:HG22 | 1.81                     | 0.62              |
| 1:B:57:VAL:O     | 1:B:61:GLN:HG3   | 1.99                     | 0.62              |
| 1:C:267:ASP:OD1  | 1:C:270:LYS:NZ   | 2.30                     | 0.62              |
| 1:A:77:ILE:HG23  | 1:A:154:LEU:HD22 | 1.82                     | 0.62              |
| 1:C:288:SER:HB3  | 1:C:291:ARG:O    | 2.00                     | 0.61              |
| 1:B:72:PRO:CB    | 1:B:77:ILE:HD11  | 2.28                     | 0.61              |
| 1:A:77:ILE:HG21  | 1:A:151:SER:HA   | 1.82                     | 0.61              |
| 1:B:241:GLN:HB2  | 1:B:242:PRO:HA   | 1.83                     | 0.61              |
| 1:C:205:HIS:CE1  | 1:C:244:GLY:O    | 2.51                     | 0.61              |
| 1:B:280:PRO:HB3  | 1:B:301:THR:O    | 2.00                     | 0.61              |
| 1:A:146:LEU:C    | 1:A:148:LEU:N    | 2.56                     | 0.61              |
| 1:B:83:GLN:O     | 1:B:86:ARG:HB2   | 2.00                     | 0.61              |
| 1:C:142:ASN:HD22 | 1:C:145:LYS:HD2  | 1.64                     | 0.60              |
| 1:C:299:TYR:OH   | 1:C:307:LEU:HD12 | 2.01                     | 0.60              |
| 1:B:243:TRP:C    | 1:B:243:TRP:CD1  | 2.79                     | 0.60              |
| 1:B:153:MET:HG2  | 1:B:223:THR:HG22 | 1.82                     | 0.60              |
| 1:B:215:ALA:O    | 1:B:218:SER:HB3  | 2.02                     | 0.60              |
| 1:A:285:PHE:CE2  | 1:A:320:LEU:HD11 | 2.37                     | 0.60              |
| 1:C:257:HIS:HD2  | 1:C:259:GLY:H    | 1.49                     | 0.60              |
| 1:B:241:GLN:HG3  | 1:B:315:PRO:HB3  | 1.83                     | 0.60              |
| 1:C:115:MET:O    | 1:C:118:SER:HB2  | 2.01                     | 0.60              |
| 1:B:113:SER:OG   | 1:B:225:ASN:HB3  | 2.02                     | 0.60              |
| 1:C:234:ASP:O    | 1:C:237:THR:OG1  | 2.19                     | 0.60              |
| 1:A:160:ILE:CG2  | 1:A:166:PHE:HE1  | 2.15                     | 0.60              |
| 1:A:196:VAL:O    | 1:A:199:GLN:HB2  | 2.01                     | 0.60              |
| 1:A:128:GLY:O    | 1:A:131:ARG:HB2  | 2.02                     | 0.59              |
| 1:A:174:THR:CG2  | 1:A:238:ARG:HD3  | 2.24                     | 0.59              |
| 1:C:323:GLY:HA3  | 1:C:329:TYR:CD2  | 2.37                     | 0.59              |
| 1:A:216:LEU:HB2  | 1:A:250:TRP:CH2  | 2.38                     | 0.59              |
| 1:B:263:PHE:O    | 1:B:264:LEU:CD1  | 2.47                     | 0.59              |
| 1:A:132:MET:HB2  | 1:A:133:TYR:CE1  | 2.37                     | 0.59              |
| 1:C:145:LYS:O    | 1:C:149:ILE:HG13 | 2.02                     | 0.59              |
| 1:C:65:LEU:HD23  | 1:C:133:TYR:CD1  | 2.38                     | 0.59              |
| 1:A:332:PRO:HD3  | 1:A:338:ASN:ND2  | 2.16                     | 0.58              |
| 1:A:143:LEU:O    | 1:A:146:LEU:HB2  | 2.03                     | 0.58              |
| 1:C:243:TRP:O    | 1:C:246:ILE:N    | 2.34                     | 0.58              |
| 1:A:268:GLU:O    | 1:A:271:ALA:HB3  | 2.02                     | 0.58              |
| 1:A:69:ASN:CB    | 1:A:73:TYR:HD2   | 2.16                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:77:ILE:HG23  | 1:B:154:LEU:HD22 | 1.84                     | 0.58              |
| 1:B:166:PHE:CZ   | 1:B:168:GLY:HA3  | 2.39                     | 0.58              |
| 1:C:65:LEU:HD23  | 1:C:133:TYR:CE1  | 2.39                     | 0.58              |
| 1:B:111:ILE:O    | 1:B:115:MET:HG2  | 2.03                     | 0.58              |
| 1:A:322:ASP:O    | 1:A:325:ARG:N    | 2.37                     | 0.58              |
| 1:B:220:ILE:HG12 | 1:B:236:PHE:CD1  | 2.39                     | 0.58              |
| 1:B:270:LYS:HG2  | 1:B:306:ILE:HG21 | 1.86                     | 0.58              |
| 1:B:73:TYR:O     | 1:B:76:ASP:N     | 2.32                     | 0.58              |
| 1:A:140:ARG:O    | 1:A:143:LEU:HB3  | 2.04                     | 0.57              |
| 1:C:253:LEU:HD22 | 1:C:316:LEU:CD2  | 2.34                     | 0.57              |
| 1:C:290:THR:O    | 1:C:291:ARG:HG3  | 2.04                     | 0.57              |
| 1:A:149:ILE:HD13 | 1:A:224:CYS:SG   | 2.44                     | 0.57              |
| 1:C:50:TRP:HA    | 1:C:53:MET:HE3   | 1.86                     | 0.57              |
| 1:B:270:LYS:HA   | 1:B:306:ILE:HD13 | 1.86                     | 0.57              |
| 1:C:43:ARG:HA    | 1:C:46:VAL:HG22  | 1.85                     | 0.57              |
| 1:C:251:ASN:HA   | 1:C:255:VAL:HB   | 1.86                     | 0.57              |
| 1:C:252:PHE:O    | 1:C:257:HIS:HB2  | 2.04                     | 0.57              |
| 1:C:269:VAL:HG21 | 1:C:286:ARG:NE   | 2.17                     | 0.57              |
| 1:B:57:VAL:O     | 1:B:61:GLN:CG    | 2.52                     | 0.57              |
| 1:C:74:ILE:O     | 1:C:74:ILE:HG12  | 2.03                     | 0.57              |
| 1:A:245:SER:O    | 1:A:249:ASN:OD1  | 2.22                     | 0.56              |
| 1:B:106:TYR:OH   | 1:B:156:GLU:HG2  | 2.05                     | 0.56              |
| 1:A:47:GLU:O     | 1:A:51:LYS:HB2   | 2.05                     | 0.56              |
| 1:C:257:HIS:CD2  | 1:C:258:PRO:HD2  | 2.40                     | 0.56              |
| 1:A:177:ASP:HB3  | 1:A:243:TRP:CD1  | 2.41                     | 0.56              |
| 1:B:235:ILE:HG23 | 1:B:293:GLY:HA2  | 1.87                     | 0.56              |
| 1:B:240:PHE:CE1  | 1:B:254:ALA:HB2  | 2.41                     | 0.56              |
| 1:B:262:ALA:O    | 1:B:287:LEU:N    | 2.38                     | 0.56              |
| 1:B:335:ARG:HG3  | 1:B:335:ARG:NH1  | 2.16                     | 0.56              |
| 1:C:60:CYS:O     | 1:C:65:LEU:HD12  | 2.05                     | 0.56              |
| 1:A:276:TYR:O    | 1:A:277:SER:C    | 2.48                     | 0.56              |
| 1:C:266:TYR:CD2  | 1:C:270:LYS:NZ   | 2.74                     | 0.56              |
| 1:A:146:LEU:O    | 1:A:148:LEU:N    | 2.38                     | 0.56              |
| 1:B:110:TYR:O    | 1:B:114:LEU:N    | 2.36                     | 0.56              |
| 1:B:133:TYR:N    | 1:B:133:TYR:CD1  | 2.73                     | 0.56              |
| 1:B:261:MET:N    | 1:B:285:PHE:O    | 2.39                     | 0.56              |
| 1:B:296:ALA:HA   | 1:B:310:ILE:HG23 | 1.87                     | 0.56              |
| 1:A:266:TYR:O    | 1:A:270:LYS:HG3  | 2.06                     | 0.56              |
| 1:A:60:CYS:O     | 1:A:65:LEU:HD12  | 2.06                     | 0.55              |
| 1:B:52:LEU:O     | 1:B:55:LYS:HB2   | 2.06                     | 0.55              |
| 1:B:72:PRO:CG    | 1:B:147:SER:HB3  | 2.36                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:197:PHE:O    | 1:C:200:CYS:HB2  | 2.06                     | 0.55              |
| 1:A:280:PRO:HB3  | 1:A:301:THR:C    | 2.31                     | 0.55              |
| 1:A:191:ILE:HA   | 1:A:229:SER:HA   | 1.88                     | 0.55              |
| 1:B:44:ARG:O     | 1:B:47:GLU:HB2   | 2.05                     | 0.55              |
| 1:A:146:LEU:O    | 1:A:147:SER:C    | 2.49                     | 0.55              |
| 1:B:57:VAL:HG13  | 1:B:75:LEU:HD22  | 1.87                     | 0.55              |
| 1:B:233:PHE:CE2  | 1:B:237:THR:HG21 | 2.41                     | 0.55              |
| 1:C:84:HIS:O     | 1:C:85:LEU:C     | 2.49                     | 0.55              |
| 1:B:240:PHE:HE1  | 1:B:254:ALA:HB2  | 1.71                     | 0.55              |
| 1:C:142:ASN:O    | 1:C:145:LYS:N    | 2.39                     | 0.55              |
| 1:A:325:ARG:C    | 1:A:327:GLY:N    | 2.60                     | 0.55              |
| 1:B:220:ILE:HG12 | 1:B:236:PHE:CE1  | 2.41                     | 0.55              |
| 1:C:217:LYS:O    | 1:C:221:ASP:HB2  | 2.07                     | 0.55              |
| 1:B:101:LEU:HD21 | 1:B:107:PHE:CZ   | 2.42                     | 0.55              |
| 1:C:92:TYR:CB    | 1:C:101:LEU:HD22 | 2.36                     | 0.55              |
| 1:B:76:ASP:O     | 1:B:80:ASP:OD2   | 2.23                     | 0.55              |
| 1:B:176:ALA:O    | 1:B:180:GLU:N    | 2.32                     | 0.55              |
| 1:C:317:PHE:O    | 1:C:321:ILE:HG13 | 2.07                     | 0.55              |
| 1:A:132:MET:C    | 1:A:133:TYR:CD1  | 2.85                     | 0.54              |
| 1:A:215:ALA:O    | 1:A:218:SER:HB3  | 2.08                     | 0.54              |
| 1:B:273:LEU:HB2  | 1:B:306:ILE:CD1  | 2.37                     | 0.54              |
| 1:B:323:GLY:HA3  | 1:B:329:TYR:CD2  | 2.42                     | 0.54              |
| 1:C:142:ASN:O    | 1:C:145:LYS:HB2  | 2.08                     | 0.54              |
| 1:C:214:MET:HA   | 1:C:217:LYS:HB3  | 1.89                     | 0.54              |
| 1:C:318:GLN:NE2  | 1:C:318:GLN:HA   | 2.22                     | 0.54              |
| 1:A:105:GLU:O    | 1:A:109:ILE:HG13 | 2.07                     | 0.54              |
| 1:B:205:HIS:CE1  | 1:B:244:GLY:O    | 2.58                     | 0.54              |
| 1:C:318:GLN:HA   | 1:C:318:GLN:HE21 | 1.71                     | 0.54              |
| 1:B:82:TYR:O     | 1:B:86:ARG:HG2   | 2.08                     | 0.54              |
| 1:A:140:ARG:O    | 1:A:143:LEU:N    | 2.40                     | 0.54              |
| 1:B:104:ASN:HB3  | 1:B:107:PHE:CB   | 2.38                     | 0.54              |
| 1:B:268:GLU:O    | 1:B:269:VAL:C    | 2.49                     | 0.54              |
| 1:B:266:TYR:CE2  | 1:B:270:LYS:HD3  | 2.42                     | 0.54              |
| 1:C:191:ILE:HG12 | 1:C:227:TYR:CD2  | 2.41                     | 0.54              |
| 1:A:332:PRO:HD3  | 1:A:338:ASN:CB   | 2.38                     | 0.54              |
| 1:C:62:ASN:O     | 1:C:65:LEU:HG    | 2.07                     | 0.54              |
| 1:C:121:ALA:O    | 1:C:124:LEU:HB3  | 2.08                     | 0.54              |
| 1:B:201:LEU:O    | 1:B:205:HIS:N    | 2.36                     | 0.54              |
| 1:B:283:TYR:CE1  | 1:B:329:TYR:HB3  | 2.43                     | 0.54              |
| 1:C:251:ASN:HA   | 1:C:255:VAL:CG2  | 2.38                     | 0.53              |
| 1:A:45:THR:O     | 1:A:115:MET:HE1  | 2.07                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:265:THR:HG22 | 1:A:266:TYR:N    | 2.22                     | 0.53              |
| 1:A:282:SER:OG   | 1:A:334:GLY:HA2  | 2.08                     | 0.53              |
| 1:B:301:THR:C    | 1:B:303:ASP:N    | 2.64                     | 0.53              |
| 1:C:68:LYS:C     | 1:C:70:SER:N     | 2.66                     | 0.53              |
| 1:B:161:PHE:CE1  | 1:B:166:PHE:HD1  | 2.27                     | 0.53              |
| 1:B:235:ILE:HD13 | 1:B:292:LEU:HB3  | 1.91                     | 0.53              |
| 1:B:291:ARG:HB3  | 1:B:291:ARG:NH1  | 2.22                     | 0.53              |
| 1:B:318:GLN:O    | 1:B:321:ILE:N    | 2.42                     | 0.53              |
| 1:A:74:ILE:HB    | 1:A:147:SER:OG   | 2.08                     | 0.53              |
| 1:B:253:LEU:O    | 1:B:260:TYR:HB2  | 2.08                     | 0.53              |
| 1:C:273:LEU:HB2  | 1:C:306:ILE:HD13 | 1.89                     | 0.53              |
| 1:A:161:PHE:HA   | 1:A:165:GLN:O    | 2.07                     | 0.53              |
| 1:B:144:THR:HA   | 1:B:147:SER:HB2  | 1.91                     | 0.53              |
| 1:C:281:GLY:O    | 1:C:282:SER:C    | 2.51                     | 0.53              |
| 1:B:52:LEU:HD21  | 1:B:119:LYS:CE   | 2.39                     | 0.53              |
| 1:B:156:GLU:HA   | 1:B:231:PHE:CD2  | 2.43                     | 0.53              |
| 1:A:123:ARG:O    | 1:A:126:LYS:HB3  | 2.09                     | 0.53              |
| 1:B:193:PRO:HG2  | 1:B:196:VAL:CG2  | 2.38                     | 0.53              |
| 1:A:264:LEU:O    | 1:A:286:ARG:NH1  | 2.40                     | 0.52              |
| 1:C:198:ARG:HG3  | 1:C:207:ILE:CD1  | 2.39                     | 0.52              |
| 1:A:109:ILE:HD12 | 1:A:191:ILE:HD13 | 1.91                     | 0.52              |
| 1:B:73:TYR:HB2   | 1:B:76:ASP:HB2   | 1.91                     | 0.52              |
| 1:C:60:CYS:C     | 1:C:62:ASN:H     | 2.17                     | 0.52              |
| 1:A:77:ILE:HD12  | 1:A:154:LEU:HD23 | 1.91                     | 0.52              |
| 1:B:162:PRO:CD   | 1:B:167:GLN:HG3  | 2.39                     | 0.52              |
| 1:B:270:LYS:HG2  | 1:B:306:ILE:CG2  | 2.39                     | 0.52              |
| 1:B:216:LEU:HA   | 1:B:250:TRP:CZ2  | 2.44                     | 0.52              |
| 1:B:272:ARG:HG3  | 1:B:272:ARG:HH11 | 1.73                     | 0.52              |
| 1:A:316:LEU:HG   | 1:A:320:LEU:CD1  | 2.38                     | 0.52              |
| 1:B:161:PHE:CZ   | 1:B:166:PHE:CD1  | 2.98                     | 0.52              |
| 1:C:196:VAL:O    | 1:C:200:CYS:SG   | 2.52                     | 0.52              |
| 1:A:82:TYR:O     | 1:A:86:ARG:HG2   | 2.09                     | 0.52              |
| 1:A:301:THR:C    | 1:A:303:ASP:N    | 2.67                     | 0.52              |
| 1:B:49:THR:HA    | 1:B:115:MET:SD   | 2.50                     | 0.52              |
| 1:B:118:SER:O    | 1:B:121:ALA:HB3  | 2.10                     | 0.52              |
| 1:B:260:TYR:HA   | 1:B:285:PHE:CE1  | 2.45                     | 0.52              |
| 1:A:326:GLU:HB2  | 1:A:328:PHE:CE2  | 2.45                     | 0.52              |
| 1:B:260:TYR:HA   | 1:B:285:PHE:CD1  | 2.45                     | 0.52              |
| 1:B:205:HIS:HB3  | 1:B:247:LEU:CD1  | 2.39                     | 0.52              |
| 1:A:263:PHE:O    | 1:A:264:LEU:CD1  | 2.41                     | 0.51              |
| 1:A:202:HIS:HD2  | 1:A:207:ILE:H    | 1.58                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:333:ASP:O    | 1:C:333:ASP:OD2  | 2.28                     | 0.51              |
| 1:C:264:LEU:CB   | 1:C:286:ARG:HD3  | 2.40                     | 0.51              |
| 1:C:53:MET:O     | 1:C:54:ASP:C     | 2.53                     | 0.51              |
| 1:B:143:LEU:O    | 1:B:144:THR:C    | 2.50                     | 0.51              |
| 1:A:195:LYS:O    | 1:A:199:GLN:HG3  | 2.11                     | 0.51              |
| 1:B:72:PRO:HD3   | 1:B:148:LEU:CD1  | 2.41                     | 0.51              |
| 1:C:216:LEU:HA   | 1:C:250:TRP:CZ2  | 2.45                     | 0.51              |
| 1:A:323:GLY:O    | 1:A:328:PHE:HB2  | 2.10                     | 0.51              |
| 1:B:178:ALA:O    | 1:B:181:PHE:HB3  | 2.11                     | 0.51              |
| 1:B:272:ARG:HG3  | 1:B:272:ARG:NH1  | 2.26                     | 0.51              |
| 1:A:52:LEU:CD2   | 1:A:119:LYS:CG   | 2.84                     | 0.51              |
| 1:A:152:HIS:HD2  | 1:A:292:LEU:HD11 | 1.74                     | 0.51              |
| 1:A:251:ASN:HA   | 1:A:255:VAL:CG2  | 2.41                     | 0.51              |
| 1:C:216:LEU:CD1  | 1:C:220:ILE:HD11 | 2.41                     | 0.51              |
| 1:C:289:CYS:SG   | 1:C:290:THR:HG23 | 2.51                     | 0.51              |
| 1:A:173:ILE:HG23 | 1:A:234:ASP:OD1  | 2.10                     | 0.50              |
| 1:A:77:ILE:HG23  | 1:A:154:LEU:CD2  | 2.41                     | 0.50              |
| 1:C:60:CYS:C     | 1:C:62:ASN:N     | 2.69                     | 0.50              |
| 1:C:64:LYS:O     | 1:C:133:TYR:HB3  | 2.11                     | 0.50              |
| 1:C:283:TYR:CE1  | 1:C:338:ASN:ND2  | 2.80                     | 0.50              |
| 1:C:65:LEU:O     | 1:C:66:GLN:CG    | 2.59                     | 0.50              |
| 1:C:215:ALA:HB1  | 1:C:363:TYR:HD2  | 1.75                     | 0.50              |
| 1:A:49:THR:O     | 1:A:53:MET:HG3   | 2.11                     | 0.50              |
| 1:A:153:MET:HG2  | 1:A:223:THR:HG22 | 1.94                     | 0.50              |
| 1:A:239:LEU:HD13 | 1:A:287:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:286:ARG:HD2  | 1:A:287:LEU:O    | 2.11                     | 0.50              |
| 1:C:60:CYS:HA    | 1:C:65:LEU:HD11  | 1.94                     | 0.50              |
| 1:C:265:THR:HG22 | 1:C:267:ASP:H    | 1.77                     | 0.50              |
| 1:C:178:ALA:O    | 1:C:181:PHE:HB3  | 2.12                     | 0.50              |
| 1:C:260:TYR:HA   | 1:C:285:PHE:CE1  | 2.47                     | 0.50              |
| 1:B:52:LEU:N     | 1:B:52:LEU:HD12  | 2.26                     | 0.49              |
| 1:B:144:THR:O    | 1:B:145:LYS:C    | 2.55                     | 0.49              |
| 1:C:76:ASP:O     | 1:C:79:PRO:HD2   | 2.12                     | 0.49              |
| 1:B:52:LEU:HD21  | 1:B:119:LYS:HE2  | 1.94                     | 0.49              |
| 1:C:335:ARG:HG3  | 1:C:335:ARG:HH11 | 1.78                     | 0.49              |
| 1:B:291:ARG:CB   | 1:B:291:ARG:CZ   | 2.89                     | 0.49              |
| 1:A:69:ASN:CB    | 1:A:73:TYR:CD2   | 2.95                     | 0.49              |
| 1:B:166:PHE:CZ   | 1:B:190:THR:HG21 | 2.46                     | 0.49              |
| 1:A:132:MET:CB   | 1:A:133:TYR:CE1  | 2.95                     | 0.49              |
| 1:A:197:PHE:O    | 1:A:200:CYS:N    | 2.44                     | 0.49              |
| 1:A:266:TYR:CD1  | 1:A:308:GLN:OE1  | 2.65                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:73:TYR:O     | 1:C:77:ILE:HG13  | 2.13                     | 0.49              |
| 1:A:88:ILE:HA    | 1:A:164:GLY:O    | 2.13                     | 0.49              |
| 1:B:47:GLU:O     | 1:B:50:TRP:HB2   | 2.13                     | 0.49              |
| 1:B:67:LEU:HD23  | 1:B:140:ARG:HH22 | 1.78                     | 0.49              |
| 1:A:295:TRP:O    | 1:A:310:ILE:HG22 | 2.13                     | 0.49              |
| 1:C:289:CYS:HA   | 1:C:292:LEU:HD21 | 1.95                     | 0.49              |
| 1:B:326:GLU:OE1  | 1:B:326:GLU:CA   | 2.61                     | 0.49              |
| 1:C:297:ILE:HG21 | 1:C:329:TYR:CZ   | 2.47                     | 0.49              |
| 1:A:231:PHE:O    | 1:A:232:GLU:C    | 2.56                     | 0.48              |
| 1:A:318:GLN:O    | 1:A:319:ALA:C    | 2.55                     | 0.48              |
| 1:A:326:GLU:HB2  | 1:A:328:PHE:CD2  | 2.47                     | 0.48              |
| 1:C:165:GLN:HG2  | 1:C:166:PHE:N    | 2.27                     | 0.48              |
| 1:A:152:HIS:NE2  | 1:A:292:LEU:HD21 | 2.27                     | 0.48              |
| 1:B:78:LEU:CB    | 1:B:79:PRO:HD3   | 2.43                     | 0.48              |
| 1:B:268:GLU:HA   | 1:B:271:ALA:HB3  | 1.95                     | 0.48              |
| 1:C:195:LYS:O    | 1:C:199:GLN:HG3  | 2.13                     | 0.48              |
| 1:A:222:LEU:N    | 1:A:232:GLU:OE2  | 2.46                     | 0.48              |
| 1:A:331:TYR:O    | 1:A:332:PRO:C    | 2.54                     | 0.48              |
| 1:A:276:TYR:O    | 1:A:279:LYS:N    | 2.45                     | 0.48              |
| 1:A:283:TYR:OH   | 1:A:338:ASN:ND2  | 2.43                     | 0.48              |
| 1:B:67:LEU:HD23  | 1:B:140:ARG:NH2  | 2.28                     | 0.48              |
| 1:B:111:ILE:O    | 1:B:114:LEU:N    | 2.46                     | 0.48              |
| 1:A:273:LEU:C    | 1:A:306:ILE:HD11 | 2.37                     | 0.48              |
| 1:B:186:PHE:O    | 1:B:189:LYS:HD2  | 2.13                     | 0.48              |
| 1:B:298:GLY:O    | 1:B:299:TYR:HB3  | 2.12                     | 0.48              |
| 1:C:283:TYR:HE1  | 1:C:338:ASN:HD22 | 1.61                     | 0.48              |
| 1:A:214:MET:O    | 1:A:217:LYS:HB3  | 2.14                     | 0.48              |
| 1:C:68:LYS:C     | 1:C:70:SER:H     | 2.22                     | 0.48              |
| 1:C:264:LEU:HB2  | 1:C:286:ARG:HD3  | 1.96                     | 0.48              |
| 1:A:65:LEU:HD11  | 1:A:125:PHE:CE1  | 2.49                     | 0.48              |
| 1:B:144:THR:O    | 1:B:147:SER:N    | 2.47                     | 0.48              |
| 1:B:268:GLU:O    | 1:B:272:ARG:N    | 2.34                     | 0.48              |
| 1:B:301:THR:C    | 1:B:303:ASP:H    | 2.22                     | 0.48              |
| 1:A:71:PRO:HA    | 1:A:72:PRO:HA    | 1.59                     | 0.48              |
| 1:B:325:ARG:C    | 1:B:327:GLY:N    | 2.71                     | 0.47              |
| 1:C:362:LEU:O    | 1:C:365:GLU:HB2  | 2.14                     | 0.47              |
| 1:A:245:SER:O    | 1:A:249:ASN:CG   | 2.57                     | 0.47              |
| 1:A:258:PRO:HG2  | 1:A:332:PRO:CB   | 2.40                     | 0.47              |
| 1:A:146:LEU:O    | 1:A:149:ILE:N    | 2.47                     | 0.47              |
| 1:A:322:ASP:O    | 1:A:325:ARG:HB2  | 2.13                     | 0.47              |
| 1:B:261:MET:HB2  | 1:B:286:ARG:HB3  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:290:THR:C    | 1:B:291:ARG:HG3  | 2.38                     | 0.47              |
| 1:C:173:ILE:HD11 | 1:C:230:VAL:HG23 | 1.96                     | 0.47              |
| 1:B:279:LYS:O    | 1:B:279:LYS:HG2  | 2.13                     | 0.47              |
| 1:B:325:ARG:O    | 1:B:327:GLY:N    | 2.47                     | 0.47              |
| 1:C:279:LYS:HG2  | 1:C:279:LYS:O    | 2.14                     | 0.47              |
| 1:A:332:PRO:CD   | 1:A:338:ASN:HB2  | 2.45                     | 0.47              |
| 1:C:205:HIS:HB3  | 1:C:247:LEU:HG   | 1.96                     | 0.47              |
| 1:A:183:ARG:O    | 1:A:184:LYS:C    | 2.58                     | 0.47              |
| 1:C:223:THR:O    | 1:C:224:CYS:HB2  | 2.14                     | 0.47              |
| 1:A:46:VAL:HA    | 1:A:49:THR:CB    | 2.44                     | 0.47              |
| 1:A:283:TYR:HB2  | 1:A:298:GLY:O    | 2.14                     | 0.47              |
| 1:A:306:ILE:HG22 | 1:A:306:ILE:O    | 2.14                     | 0.47              |
| 1:B:50:TRP:O     | 1:B:51:LYS:C     | 2.58                     | 0.47              |
| 1:B:52:LEU:N     | 1:B:52:LEU:CD1   | 2.78                     | 0.47              |
| 1:B:234:ASP:O    | 1:B:238:ARG:CG   | 2.61                     | 0.47              |
| 1:C:202:HIS:CD2  | 1:C:207:ILE:H    | 2.30                     | 0.47              |
| 1:B:325:ARG:C    | 1:B:327:GLY:H    | 2.23                     | 0.47              |
| 1:B:114:LEU:HD12 | 1:B:114:LEU:HA   | 1.61                     | 0.47              |
| 1:B:186:PHE:HB3  | 1:B:189:LYS:HD2  | 1.96                     | 0.47              |
| 1:B:317:PHE:CD2  | 1:B:318:GLN:N    | 2.82                     | 0.47              |
| 1:B:326:GLU:CB   | 1:B:328:PHE:CE2  | 2.97                     | 0.47              |
| 1:C:265:THR:N    | 1:C:268:GLU:OE1  | 2.48                     | 0.47              |
| 1:C:283:TYR:O    | 1:C:284:ILE:HG23 | 2.15                     | 0.47              |
| 1:A:50:TRP:HH2   | 1:A:86:ARG:HH11  | 1.63                     | 0.47              |
| 1:B:191:ILE:HG13 | 1:B:229:SER:HB3  | 1.96                     | 0.47              |
| 1:C:178:ALA:HB1  | 1:C:237:THR:HG21 | 1.97                     | 0.47              |
| 1:C:241:GLN:CG   | 1:C:315:PRO:HB3  | 2.38                     | 0.47              |
| 1:A:183:ARG:O    | 1:A:187:GLY:CA   | 2.63                     | 0.46              |
| 1:A:216:LEU:HA   | 1:A:250:TRP:CZ2  | 2.51                     | 0.46              |
| 1:A:261:MET:O    | 1:A:262:ALA:C    | 2.58                     | 0.46              |
| 1:B:58:ARG:O     | 1:B:61:GLN:HB2   | 2.14                     | 0.46              |
| 1:C:269:VAL:CG2  | 1:C:286:ARG:HE   | 2.23                     | 0.46              |
| 1:B:250:TRP:O    | 1:B:255:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:65:LEU:O     | 1:A:66:GLN:C     | 2.58                     | 0.46              |
| 1:C:159:ALA:O    | 1:C:162:PRO:HD3  | 2.15                     | 0.46              |
| 1:A:246:ILE:O    | 1:A:249:ASN:ND2  | 2.48                     | 0.46              |
| 1:B:152:HIS:O    | 1:B:155:ALA:N    | 2.48                     | 0.46              |
| 1:C:266:TYR:O    | 1:C:266:TYR:CD1  | 2.68                     | 0.46              |
| 1:A:65:LEU:HD11  | 1:A:125:PHE:HE1  | 1.81                     | 0.46              |
| 1:B:105:GLU:O    | 1:B:105:GLU:HG2  | 2.15                     | 0.46              |
| 1:C:216:LEU:HB2  | 1:C:250:TRP:CH2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:77:ILE:HG23  | 1:B:154:LEU:CD2  | 2.45                     | 0.46              |
| 1:B:325:ARG:O    | 1:B:326:GLU:C    | 2.57                     | 0.46              |
| 1:C:110:TYR:CE1  | 1:C:157:ILE:CB   | 2.98                     | 0.46              |
| 1:A:145:LYS:O    | 1:A:148:LEU:HB3  | 2.16                     | 0.46              |
| 1:C:77:ILE:HD13  | 1:C:151:SER:CA   | 2.43                     | 0.46              |
| 1:A:318:GLN:OE1  | 1:A:322:ASP:OD1  | 2.35                     | 0.46              |
| 1:B:124:LEU:HD21 | 1:B:139:ASP:O    | 2.16                     | 0.46              |
| 1:C:60:CYS:HA    | 1:C:65:LEU:CD1   | 2.45                     | 0.46              |
| 1:C:123:ARG:O    | 1:C:126:LYS:HB3  | 2.16                     | 0.46              |
| 1:A:266:TYR:CD2  | 1:A:270:LYS:NZ   | 2.83                     | 0.45              |
| 1:A:291:ARG:O    | 1:A:294:GLN:HB2  | 2.16                     | 0.45              |
| 1:B:162:PRO:HD2  | 1:B:167:GLN:HG3  | 1.98                     | 0.45              |
| 1:C:80:ASP:O     | 1:C:83:GLN:HB2   | 2.16                     | 0.45              |
| 1:A:52:LEU:CD2   | 1:A:119:LYS:HG2  | 2.30                     | 0.45              |
| 1:A:154:LEU:HD11 | 1:A:158:LYS:HE3  | 1.98                     | 0.45              |
| 1:A:239:LEU:HD21 | 1:A:293:GLY:C    | 2.41                     | 0.45              |
| 1:C:57:VAL:O     | 1:C:61:GLN:HG3   | 2.16                     | 0.45              |
| 1:B:192:VAL:CG2  | 1:B:197:PHE:HB2  | 2.46                     | 0.45              |
| 1:C:191:ILE:HA   | 1:C:229:SER:HA   | 1.98                     | 0.45              |
| 1:A:183:ARG:O    | 1:A:187:GLY:N    | 2.50                     | 0.45              |
| 1:B:71:PRO:HD3   | 1:B:73:TYR:OH    | 2.17                     | 0.45              |
| 1:C:240:PHE:O    | 1:C:249:ASN:ND2  | 2.49                     | 0.45              |
| 1:C:243:TRP:O    | 1:C:246:ILE:CB   | 2.65                     | 0.45              |
| 1:A:202:HIS:CD2  | 1:A:207:ILE:H    | 2.34                     | 0.45              |
| 1:B:52:LEU:HD23  | 1:B:119:LYS:HG3  | 1.99                     | 0.45              |
| 1:C:253:LEU:HD13 | 1:C:316:LEU:HD23 | 1.99                     | 0.45              |
| 1:A:78:LEU:CB    | 1:A:79:PRO:HD3   | 2.47                     | 0.45              |
| 1:B:173:ILE:O    | 1:B:174:THR:C    | 2.59                     | 0.45              |
| 1:B:205:HIS:HB3  | 1:B:247:LEU:HG   | 1.99                     | 0.45              |
| 1:C:289:CYS:HA   | 1:C:292:LEU:HD23 | 1.99                     | 0.45              |
| 1:C:322:ASP:O    | 1:C:326:GLU:CB   | 2.64                     | 0.45              |
| 1:A:132:MET:HB2  | 1:A:133:TYR:CZ   | 2.51                     | 0.45              |
| 1:B:233:PHE:O    | 1:B:237:THR:HG23 | 2.16                     | 0.45              |
| 1:C:301:THR:N    | 1:C:305:ASN:O    | 2.47                     | 0.45              |
| 1:A:146:LEU:C    | 1:A:148:LEU:H    | 2.22                     | 0.45              |
| 1:B:57:VAL:HG23  | 1:B:78:LEU:HD23  | 1.98                     | 0.45              |
| 1:C:297:ILE:O    | 1:C:308:GLN:HA   | 2.17                     | 0.45              |
| 1:A:197:PHE:O    | 1:A:198:ARG:C    | 2.60                     | 0.45              |
| 1:A:261:MET:O    | 1:A:264:LEU:CD1  | 2.62                     | 0.44              |
| 1:A:316:LEU:O    | 1:A:317:PHE:C    | 2.59                     | 0.44              |
| 1:B:276:TYR:O    | 1:B:300:VAL:HG21 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:323:GLY:HA3  | 1:A:329:TYR:CD2  | 2.51                     | 0.44              |
| 1:B:208:SER:N    | 1:B:212:GLU:OE1  | 2.47                     | 0.44              |
| 1:C:202:HIS:C    | 1:C:204:VAL:N    | 2.71                     | 0.44              |
| 1:B:57:VAL:HG13  | 1:B:75:LEU:HD23  | 1.95                     | 0.44              |
| 1:B:194:TRP:CE3  | 1:B:228:ILE:HD11 | 2.45                     | 0.44              |
| 1:B:253:LEU:O    | 1:B:257:HIS:HB3  | 2.18                     | 0.44              |
| 1:A:176:ALA:O    | 1:A:177:ASP:C    | 2.59                     | 0.44              |
| 1:A:182:TRP:CH2  | 1:A:230:VAL:HA   | 2.53                     | 0.44              |
| 1:B:138:GLN:HG3  | 1:B:138:GLN:O    | 2.16                     | 0.44              |
| 1:C:104:ASN:HB3  | 1:C:107:PHE:CB   | 2.47                     | 0.44              |
| 1:A:126:LYS:O    | 1:A:129:LYS:HD3  | 2.17                     | 0.44              |
| 1:B:265:THR:HB   | 1:B:268:GLU:OE1  | 2.18                     | 0.44              |
| 1:B:333:ASP:C    | 1:B:335:ARG:H    | 2.26                     | 0.44              |
| 1:C:74:ILE:O     | 1:C:74:ILE:CG1   | 2.66                     | 0.44              |
| 1:A:265:THR:N    | 1:A:268:GLU:OE1  | 2.46                     | 0.44              |
| 1:C:81:THR:O     | 1:C:82:TYR:C     | 2.61                     | 0.44              |
| 1:C:269:VAL:CG2  | 1:C:286:ARG:NE   | 2.80                     | 0.44              |
| 1:A:260:TYR:OH   | 1:A:262:ALA:HA   | 2.17                     | 0.44              |
| 1:A:285:PHE:CE2  | 1:A:320:LEU:CD1  | 3.01                     | 0.44              |
| 1:B:148:LEU:O    | 1:B:151:SER:HB3  | 2.18                     | 0.44              |
| 1:C:296:ALA:HA   | 1:C:310:ILE:HG22 | 1.99                     | 0.44              |
| 1:C:300:VAL:HA   | 1:C:305:ASN:O    | 2.18                     | 0.44              |
| 1:A:173:ILE:HG23 | 1:A:234:ASP:CB   | 2.47                     | 0.44              |
| 1:B:227:TYR:O    | 1:B:228:ILE:HD13 | 2.16                     | 0.44              |
| 1:C:156:GLU:O    | 1:C:157:ILE:C    | 2.61                     | 0.44              |
| 1:A:237:THR:O    | 1:A:237:THR:HG22 | 2.18                     | 0.43              |
| 1:A:185:PHE:CE2  | 1:A:200:CYS:SG   | 3.11                     | 0.43              |
| 1:B:71:PRO:HA    | 1:B:72:PRO:HA    | 1.60                     | 0.43              |
| 1:B:268:GLU:O    | 1:B:271:ALA:N    | 2.52                     | 0.43              |
| 1:B:185:PHE:O    | 1:B:185:PHE:CD2  | 2.72                     | 0.43              |
| 1:B:190:THR:HG22 | 1:B:190:THR:O    | 2.18                     | 0.43              |
| 1:B:251:ASN:HA   | 1:B:255:VAL:HG23 | 2.01                     | 0.43              |
| 1:C:181:PHE:CG   | 1:C:243:TRP:CH2  | 3.06                     | 0.43              |
| 1:A:60:CYS:HA    | 1:A:65:LEU:HD12  | 2.00                     | 0.43              |
| 1:B:83:GLN:O     | 1:B:86:ARG:CB    | 2.67                     | 0.43              |
| 1:A:238:ARG:O    | 1:A:241:GLN:NE2  | 2.33                     | 0.43              |
| 1:A:251:ASN:HA   | 1:A:255:VAL:HG21 | 2.00                     | 0.43              |
| 1:B:192:VAL:HG23 | 1:B:197:PHE:HB2  | 2.01                     | 0.43              |
| 1:B:291:ARG:CG   | 1:B:291:ARG:HH11 | 2.31                     | 0.43              |
| 1:A:290:THR:C    | 1:A:291:ARG:HG3  | 2.39                     | 0.43              |
| 1:B:235:ILE:O    | 1:B:238:ARG:N    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:49:THR:CA    | 1:B:115:MET:SD   | 3.07                     | 0.43              |
| 1:B:318:GLN:O    | 1:B:319:ALA:C    | 2.62                     | 0.43              |
| 1:C:251:ASN:HA   | 1:C:255:VAL:CB   | 2.48                     | 0.43              |
| 1:C:362:LEU:HA   | 1:C:365:GLU:HB2  | 2.01                     | 0.43              |
| 1:A:65:LEU:HD23  | 1:A:133:TYR:HD1  | 1.84                     | 0.43              |
| 1:A:182:TRP:O    | 1:A:186:PHE:N    | 2.52                     | 0.43              |
| 1:A:193:PRO:HG2  | 1:A:196:VAL:CG2  | 2.48                     | 0.43              |
| 1:C:110:TYR:O    | 1:C:110:TYR:CD2  | 2.72                     | 0.43              |
| 1:C:265:THR:O    | 1:C:268:GLU:HB2  | 2.19                     | 0.43              |
| 1:C:272:ARG:HG3  | 1:C:272:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:122:ILE:O    | 1:A:125:PHE:N    | 2.52                     | 0.43              |
| 1:A:198:ARG:O    | 1:A:202:HIS:HB2  | 2.19                     | 0.43              |
| 1:A:231:PHE:C    | 1:A:233:PHE:N    | 2.73                     | 0.43              |
| 1:B:161:PHE:CE1  | 1:B:166:PHE:CD1  | 3.06                     | 0.42              |
| 1:B:216:LEU:HB2  | 1:B:250:TRP:CH2  | 2.54                     | 0.42              |
| 1:C:171:PHE:CD2  | 1:C:171:PHE:C    | 2.97                     | 0.42              |
| 1:B:236:PHE:O    | 1:B:237:THR:C    | 2.62                     | 0.42              |
| 1:C:174:THR:CB   | 1:C:238:ARG:HD3  | 2.49                     | 0.42              |
| 1:C:217:LYS:O    | 1:C:221:ASP:CB   | 2.67                     | 0.42              |
| 1:A:103:GLU:O    | 1:A:104:ASN:C    | 2.62                     | 0.42              |
| 1:C:78:LEU:O     | 1:C:81:THR:HB    | 2.19                     | 0.42              |
| 1:C:150:PHE:O    | 1:C:151:SER:C    | 2.61                     | 0.42              |
| 1:C:254:ALA:HA   | 1:C:260:TYR:CG   | 2.54                     | 0.42              |
| 1:B:273:LEU:HB2  | 1:B:306:ILE:HD13 | 2.01                     | 0.42              |
| 1:C:291:ARG:NH2  | 1:C:294:GLN:OE1  | 2.52                     | 0.42              |
| 1:A:59:LEU:HD11  | 1:A:122:ILE:HG23 | 2.01                     | 0.42              |
| 1:A:173:ILE:CG2  | 1:A:234:ASP:OD1  | 2.67                     | 0.42              |
| 1:A:183:ARG:O    | 1:A:187:GLY:HA2  | 2.19                     | 0.42              |
| 1:A:280:PRO:HA   | 1:A:300:VAL:HG12 | 2.01                     | 0.42              |
| 1:B:200:CYS:O    | 1:B:203:GLU:N    | 2.48                     | 0.42              |
| 1:B:257:HIS:HA   | 1:B:258:PRO:HD2  | 1.90                     | 0.42              |
| 1:C:123:ARG:O    | 1:C:127:GLU:HG2  | 2.18                     | 0.42              |
| 1:C:207:ILE:O    | 1:C:208:SER:C    | 2.61                     | 0.42              |
| 1:A:195:LYS:C    | 1:A:195:LYS:CD   | 2.92                     | 0.42              |
| 1:B:251:ASN:HA   | 1:B:255:VAL:CG2  | 2.50                     | 0.42              |
| 1:C:220:ILE:HG12 | 1:C:236:PHE:CD1  | 2.55                     | 0.42              |
| 1:C:272:ARG:HD3  | 1:C:284:ILE:HD13 | 2.00                     | 0.42              |
| 1:C:272:ARG:HG3  | 1:C:272:ARG:HH11 | 1.83                     | 0.42              |
| 1:A:57:VAL:O     | 1:A:57:VAL:HG12  | 2.20                     | 0.42              |
| 1:A:195:LYS:CD   | 1:A:196:VAL:N    | 2.76                     | 0.42              |
| 1:A:285:PHE:CD1  | 1:A:316:LEU:HD21 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:286:ARG:CD   | 1:A:287:LEU:O    | 2.68                     | 0.42              |
| 1:C:72:PRO:HG2   | 1:C:147:SER:CB   | 2.44                     | 0.42              |
| 1:C:114:LEU:HA   | 1:C:114:LEU:HD12 | 1.77                     | 0.42              |
| 1:A:60:CYS:HA    | 1:A:65:LEU:CD1   | 2.50                     | 0.41              |
| 1:A:122:ILE:O    | 1:A:123:ARG:C    | 2.63                     | 0.41              |
| 1:A:286:ARG:HE   | 1:A:296:ALA:HB3  | 1.84                     | 0.41              |
| 1:B:142:ASN:O    | 1:B:145:LYS:CB   | 2.51                     | 0.41              |
| 1:B:154:LEU:O    | 1:B:158:LYS:HG3  | 2.20                     | 0.41              |
| 1:C:161:PHE:CZ   | 1:C:166:PHE:CD1  | 3.07                     | 0.41              |
| 1:C:203:GLU:OE1  | 1:C:203:GLU:HA   | 2.11                     | 0.41              |
| 1:A:76:ASP:CA    | 1:A:79:PRO:HD2   | 2.50                     | 0.41              |
| 1:A:115:MET:O    | 1:A:116:LYS:C    | 2.61                     | 0.41              |
| 1:A:257:HIS:HA   | 1:A:258:PRO:HD2  | 1.87                     | 0.41              |
| 1:A:322:ASP:O    | 1:A:323:GLY:C    | 2.61                     | 0.41              |
| 1:B:74:ILE:O     | 1:B:78:LEU:HB2   | 2.21                     | 0.41              |
| 1:B:261:MET:O    | 1:B:262:ALA:CB   | 2.64                     | 0.41              |
| 1:C:64:LYS:HE3   | 1:C:133:TYR:CD2  | 2.55                     | 0.41              |
| 1:C:72:PRO:CG    | 1:C:147:SER:HB3  | 2.46                     | 0.41              |
| 1:C:332:PRO:HD2  | 1:C:338:ASN:HB2  | 2.01                     | 0.41              |
| 1:A:178:ALA:HB1  | 1:A:237:THR:HG21 | 2.00                     | 0.41              |
| 1:A:230:VAL:O    | 1:A:233:PHE:HB3  | 2.20                     | 0.41              |
| 1:B:71:PRO:HG3   | 1:B:73:TYR:CE1   | 2.56                     | 0.41              |
| 1:A:114:LEU:HD12 | 1:A:114:LEU:HA   | 1.83                     | 0.41              |
| 1:B:264:LEU:CB   | 1:B:286:ARG:HD3  | 2.50                     | 0.41              |
| 1:C:140:ARG:NH1  | 1:C:143:LEU:HD23 | 2.35                     | 0.41              |
| 1:C:257:HIS:CD2  | 1:C:259:GLY:H    | 2.34                     | 0.41              |
| 1:C:299:TYR:O    | 1:C:306:ILE:HA   | 2.20                     | 0.41              |
| 1:A:130:GLU:H    | 1:A:130:GLU:HG3  | 1.39                     | 0.41              |
| 1:A:160:ILE:CG2  | 1:A:166:PHE:CE1  | 2.96                     | 0.41              |
| 1:B:75:LEU:O     | 1:B:79:PRO:HG2   | 2.19                     | 0.41              |
| 1:B:215:ALA:HB1  | 1:B:363:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:205:HIS:HE1  | 1:A:244:GLY:O    | 2.03                     | 0.41              |
| 1:B:111:ILE:O    | 1:B:112:ASP:C    | 2.62                     | 0.41              |
| 1:B:235:ILE:HG23 | 1:B:293:GLY:CA   | 2.48                     | 0.41              |
| 1:B:266:TYR:CD1  | 1:B:308:GLN:OE1  | 2.74                     | 0.41              |
| 1:C:191:ILE:O    | 1:C:191:ILE:HG23 | 2.21                     | 0.41              |
| 1:B:78:LEU:HB3   | 1:B:79:PRO:HD3   | 2.02                     | 0.41              |
| 1:C:65:LEU:O     | 1:C:66:GLN:HG3   | 2.20                     | 0.41              |
| 1:C:76:ASP:C     | 1:C:79:PRO:HD2   | 2.45                     | 0.41              |
| 1:A:205:HIS:CE1  | 1:A:244:GLY:O    | 2.74                     | 0.41              |
| 1:C:106:TYR:HA   | 1:C:109:ILE:HG22 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:241:GLN:HB2  | 1:C:242:PRO:HA   | 2.02                     | 0.41              |
| 1:A:139:ASP:O    | 1:A:142:ASN:HB2  | 2.21                     | 0.41              |
| 1:B:238:ARG:HH11 | 1:B:238:ARG:HD2  | 1.73                     | 0.41              |
| 1:B:291:ARG:NH1  | 1:B:291:ARG:CB   | 2.84                     | 0.41              |
| 1:C:140:ARG:O    | 1:C:143:LEU:HB3  | 2.20                     | 0.41              |
| 1:C:177:ASP:HB3  | 1:C:243:TRP:CD1  | 2.56                     | 0.41              |
| 1:C:283:TYR:CD1  | 1:C:329:TYR:HB3  | 2.56                     | 0.41              |
| 1:A:188:ASP:OD1  | 1:A:188:ASP:N    | 2.49                     | 0.41              |
| 1:B:142:ASN:O    | 1:B:143:LEU:C    | 2.63                     | 0.41              |
| 1:B:235:ILE:HG22 | 1:B:239:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:256:THR:OG1  | 1:B:257:HIS:N    | 2.54                     | 0.41              |
| 1:B:286:ARG:HH21 | 1:B:308:GLN:NE2  | 2.07                     | 0.41              |
| 1:C:191:ILE:HD11 | 1:C:227:TYR:HB3  | 2.03                     | 0.41              |
| 1:C:299:TYR:CE2  | 1:C:301:THR:CG2  | 3.04                     | 0.41              |
| 1:A:162:PRO:O    | 1:A:162:PRO:HG2  | 2.21                     | 0.40              |
| 1:A:217:LYS:NZ   | 1:A:226:ASP:HA   | 2.36                     | 0.40              |
| 1:B:59:LEU:HD22  | 1:B:125:PHE:CG   | 2.56                     | 0.40              |
| 1:B:193:PRO:CG   | 1:B:196:VAL:CG2  | 3.00                     | 0.40              |
| 1:A:249:ASN:O    | 1:A:250:TRP:C    | 2.64                     | 0.40              |
| 1:A:286:ARG:O    | 1:A:295:TRP:HA   | 2.21                     | 0.40              |
| 1:C:47:GLU:O     | 1:C:50:TRP:HB2   | 2.22                     | 0.40              |
| 1:C:48:LYS:HA    | 1:C:51:LYS:HE2   | 2.03                     | 0.40              |
| 1:A:52:LEU:CD2   | 1:A:119:LYS:HG3  | 2.51                     | 0.40              |
| 1:A:113:SER:HG   | 1:A:225:ASN:HB3  | 1.86                     | 0.40              |
| 1:B:185:PHE:CD2  | 1:B:185:PHE:C    | 2.99                     | 0.40              |
| 1:B:327:GLY:HA2  | 1:B:330:LEU:HD21 | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|-----------|----------|-------------|----|
| 1   | A     | 281/394 (71%)  | 231 (82%) | 41 (15%)  | 9 (3%)   | 3           | 18 |
| 1   | B     | 284/394 (72%)  | 222 (78%) | 59 (21%)  | 3 (1%)   | 11          | 39 |
| 1   | C     | 282/394 (72%)  | 238 (84%) | 38 (14%)  | 6 (2%)   | 5           | 25 |
| All | All   | 847/1182 (72%) | 691 (82%) | 138 (16%) | 18 (2%)  | 5           | 25 |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 246 | ILE  |
| 1   | C     | 200 | CYS  |
| 1   | C     | 246 | ILE  |
| 1   | A     | 147 | SER  |
| 1   | A     | 184 | LYS  |
| 1   | A     | 196 | VAL  |
| 1   | B     | 191 | ILE  |
| 1   | B     | 326 | GLU  |
| 1   | A     | 208 | SER  |
| 1   | C     | 174 | THR  |
| 1   | A     | 69  | ASN  |
| 1   | A     | 132 | MET  |
| 1   | A     | 197 | PHE  |
| 1   | A     | 336 | SER  |
| 1   | C     | 104 | ASN  |
| 1   | C     | 243 | TRP  |
| 1   | B     | 184 | LYS  |
| 1   | C     | 224 | CYS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 208/352 (59%) | 187 (90%) | 21 (10%) | 7           | 28 |
| 1   | B     | 212/352 (60%) | 202 (95%) | 10 (5%)  | 23          | 55 |
| 1   | C     | 208/352 (59%) | 194 (93%) | 14 (7%)  | 15          | 43 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| All | All   | 628/1056 (60%) | 583 (93%) | 45 (7%)  | 13          | 40 |

All (45) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | VAL  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 58  | ARG  |
| 1   | A     | 78  | LEU  |
| 1   | A     | 113 | SER  |
| 1   | A     | 123 | ARG  |
| 1   | A     | 126 | LYS  |
| 1   | A     | 130 | GLU  |
| 1   | A     | 133 | TYR  |
| 1   | A     | 153 | MET  |
| 1   | A     | 169 | ASP  |
| 1   | A     | 188 | ASP  |
| 1   | A     | 195 | LYS  |
| 1   | A     | 200 | CYS  |
| 1   | A     | 245 | SER  |
| 1   | A     | 248 | ARG  |
| 1   | A     | 249 | ASN  |
| 1   | A     | 286 | ARG  |
| 1   | A     | 310 | ILE  |
| 1   | A     | 317 | PHE  |
| 1   | A     | 330 | LEU  |
| 1   | B     | 63  | PRO  |
| 1   | B     | 113 | SER  |
| 1   | B     | 133 | TYR  |
| 1   | B     | 148 | LEU  |
| 1   | B     | 192 | VAL  |
| 1   | B     | 219 | THR  |
| 1   | B     | 291 | ARG  |
| 1   | B     | 301 | THR  |
| 1   | B     | 309 | THR  |
| 1   | B     | 310 | ILE  |
| 1   | C     | 46  | VAL  |
| 1   | C     | 47  | GLU  |
| 1   | C     | 52  | LEU  |
| 1   | C     | 60  | CYS  |
| 1   | C     | 67  | LEU  |
| 1   | C     | 70  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 127 | GLU  |
| 1   | C     | 142 | ASN  |
| 1   | C     | 148 | LEU  |
| 1   | C     | 229 | SER  |
| 1   | C     | 264 | LEU  |
| 1   | C     | 272 | ARG  |
| 1   | C     | 309 | THR  |
| 1   | C     | 310 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 142 | ASN  |
| 1   | A     | 202 | HIS  |
| 1   | A     | 205 | HIS  |
| 1   | A     | 257 | HIS  |
| 1   | A     | 305 | ASN  |
| 1   | A     | 318 | GLN  |
| 1   | A     | 338 | ASN  |
| 1   | B     | 142 | ASN  |
| 1   | B     | 152 | HIS  |
| 1   | B     | 167 | GLN  |
| 1   | B     | 202 | HIS  |
| 1   | B     | 205 | HIS  |
| 1   | B     | 249 | ASN  |
| 1   | B     | 251 | ASN  |
| 1   | B     | 305 | ASN  |
| 1   | B     | 308 | GLN  |
| 1   | B     | 318 | GLN  |
| 1   | C     | 142 | ASN  |
| 1   | C     | 167 | GLN  |
| 1   | C     | 202 | HIS  |
| 1   | C     | 205 | HIS  |
| 1   | C     | 249 | ASN  |
| 1   | C     | 257 | HIS  |
| 1   | C     | 305 | ASN  |
| 1   | C     | 308 | GLN  |
| 1   | C     | 318 | GLN  |
| 1   | C     | 338 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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     | 287/394 (72%)  | -0.76  | 1 (0%) 90 80 | 43, 43, 46, 46        | 0     |
| 1   | B     | 294/394 (74%)  | -0.78  | 0 100 100    | 40, 47, 55, 55        | 0     |
| 1   | C     | 292/394 (74%)  | -0.54  | 2 (0%) 84 68 | 47, 59, 101, 101      | 0     |
| All | All   | 873/1182 (73%) | -0.69  | 3 (0%) 90 80 | 40, 47, 89, 101       | 0     |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 62  | ASN  | 3.8  |
| 1   | C     | 60  | CYS  | 3.0  |
| 1   | A     | 210 | GLY  | 2.3  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.