



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:58 AM UTC

PDB ID : 2QPD / pdb\_00002qpd  
Title : An unexpected outcome of surface-engineering an integral membrane protein: Improved crystallization of cytochrome ba3 oxidase from *Thermus thermophilus*  
Authors : Liu, B.; Luna, V.M.; Chen, Y.; Stout, C.D.; Fee, J.A.  
Deposited on : 2007-07-23  
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

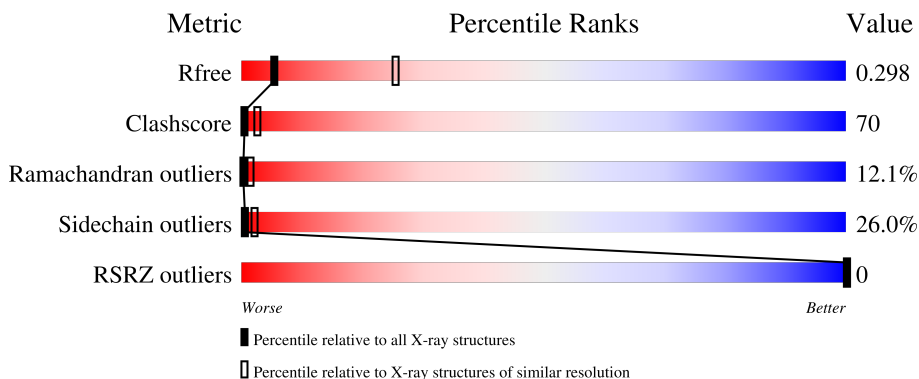
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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                      | 1605 (3.30-3.22)                                      |
| Clashscore            | 190562                      | 1660 (3.30-3.22)                                      |
| Ramachandran outliers | 187476                      | 1630 (3.30-3.22)                                      |
| Sidechain outliers    | 187428                      | 1629 (3.30-3.22)                                      |
| RSRZ outliers         | 180081                      | 1605 (3.30-3.22)                                      |

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     | 568    |                  |
| 2   | B     | 168    |                  |
| 3   | C     | 34     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 6   | HAS  | A     | 801 | X         | -        | X       | -                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6077 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 Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 557      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4409  | 2985 | 709 | 699 | 16 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | -5      | MET      | -      | expression tag      | UNP Q5SJ79 |
| A     | -4      | HIS      | -      | expression tag      | UNP Q5SJ79 |
| A     | -3      | HIS      | -      | expression tag      | UNP Q5SJ79 |
| A     | -2      | HIS      | -      | expression tag      | UNP Q5SJ79 |
| A     | -1      | HIS      | -      | expression tag      | UNP Q5SJ79 |
| A     | 0       | HIS      | -      | expression tag      | UNP Q5SJ79 |
| A     | 1       | HIS      | -      | expression tag      | UNP Q5SJ79 |
| A     | 258     | ARG      | LYS    | engineered mutation | UNP Q5SJ79 |

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 844 | 216 | 234 | 4 |         |         |       |

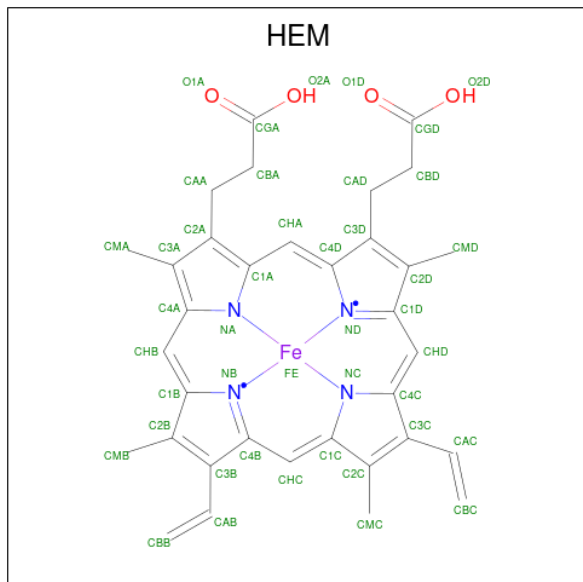
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 3   | C     | 33       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 259   | 179 | 39 | 41 |         |         |       |

- Molecule 4 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

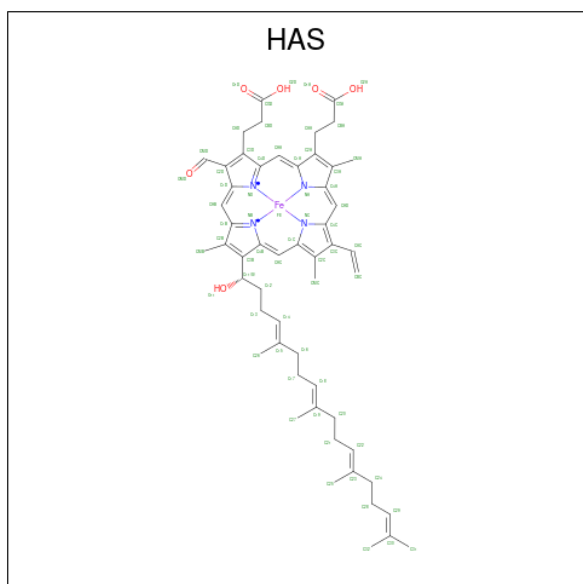
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



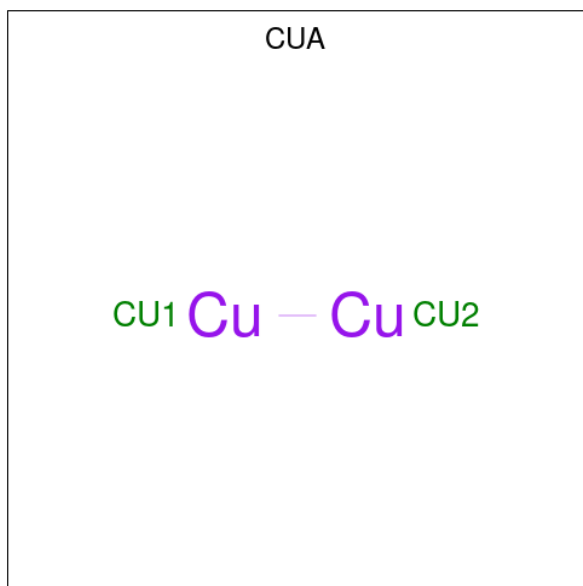
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 5   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula:  $\text{C}_{54}\text{H}_{64}\text{FeN}_4\text{O}_6$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 6   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 65    | 54 | 1  | 4 | 6 |         |         |

- Molecule 7 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula:  $\text{Cu}_2$ ).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | B     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

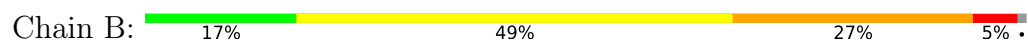
### 3 Residue-property plots

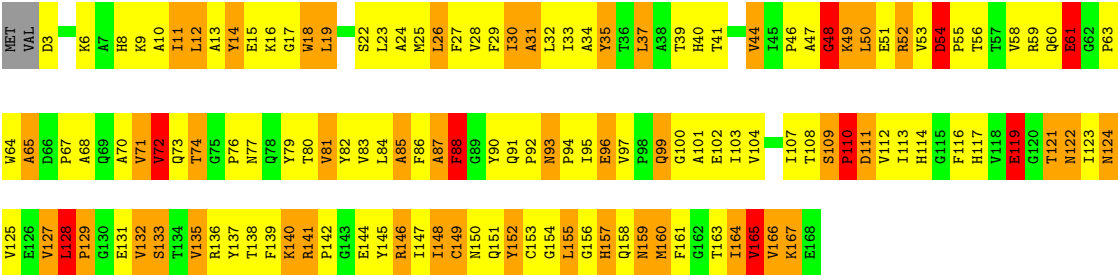
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytochrome c oxidase subunit 1

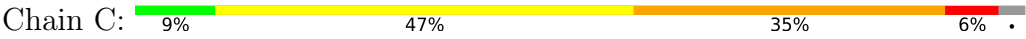


#### • Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 3: Cytochrome c oxidase polypeptide 2A



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 115.19Å 115.19Å 149.14Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.98 – 3.25<br>19.98 – 3.25                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 77.2 (19.98-3.25)<br>82.2 (19.98-3.25)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.03                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.25 (at 3.04Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.215 , 0.307<br>0.189 , 0.298                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 780 reflections (3.82%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 114.7                                                       | Xtriage          |
| Anisotropy                                                              | 0.167                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.25 , 71.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 6077                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 44.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

Bond lengths and bond angles in the following residue types are not validated in this section: HAS, CU1, HEM, CUA

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 1.32         | 21/4566 (0.5%) | 1.60        | 83/6266 (1.3%)  |
| 2   | B     | 1.38         | 12/1335 (0.9%) | 1.67        | 30/1822 (1.6%)  |
| 3   | C     | 1.43         | 2/265 (0.8%)   | 1.45        | 3/359 (0.8%)    |
| All | All   | 1.34         | 35/6166 (0.6%) | 1.61        | 116/8447 (1.4%) |

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                   | 4                   |
| 2   | B     | 0                   | 3                   |
| All | All   | 0                   | 7                   |

All (35) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 72  | VAL  | CA-CB | 7.35  | 1.64        | 1.54     |
| 1   | A     | 447 | VAL  | CA-CB | 6.67  | 1.62        | 1.54     |
| 2   | B     | 73  | GLN  | CA-C  | 6.49  | 1.61        | 1.52     |
| 2   | B     | 52  | ARG  | CA-C  | 6.31  | 1.60        | 1.52     |
| 1   | A     | 205 | VAL  | CA-CB | 6.28  | 1.60        | 1.54     |
| 2   | B     | 73  | GLN  | N-CA  | 6.13  | 1.54        | 1.46     |
| 1   | A     | 62  | VAL  | CA-CB | 6.03  | 1.60        | 1.53     |
| 2   | B     | 121 | THR  | CA-C  | 6.03  | 1.59        | 1.53     |
| 3   | C     | 21  | VAL  | CA-CB | 5.97  | 1.62        | 1.54     |
| 1   | A     | 447 | VAL  | CA-C  | 5.91  | 1.57        | 1.53     |
| 1   | A     | 250 | ILE  | CA-CB | -5.87 | 1.49        | 1.55     |
| 1   | A     | 8   | ILE  | CA-CB | 5.85  | 1.63        | 1.54     |
| 2   | B     | 127 | VAL  | CA-CB | 5.81  | 1.60        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 158 | VAL  | CA-CB | 5.80  | 1.62        | 1.54     |
| 1   | A     | 300 | VAL  | CA-CB | -5.76 | 1.47        | 1.54     |
| 1   | A     | 209 | LEU  | CA-C  | 5.74  | 1.60        | 1.52     |
| 1   | A     | 305 | VAL  | CA-CB | 5.61  | 1.60        | 1.54     |
| 2   | B     | 35  | TYR  | N-CA  | -5.60 | 1.39        | 1.46     |
| 1   | A     | 213 | PHE  | N-CA  | 5.60  | 1.53        | 1.46     |
| 1   | A     | 207 | PHE  | CA-C  | -5.53 | 1.48        | 1.52     |
| 1   | A     | 83  | LEU  | N-CA  | -5.52 | 1.39        | 1.46     |
| 2   | B     | 125 | VAL  | CA-CB | 5.50  | 1.61        | 1.54     |
| 1   | A     | 459 | ALA  | CA-CB | -5.43 | 1.45        | 1.53     |
| 2   | B     | 148 | ILE  | CA-CB | -5.32 | 1.47        | 1.54     |
| 1   | A     | 361 | ALA  | CA-C  | 5.29  | 1.60        | 1.52     |
| 1   | A     | 547 | VAL  | CA-CB | 5.29  | 1.61        | 1.54     |
| 1   | A     | 527 | ILE  | CA-CB | 5.27  | 1.61        | 1.54     |
| 2   | B     | 93  | ASN  | N-CA  | -5.25 | 1.41        | 1.46     |
| 1   | A     | 310 | LEU  | CA-C  | -5.16 | 1.46        | 1.52     |
| 2   | B     | 80  | THR  | CA-CB | 5.12  | 1.60        | 1.53     |
| 3   | C     | 4   | LYS  | CA-C  | 5.08  | 1.58        | 1.52     |
| 1   | A     | 391 | SER  | N-CA  | 5.07  | 1.52        | 1.46     |
| 2   | B     | 81  | VAL  | CA-CB | 5.06  | 1.59        | 1.53     |
| 1   | A     | 49  | VAL  | N-CA  | -5.01 | 1.40        | 1.46     |
| 1   | A     | 303 | LEU  | N-CA  | -5.00 | 1.40        | 1.46     |

All (116) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 339 | LEU  | CA-C-N  | 11.37  | 134.06      | 119.84   |
| 1   | A     | 339 | LEU  | C-N-CA  | 11.37  | 134.06      | 119.84   |
| 1   | A     | 44  | LEU  | N-CA-C  | -10.52 | 100.58      | 113.41   |
| 1   | A     | 514 | GLY  | CA-C-N  | 10.36  | 132.79      | 119.84   |
| 1   | A     | 514 | GLY  | C-N-CA  | 10.36  | 132.79      | 119.84   |
| 1   | A     | 220 | ASP  | CA-C-N  | 10.24  | 130.54      | 119.28   |
| 1   | A     | 220 | ASP  | C-N-CA  | 10.24  | 130.54      | 119.28   |
| 1   | A     | 437 | VAL  | CB-CA-C | -9.20  | 99.99       | 112.04   |
| 1   | A     | 348 | ALA  | CA-C-N  | -9.10  | 109.27      | 119.28   |
| 1   | A     | 348 | ALA  | C-N-CA  | -9.10  | 109.27      | 119.28   |
| 2   | B     | 155 | LEU  | N-CA-C  | 9.02   | 122.28      | 111.82   |
| 2   | B     | 121 | THR  | N-CA-C  | 8.50   | 119.80      | 108.07   |
| 3   | C     | 10  | ALA  | N-CA-C  | -8.43  | 101.13      | 111.33   |
| 2   | B     | 54  | ASP  | CA-C-N  | 7.95   | 127.61      | 119.82   |
| 2   | B     | 54  | ASP  | C-N-CA  | 7.95   | 127.61      | 119.82   |
| 1   | A     | 336 | ILE  | N-CA-C  | 7.60   | 118.19      | 110.82   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 141 | ARG  | CA-C-N   | -7.55 | 112.55      | 120.03   |
| 2   | B     | 141 | ARG  | C-N-CA   | -7.55 | 112.55      | 120.03   |
| 1   | A     | 343 | ASN  | CA-C-N   | 7.37  | 126.63      | 118.97   |
| 1   | A     | 343 | ASN  | C-N-CA   | 7.37  | 126.63      | 118.97   |
| 1   | A     | 506 | LEU  | CA-C-N   | -7.36 | 110.64      | 119.84   |
| 1   | A     | 506 | LEU  | C-N-CA   | -7.36 | 110.64      | 119.84   |
| 1   | A     | 266 | ARG  | N-CA-C   | -7.31 | 102.69      | 111.69   |
| 1   | A     | 261 | SER  | N-CA-C   | 7.15  | 119.35      | 107.20   |
| 2   | B     | 146 | ARG  | CB-CG-CD | -7.12 | 94.92       | 111.30   |
| 1   | A     | 274 | LEU  | N-CA-C   | 7.08  | 118.64      | 111.07   |
| 2   | B     | 109 | SER  | CA-C-N   | 7.02  | 128.61      | 119.84   |
| 2   | B     | 109 | SER  | C-N-CA   | 7.02  | 128.61      | 119.84   |
| 1   | A     | 306 | ALA  | N-CA-C   | -7.00 | 103.41      | 112.23   |
| 1   | A     | 446 | ASN  | CA-C-N   | -6.96 | 115.78      | 123.02   |
| 1   | A     | 446 | ASN  | C-N-CA   | -6.96 | 115.78      | 123.02   |
| 2   | B     | 132 | VAL  | CA-C-N   | 6.93  | 130.59      | 120.82   |
| 2   | B     | 132 | VAL  | C-N-CA   | 6.93  | 130.59      | 120.82   |
| 1   | A     | 247 | ILE  | N-CA-C   | 6.84  | 116.99      | 110.42   |
| 1   | A     | 254 | GLN  | N-CA-C   | -6.73 | 103.87      | 111.07   |
| 2   | B     | 61  | GLU  | N-CA-C   | 6.72  | 119.16      | 109.14   |
| 2   | B     | 52  | ARG  | N-CA-C   | 6.70  | 119.95      | 110.23   |
| 1   | A     | 29  | PHE  | N-CA-C   | 6.68  | 118.22      | 111.07   |
| 1   | A     | 393 | VAL  | CB-CA-C  | -6.66 | 103.17      | 111.70   |
| 1   | A     | 471 | VAL  | CB-CA-C  | -6.66 | 103.35      | 111.88   |
| 1   | A     | 218 | GLY  | N-CA-C   | 6.64  | 122.15      | 110.80   |
| 2   | B     | 79  | TYR  | CB-CA-C  | -6.62 | 102.46      | 110.94   |
| 1   | A     | 140 | LYS  | N-CA-C   | 6.61  | 120.64      | 107.62   |
| 1   | A     | 174 | ASN  | CA-C-N   | 6.61  | 127.60      | 120.13   |
| 1   | A     | 174 | ASN  | C-N-CA   | 6.61  | 127.60      | 120.13   |
| 1   | A     | 124 | LEU  | N-CA-C   | 6.55  | 118.50      | 111.36   |
| 2   | B     | 85  | ALA  | N-CA-C   | -6.50 | 100.86      | 110.48   |
| 1   | A     | 504 | ALA  | N-CA-C   | 6.39  | 123.92      | 109.81   |
| 1   | A     | 15  | TYR  | CA-C-N   | 6.38  | 127.82      | 119.84   |
| 1   | A     | 15  | TYR  | C-N-CA   | 6.38  | 127.82      | 119.84   |
| 1   | A     | 498 | LYS  | CA-C-N   | 6.32  | 127.74      | 119.84   |
| 1   | A     | 498 | LYS  | C-N-CA   | 6.32  | 127.74      | 119.84   |
| 1   | A     | 297 | ILE  | N-CA-C   | 6.32  | 116.36      | 110.42   |
| 2   | B     | 128 | LEU  | CA-C-N   | 6.23  | 127.63      | 119.84   |
| 2   | B     | 128 | LEU  | C-N-CA   | 6.23  | 127.63      | 119.84   |
| 2   | B     | 65  | ALA  | N-CA-C   | -6.20 | 103.25      | 111.24   |
| 3   | C     | 31  | PHE  | N-CA-C   | 6.12  | 117.64      | 110.97   |
| 1   | A     | 179 | THR  | CA-C-N   | -6.08 | 113.70      | 119.85   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 179 | THR  | C-N-CA    | -6.08 | 113.70      | 119.85   |
| 1   | A     | 215 | LEU  | N-CA-C    | 5.99  | 120.77      | 112.45   |
| 1   | A     | 310 | LEU  | N-CA-C    | -5.99 | 104.45      | 110.97   |
| 1   | A     | 265 | ALA  | N-CA-C    | -5.97 | 106.32      | 113.97   |
| 1   | A     | 466 | PRO  | N-CA-C    | -5.97 | 104.86      | 113.75   |
| 1   | A     | 22  | LEU  | CA-CB-CG  | -5.96 | 95.43       | 116.30   |
| 1   | A     | 225 | ARG  | NE-CZ-NH2 | 5.89  | 124.50      | 119.20   |
| 1   | A     | 393 | VAL  | N-CA-CB   | 5.85  | 116.76      | 110.62   |
| 1   | A     | 447 | VAL  | CB-CA-C   | 5.82  | 117.47      | 110.78   |
| 2   | B     | 68  | ALA  | N-CA-C    | -5.80 | 104.15      | 111.11   |
| 1   | A     | 249 | THR  | CB-CA-C   | -5.79 | 99.34       | 109.07   |
| 1   | A     | 527 | ILE  | CA-C-N    | 5.79  | 126.51      | 120.03   |
| 1   | A     | 527 | ILE  | C-N-CA    | 5.79  | 126.51      | 120.03   |
| 1   | A     | 45  | ASN  | N-CA-C    | -5.79 | 104.17      | 111.11   |
| 2   | B     | 122 | ASN  | N-CA-C    | -5.77 | 104.78      | 113.89   |
| 2   | B     | 156 | GLY  | N-CA-C    | -5.77 | 106.26      | 115.66   |
| 1   | A     | 427 | LEU  | N-CA-C    | -5.71 | 106.08      | 113.16   |
| 1   | A     | 247 | ILE  | CA-C-N    | 5.67  | 127.81      | 120.44   |
| 1   | A     | 247 | ILE  | C-N-CA    | 5.67  | 127.81      | 120.44   |
| 1   | A     | 52  | TYR  | CA-C-N    | 5.66  | 124.85      | 118.97   |
| 1   | A     | 52  | TYR  | C-N-CA    | 5.66  | 124.85      | 118.97   |
| 1   | A     | 284 | GLN  | N-CA-C    | -5.63 | 103.92      | 112.99   |
| 2   | B     | 164 | ILE  | N-CA-C    | -5.62 | 99.40       | 107.78   |
| 1   | A     | 341 | TRP  | CA-CB-CG  | -5.62 | 102.93      | 113.60   |
| 1   | A     | 297 | ILE  | CB-CA-C   | -5.61 | 104.63      | 111.87   |
| 1   | A     | 298 | HIS  | N-CA-C    | -5.60 | 106.15      | 112.87   |
| 1   | A     | 465 | VAL  | CA-C-N    | -5.55 | 112.99      | 119.32   |
| 1   | A     | 465 | VAL  | C-N-CA    | -5.55 | 112.99      | 119.32   |
| 1   | A     | 512 | ILE  | N-CA-C    | -5.55 | 97.80       | 109.34   |
| 1   | A     | 205 | VAL  | N-CA-CB   | 5.50  | 116.39      | 110.62   |
| 2   | B     | 50  | LEU  | CA-CB-CG  | 5.43  | 135.32      | 116.30   |
| 2   | B     | 165 | VAL  | CB-CA-C   | -5.42 | 103.46      | 110.84   |
| 1   | A     | 413 | ILE  | N-CA-CB   | 5.42  | 116.84      | 110.82   |
| 2   | B     | 132 | VAL  | N-CA-C    | 5.40  | 115.30      | 106.72   |
| 1   | A     | 340 | PRO  | N-CA-C    | 5.39  | 123.58      | 112.47   |
| 2   | B     | 125 | VAL  | CA-C-N    | -5.38 | 114.61      | 122.19   |
| 2   | B     | 125 | VAL  | C-N-CA    | -5.38 | 114.61      | 122.19   |
| 2   | B     | 53  | VAL  | CB-CA-C   | -5.37 | 103.07      | 110.91   |
| 1   | A     | 476 | VAL  | N-CA-C    | 5.33  | 115.55      | 110.53   |
| 1   | A     | 374 | VAL  | N-CA-C    | 5.32  | 119.49      | 112.04   |
| 1   | A     | 447 | VAL  | CA-C-O    | 5.31  | 123.08      | 119.20   |
| 1   | A     | 53  | PRO  | N-CA-C    | -5.22 | 106.00      | 113.47   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 165 | ASP  | N-CA-C   | -5.20 | 105.31      | 110.97   |
| 1   | A     | 327 | ARG  | CA-C-N   | -5.19 | 117.80      | 123.30   |
| 1   | A     | 327 | ARG  | C-N-CA   | -5.19 | 117.80      | 123.30   |
| 1   | A     | 299 | SER  | N-CA-C   | -5.17 | 105.29      | 111.03   |
| 2   | B     | 128 | LEU  | CA-CB-CG | 5.16  | 134.36      | 116.30   |
| 1   | A     | 418 | ARG  | N-CA-C   | -5.13 | 104.95      | 111.11   |
| 3   | C     | 22  | PHE  | N-CA-C   | 5.10  | 117.96      | 111.69   |
| 1   | A     | 100 | ARG  | N-CA-C   | 5.09  | 116.77      | 109.04   |
| 2   | B     | 88  | PHE  | CB-CA-C  | 5.08  | 120.52      | 110.42   |
| 1   | A     | 230 | TRP  | CA-C-N   | 5.07  | 127.34      | 120.44   |
| 1   | A     | 230 | TRP  | C-N-CA   | 5.07  | 127.34      | 120.44   |
| 1   | A     | 47  | GLY  | N-CA-C   | -5.07 | 106.28      | 112.77   |
| 1   | A     | 138 | PRO  | N-CA-C   | 5.03  | 125.17      | 112.10   |
| 1   | A     | 411 | LYS  | CA-C-N   | 5.01  | 126.10      | 119.84   |
| 1   | A     | 411 | LYS  | C-N-CA   | 5.01  | 126.10      | 119.84   |
| 1   | A     | 56  | LYS  | N-CA-C   | -5.01 | 105.90      | 111.36   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 174 | ASN  | Peptide |
| 1   | A     | 400 | SER  | Peptide |
| 1   | A     | 458 | ASP  | Peptide |
| 1   | A     | 503 | GLU  | Peptide |
| 2   | B     | 46  | PRO  | Peptide |
| 2   | B     | 48  | GLY  | Peptide |
| 2   | B     | 87  | ALA  | Peptide |

## 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     | 4409  | 0        | 4516     | 684     | 0            |
| 2   | B     | 1298  | 0        | 1280     | 166     | 0            |
| 3   | C     | 259   | 0        | 279      | 45      | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | A     | 43    | 0        | 30       | 9       | 0            |
| 6   | A     | 65    | 0        | 61       | 31      | 0            |
| 7   | B     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 6077  | 0        | 6166     | 858     | 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 70.

All (858) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:233:HIS:NE2  | 1:A:237:TYR:HE2  | 1.02                     | 1.42              |
| 1:A:233:HIS:NE2  | 1:A:237:TYR:CE2  | 1.95                     | 1.27              |
| 1:A:12:TYR:HA    | 1:A:16:PRO:HB3   | 1.21                     | 1.20              |
| 1:A:102:ASN:OD1  | 1:A:105:LEU:HG   | 1.41                     | 1.19              |
| 1:A:120:ALA:O    | 1:A:123:PRO:HD2  | 1.41                     | 1.17              |
| 1:A:300:VAL:HG13 | 2:B:30:ILE:CD1   | 1.78                     | 1.14              |
| 1:A:410:GLY:CA   | 1:A:502:ALA:HB2  | 1.77                     | 1.13              |
| 1:A:388:GLN:HA   | 1:A:388:GLN:NE2  | 1.61                     | 1.10              |
| 1:A:559:TRP:HB3  | 1:A:561:LEU:HD21 | 1.31                     | 1.10              |
| 1:A:559:TRP:HB3  | 1:A:561:LEU:CD2  | 1.85                     | 1.06              |
| 1:A:410:GLY:HA2  | 1:A:502:ALA:HB2  | 1.34                     | 1.05              |
| 2:B:97:VAL:HG23  | 2:B:166:VAL:HG12 | 1.38                     | 1.03              |
| 1:A:388:GLN:CA   | 1:A:388:GLN:HE21 | 1.68                     | 1.02              |
| 1:A:300:VAL:HG13 | 2:B:30:ILE:HD13  | 1.36                     | 1.02              |
| 1:A:526:ARG:HH21 | 1:A:529:PHE:HB2  | 1.21                     | 1.02              |
| 1:A:20:ALA:HB3   | 1:A:106:MET:HE3  | 1.45                     | 0.99              |
| 1:A:518:ARG:HH21 | 1:A:518:ARG:HG3  | 1.26                     | 0.98              |
| 1:A:385:PHE:CG   | 6:A:801:HAS:HMA1 | 1.98                     | 0.97              |
| 1:A:101:PRO:HA   | 1:A:166:LEU:HD11 | 1.46                     | 0.97              |
| 2:B:6:LYS:HE2    | 3:C:2:GLU:O      | 1.64                     | 0.96              |
| 2:B:8:HIS:O      | 2:B:11:ILE:HG22  | 1.65                     | 0.96              |
| 1:A:388:GLN:NE2  | 1:A:388:GLN:CA   | 2.25                     | 0.94              |
| 2:B:149:CYS:HB3  | 2:B:160:MET:HG2  | 1.49                     | 0.94              |
| 1:A:44:LEU:O     | 1:A:48:ASN:N     | 2.01                     | 0.93              |
| 1:A:233:HIS:CD2  | 1:A:237:TYR:HE2  | 1.84                     | 0.93              |
| 1:A:24:PHE:CD1   | 1:A:110:TRP:HD1  | 1.87                     | 0.92              |
| 1:A:300:VAL:CG1  | 2:B:30:ILE:CD1   | 2.47                     | 0.91              |
| 1:A:385:PHE:CD2  | 6:A:801:HAS:HMA1 | 2.04                     | 0.91              |
| 1:A:38:PHE:CZ    | 1:A:71:LEU:HD12  | 2.06                     | 0.90              |
| 1:A:560:ARG:O    | 1:A:560:ARG:HG3  | 1.69                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:55:LEU:O     | 1:A:55:LEU:HG    | 1.70                     | 0.89              |
| 1:A:78:ILE:HG22  | 1:A:79:VAL:N     | 1.84                     | 0.89              |
| 1:A:271:LEU:CD1  | 1:A:308:PRO:HD3  | 2.03                     | 0.88              |
| 1:A:135:PHE:O    | 1:A:137:PRO:HD3  | 1.72                     | 0.88              |
| 1:A:233:HIS:CD2  | 1:A:237:TYR:CE2  | 2.61                     | 0.88              |
| 1:A:385:PHE:HB2  | 6:A:801:HAS:HMA3 | 1.56                     | 0.88              |
| 2:B:97:VAL:HG23  | 2:B:166:VAL:CG1  | 2.04                     | 0.87              |
| 1:A:34:VAL:O     | 1:A:37:LEU:HB2   | 1.74                     | 0.87              |
| 1:A:271:LEU:HD13 | 1:A:308:PRO:HD3  | 1.57                     | 0.87              |
| 1:A:313:ALA:HB2  | 6:A:801:HAS:H273 | 1.56                     | 0.86              |
| 1:A:54:LEU:HD13  | 1:A:55:LEU:N     | 1.90                     | 0.86              |
| 1:A:54:LEU:C     | 1:A:54:LEU:HD22  | 2.00                     | 0.86              |
| 1:A:24:PHE:HD1   | 1:A:110:TRP:CD1  | 1.94                     | 0.86              |
| 1:A:313:ALA:HB2  | 6:A:801:HAS:C27  | 2.05                     | 0.86              |
| 1:A:412:PRO:HB3  | 1:A:501:LEU:HD13 | 1.58                     | 0.86              |
| 1:A:81:THR:HG1   | 1:A:239:TRP:CD1  | 1.93                     | 0.86              |
| 1:A:423:ALA:O    | 1:A:427:LEU:HB2  | 1.76                     | 0.86              |
| 1:A:486:TYR:O    | 1:A:490:SER:HB3  | 1.76                     | 0.86              |
| 1:A:192:MET:HB2  | 1:A:273:LEU:HA   | 1.57                     | 0.86              |
| 1:A:154:LEU:O    | 1:A:157:TRP:HB2  | 1.74                     | 0.85              |
| 1:A:309:SER:O    | 6:A:801:HAS:C27  | 2.24                     | 0.85              |
| 1:A:233:HIS:CE1  | 1:A:282:HIS:HE1  | 1.94                     | 0.85              |
| 1:A:410:GLY:HA3  | 1:A:502:ALA:HB2  | 1.59                     | 0.85              |
| 1:A:350:VAL:O    | 1:A:354:LEU:HD22 | 1.77                     | 0.84              |
| 1:A:300:VAL:HG13 | 2:B:30:ILE:HD11  | 1.60                     | 0.84              |
| 1:A:300:VAL:CG1  | 2:B:30:ILE:HD13  | 2.07                     | 0.84              |
| 1:A:351:LEU:HA   | 1:A:354:LEU:HD23 | 1.57                     | 0.84              |
| 1:A:233:HIS:CE1  | 1:A:282:HIS:CE1  | 2.65                     | 0.83              |
| 2:B:149:CYS:CB   | 2:B:160:MET:HG2  | 2.07                     | 0.83              |
| 1:A:24:PHE:HE1   | 1:A:110:TRP:HA   | 1.41                     | 0.83              |
| 1:A:347:VAL:HG12 | 1:A:351:LEU:HD11 | 1.61                     | 0.83              |
| 1:A:309:SER:O    | 6:A:801:HAS:H273 | 1.78                     | 0.82              |
| 1:A:233:HIS:HB3  | 1:A:234:PRO:HD2  | 1.60                     | 0.82              |
| 1:A:386:HIS:O    | 1:A:390:ALA:HB3  | 1.79                     | 0.82              |
| 1:A:174:ASN:O    | 1:A:177:LYS:HB2  | 1.80                     | 0.82              |
| 1:A:38:PHE:HZ    | 1:A:71:LEU:HD12  | 1.45                     | 0.81              |
| 1:A:89:MET:HE1   | 1:A:245:ALA:HB2  | 1.62                     | 0.81              |
| 1:A:277:THR:H    | 1:A:278:PRO:HD3  | 1.43                     | 0.81              |
| 1:A:559:TRP:CB   | 1:A:561:LEU:HD21 | 2.10                     | 0.81              |
| 1:A:105:LEU:HB2  | 1:A:162:ILE:HD11 | 1.62                     | 0.81              |
| 2:B:44:VAL:HG11  | 2:B:122:ASN:HB2  | 1.63                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:124:LEU:HD23 | 1:A:129:ALA:HB3  | 1.62                     | 0.80              |
| 1:A:234:PRO:HD3  | 1:A:276:SER:O    | 1.81                     | 0.80              |
| 1:A:498:LYS:N    | 1:A:499:PRO:HD3  | 1.97                     | 0.80              |
| 1:A:24:PHE:CD1   | 1:A:110:TRP:CD1  | 2.68                     | 0.79              |
| 1:A:63:GLN:HA    | 1:A:63:GLN:NE2   | 1.97                     | 0.79              |
| 1:A:403:TRP:CZ3  | 1:A:404:LEU:HD13 | 2.17                     | 0.79              |
| 3:C:8:ALA:O      | 3:C:11:VAL:HB    | 1.82                     | 0.79              |
| 1:A:11:VAL:O     | 1:A:13:GLU:N     | 2.15                     | 0.79              |
| 1:A:505:PRO:O    | 1:A:506:LEU:O    | 2.01                     | 0.79              |
| 1:A:146:TYR:CE2  | 1:A:208:LEU:HD22 | 2.19                     | 0.79              |
| 1:A:410:GLY:HA2  | 1:A:502:ALA:CB   | 2.12                     | 0.78              |
| 1:A:526:ARG:NH2  | 1:A:529:PHE:HB2  | 1.98                     | 0.78              |
| 1:A:294:TRP:CZ2  | 1:A:544:PRO:HD2  | 2.19                     | 0.78              |
| 1:A:184:TYR:CD2  | 1:A:266:ARG:HG2  | 2.17                     | 0.78              |
| 1:A:497:ARG:C    | 1:A:499:PRO:HD3  | 2.09                     | 0.78              |
| 1:A:385:PHE:CB   | 6:A:801:HAS:CMA  | 2.61                     | 0.77              |
| 2:B:90:TYR:OH    | 2:B:149:CYS:HB2  | 1.84                     | 0.77              |
| 1:A:340:PRO:O    | 1:A:342:ASP:N    | 2.18                     | 0.77              |
| 1:A:264:MET:HA   | 1:A:264:MET:HE2  | 1.65                     | 0.76              |
| 1:A:374:VAL:HG21 | 3:C:30:PHE:HA    | 1.67                     | 0.76              |
| 1:A:30:LEU:O     | 1:A:33:ILE:N     | 2.18                     | 0.76              |
| 1:A:472:LEU:HD22 | 1:A:472:LEU:O    | 1.84                     | 0.76              |
| 2:B:61:GLU:HA    | 2:B:65:ALA:HB2   | 1.65                     | 0.76              |
| 1:A:406:PRO:HA   | 1:A:411:LYS:O    | 1.85                     | 0.76              |
| 1:A:542:TYR:HB3  | 1:A:546:LEU:HD12 | 1.68                     | 0.76              |
| 1:A:70:THR:HG23  | 1:A:132:LEU:HA   | 1.68                     | 0.75              |
| 1:A:78:ILE:O     | 1:A:82:GLN:HB2   | 1.86                     | 0.75              |
| 2:B:11:ILE:HG23  | 2:B:12:LEU:N     | 2.01                     | 0.75              |
| 2:B:113:ILE:HG12 | 2:B:128:LEU:HD12 | 1.67                     | 0.75              |
| 1:A:135:PHE:CZ   | 1:A:228:PHE:HE1  | 2.04                     | 0.75              |
| 1:A:236:VAL:HA   | 1:A:239:TRP:CE3  | 2.21                     | 0.75              |
| 2:B:34:ALA:HA    | 2:B:37:LEU:HD22  | 1.69                     | 0.75              |
| 1:A:277:THR:N    | 1:A:278:PRO:CD   | 2.50                     | 0.75              |
| 1:A:544:PRO:O    | 1:A:548:GLN:HG3  | 1.87                     | 0.75              |
| 1:A:28:GLY:O     | 1:A:31:ALA:HB3   | 1.86                     | 0.75              |
| 1:A:187:VAL:CG1  | 1:A:527:ILE:HD12 | 2.15                     | 0.75              |
| 2:B:109:SER:HB3  | 2:B:129:PRO:HG3  | 1.69                     | 0.75              |
| 1:A:389:VAL:HG22 | 5:A:800:HEM:CBC  | 2.17                     | 0.75              |
| 1:A:297:ILE:HG22 | 1:A:298:HIS:N    | 2.01                     | 0.74              |
| 1:A:304:PHE:O    | 1:A:307:VAL:HG23 | 1.87                     | 0.74              |
| 1:A:93:PRO:HB3   | 1:A:183:THR:HG23 | 1.70                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:112:MET:HB3  | 1:A:155:SER:HB2  | 1.69                     | 0.73              |
| 1:A:236:VAL:CG2  | 1:A:237:TYR:H    | 2.02                     | 0.73              |
| 2:B:11:ILE:CG2   | 2:B:12:LEU:H     | 2.00                     | 0.73              |
| 3:C:11:VAL:HG12  | 3:C:12:ILE:N     | 2.02                     | 0.73              |
| 1:A:317:ALA:HA   | 1:A:320:LEU:HD12 | 1.70                     | 0.73              |
| 1:A:93:PRO:HG3   | 1:A:186:ALA:HB2  | 1.71                     | 0.73              |
| 1:A:122:LEU:HA   | 1:A:125:LEU:CD1  | 2.18                     | 0.73              |
| 1:A:412:PRO:HB3  | 1:A:501:LEU:CD1  | 2.19                     | 0.73              |
| 2:B:154:GLY:O    | 2:B:157:HIS:HB2  | 1.89                     | 0.73              |
| 1:A:244:TYR:OH   | 1:A:309:SER:HB3  | 1.89                     | 0.73              |
| 1:A:270:LEU:HD22 | 1:A:524:MET:HG2  | 1.71                     | 0.73              |
| 1:A:388:GLN:HE21 | 1:A:388:GLN:N    | 1.85                     | 0.73              |
| 1:A:157:TRP:CZ2  | 1:A:194:PHE:HE2  | 2.07                     | 0.73              |
| 1:A:91:TYR:CE2   | 1:A:408:LEU:HD21 | 2.22                     | 0.73              |
| 1:A:389:VAL:HA   | 1:A:393:VAL:HG23 | 1.71                     | 0.73              |
| 1:A:52:TYR:N     | 1:A:53:PRO:CD    | 2.51                     | 0.72              |
| 1:A:385:PHE:CG   | 6:A:801:HAS:CMA  | 2.73                     | 0.72              |
| 1:A:344:PRO:HG3  | 1:A:422:LEU:HD23 | 1.71                     | 0.72              |
| 1:A:364:ILE:HG22 | 1:A:365:VAL:N    | 2.04                     | 0.72              |
| 1:A:318:ALA:O    | 1:A:321:GLU:HB3  | 1.90                     | 0.72              |
| 2:B:32:LEU:O     | 2:B:35:TYR:HB3   | 1.90                     | 0.72              |
| 2:B:11:ILE:CG2   | 2:B:12:LEU:N     | 2.52                     | 0.72              |
| 1:A:499:PRO:HB3  | 1:A:502:ALA:CB   | 2.20                     | 0.71              |
| 3:C:26:VAL:O     | 3:C:29:VAL:N     | 2.22                     | 0.71              |
| 1:A:356:PHE:CE2  | 6:A:801:HAS:H162 | 2.25                     | 0.71              |
| 1:A:472:LEU:HD22 | 1:A:472:LEU:C    | 2.16                     | 0.71              |
| 1:A:482:LEU:O    | 1:A:485:ILE:N    | 2.23                     | 0.71              |
| 1:A:406:PRO:HD3  | 1:A:413:ILE:CD1  | 2.20                     | 0.71              |
| 1:A:12:TYR:CA    | 1:A:16:PRO:HB3   | 2.13                     | 0.70              |
| 1:A:544:PRO:HA   | 1:A:547:VAL:HG12 | 1.74                     | 0.70              |
| 1:A:9:SER:OG     | 1:A:11:VAL:HG23  | 1.92                     | 0.70              |
| 1:A:347:VAL:HG12 | 1:A:351:LEU:CD1  | 2.21                     | 0.70              |
| 1:A:499:PRO:HB3  | 1:A:502:ALA:HB2  | 1.73                     | 0.70              |
| 1:A:106:MET:N    | 1:A:162:ILE:HD11 | 2.07                     | 0.70              |
| 1:A:236:VAL:HG23 | 1:A:237:TYR:N    | 2.05                     | 0.70              |
| 1:A:389:VAL:HG22 | 5:A:800:HEM:HBC1 | 1.74                     | 0.70              |
| 2:B:59:ARG:O     | 2:B:65:ALA:HA    | 1.90                     | 0.70              |
| 1:A:465:VAL:HA   | 1:A:468:VAL:HG23 | 1.73                     | 0.70              |
| 1:A:366:ASN:HB3  | 6:A:801:HAS:CMD  | 2.21                     | 0.69              |
| 1:A:23:TYR:HD1   | 1:A:107:TRP:HH2  | 1.39                     | 0.69              |
| 1:A:38:PHE:O     | 1:A:39:GLY:C     | 2.35                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:505:PRO:O    | 1:A:506:LEU:C    | 2.35                     | 0.69              |
| 1:A:181:LEU:HD13 | 1:A:262:ASP:OD1  | 1.93                     | 0.69              |
| 1:A:411:LYS:HG2  | 1:A:497:ARG:HB3  | 1.74                     | 0.69              |
| 1:A:385:PHE:CB   | 6:A:801:HAS:HMA1 | 2.21                     | 0.69              |
| 1:A:89:MET:HE1   | 1:A:245:ALA:CB   | 2.23                     | 0.69              |
| 1:A:497:ARG:HH21 | 1:A:499:PRO:HG2  | 1.58                     | 0.68              |
| 1:A:24:PHE:HD1   | 1:A:110:TRP:HD1  | 1.27                     | 0.68              |
| 1:A:545:THR:O    | 1:A:549:LEU:HG   | 1.93                     | 0.68              |
| 1:A:518:ARG:HH21 | 1:A:518:ARG:CG   | 2.03                     | 0.68              |
| 1:A:233:HIS:HB3  | 1:A:234:PRO:CD   | 2.23                     | 0.68              |
| 1:A:382:PRO:HA   | 1:A:385:PHE:CZ   | 2.29                     | 0.68              |
| 1:A:370:THR:HA   | 1:A:373:TYR:CD1  | 2.29                     | 0.68              |
| 1:A:30:LEU:O     | 1:A:31:ALA:C     | 2.37                     | 0.68              |
| 1:A:122:LEU:HA   | 1:A:125:LEU:HD11 | 1.75                     | 0.68              |
| 1:A:236:VAL:HG23 | 1:A:237:TYR:H    | 1.59                     | 0.67              |
| 1:A:515:PRO:HD2  | 2:B:8:HIS:HD2    | 1.58                     | 0.67              |
| 1:A:363:GLY:O    | 1:A:366:ASN:HB2  | 1.94                     | 0.67              |
| 1:A:370:THR:HA   | 1:A:373:TYR:CE1  | 2.30                     | 0.67              |
| 1:A:97:LEU:HD22  | 1:A:170:TRP:NE1  | 2.10                     | 0.67              |
| 1:A:233:HIS:ND1  | 1:A:282:HIS:CE1  | 2.62                     | 0.67              |
| 1:A:323:ALA:O    | 1:A:327:ARG:HG3  | 1.95                     | 0.66              |
| 1:A:441:TRP:HB3  | 1:A:466:PRO:HB3  | 1.78                     | 0.66              |
| 1:A:79:VAL:HA    | 1:A:152:PHE:CZ   | 2.31                     | 0.66              |
| 2:B:149:CYS:HB3  | 2:B:160:MET:CG   | 2.24                     | 0.66              |
| 1:A:187:VAL:HG12 | 1:A:527:ILE:HD12 | 1.77                     | 0.66              |
| 1:A:251:LEU:HA   | 1:A:254:GLN:HG3  | 1.77                     | 0.66              |
| 1:A:386:HIS:HA   | 1:A:390:ALA:HB3  | 1.77                     | 0.66              |
| 3:C:26:VAL:O     | 3:C:27:TYR:C     | 2.39                     | 0.66              |
| 1:A:50:ASP:O     | 1:A:53:PRO:HD2   | 1.96                     | 0.66              |
| 2:B:84:LEU:CD1   | 2:B:108:THR:HG23 | 2.26                     | 0.66              |
| 1:A:220:ASP:HB2  | 1:A:554:ASN:C    | 2.21                     | 0.66              |
| 1:A:251:LEU:HA   | 1:A:254:GLN:CG   | 2.26                     | 0.66              |
| 1:A:386:HIS:HE1  | 5:A:800:HEM:C4D  | 2.14                     | 0.66              |
| 1:A:147:LEU:O    | 1:A:151:VAL:HG23 | 1.95                     | 0.65              |
| 1:A:388:GLN:HA   | 1:A:388:GLN:HE21 | 1.26                     | 0.65              |
| 2:B:84:LEU:HD12  | 2:B:108:THR:O    | 1.97                     | 0.65              |
| 1:A:236:VAL:CG2  | 1:A:237:TYR:N    | 2.59                     | 0.65              |
| 1:A:404:LEU:O    | 1:A:408:LEU:HB2  | 1.97                     | 0.65              |
| 1:A:526:ARG:HH21 | 1:A:529:PHE:CB   | 2.02                     | 0.65              |
| 1:A:120:ALA:O    | 1:A:123:PRO:CD   | 2.33                     | 0.65              |
| 1:A:122:LEU:O    | 1:A:123:PRO:C    | 2.37                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:9:LEU:HA     | 3:C:12:ILE:CD1   | 2.27                     | 0.65              |
| 1:A:405:LEU:O    | 1:A:406:PRO:C    | 2.37                     | 0.65              |
| 1:A:297:ILE:O    | 1:A:300:VAL:N    | 2.30                     | 0.65              |
| 1:A:321:GLU:HA   | 1:A:335:TRP:CE3  | 2.32                     | 0.65              |
| 1:A:364:ILE:O    | 1:A:365:VAL:C    | 2.38                     | 0.65              |
| 1:A:346:PHE:O    | 1:A:350:VAL:HG23 | 1.97                     | 0.65              |
| 1:A:192:MET:HB2  | 1:A:273:LEU:CA   | 2.27                     | 0.65              |
| 1:A:220:ASP:HB2  | 1:A:554:ASN:H    | 1.61                     | 0.65              |
| 1:A:385:PHE:HB2  | 6:A:801:HAS:CMA  | 2.25                     | 0.65              |
| 1:A:112:MET:CB   | 1:A:155:SER:HB2  | 2.26                     | 0.64              |
| 1:A:225:ARG:HA   | 1:A:228:PHE:HB3  | 1.80                     | 0.64              |
| 1:A:464:ALA:HB3  | 1:A:465:VAL:HG12 | 1.78                     | 0.64              |
| 1:A:523:ALA:O    | 1:A:526:ARG:HB2  | 1.98                     | 0.64              |
| 2:B:117:HIS:HD2  | 2:B:124:ASN:HB2  | 1.63                     | 0.64              |
| 2:B:153:CYS:SG   | 2:B:157:HIS:HA   | 2.37                     | 0.64              |
| 1:A:105:LEU:HD23 | 1:A:105:LEU:N    | 2.11                     | 0.64              |
| 1:A:453:ILE:HD13 | 1:A:454:ALA:N    | 2.13                     | 0.64              |
| 1:A:560:ARG:O    | 1:A:560:ARG:CG   | 2.42                     | 0.64              |
| 2:B:82:TYR:CD1   | 2:B:82:TYR:N     | 2.65                     | 0.64              |
| 1:A:192:MET:CB   | 1:A:273:LEU:HA   | 2.26                     | 0.64              |
| 1:A:511:VAL:HG12 | 1:A:512:ILE:C    | 2.23                     | 0.64              |
| 1:A:271:LEU:HD12 | 1:A:308:PRO:HD3  | 1.79                     | 0.64              |
| 3:C:13:LEU:O     | 3:C:16:THR:HB    | 1.97                     | 0.64              |
| 1:A:88:ILE:O     | 1:A:90:VAL:N     | 2.30                     | 0.64              |
| 1:A:170:TRP:CE3  | 1:A:171:LYS:HA   | 2.33                     | 0.64              |
| 1:A:410:GLY:CA   | 1:A:502:ALA:CB   | 2.68                     | 0.64              |
| 1:A:24:PHE:HE1   | 1:A:110:TRP:CA   | 2.09                     | 0.63              |
| 1:A:466:PRO:O    | 1:A:469:PHE:HB2  | 1.98                     | 0.63              |
| 2:B:152:TYR:HA   | 2:B:157:HIS:CD2  | 2.32                     | 0.63              |
| 1:A:199:GLY:HA3  | 1:A:230:TRP:CG   | 2.34                     | 0.63              |
| 1:A:23:TYR:HB3   | 1:A:110:TRP:NE1  | 2.13                     | 0.63              |
| 1:A:75:LEU:O     | 1:A:79:VAL:HB    | 1.98                     | 0.63              |
| 1:A:403:TRP:HZ3  | 1:A:404:LEU:HD13 | 1.62                     | 0.63              |
| 1:A:332:LEU:HA   | 3:C:6:LYS:HE3    | 1.81                     | 0.62              |
| 1:A:402:TYR:CE1  | 1:A:413:ILE:HG21 | 2.34                     | 0.62              |
| 1:A:550:PHE:HA   | 1:A:553:LEU:CD2  | 2.28                     | 0.62              |
| 1:A:105:LEU:HB2  | 1:A:162:ILE:CD1  | 2.28                     | 0.62              |
| 1:A:251:LEU:HD12 | 1:A:254:GLN:HG3  | 1.80                     | 0.62              |
| 1:A:343:ASN:O    | 1:A:347:VAL:HG23 | 2.00                     | 0.62              |
| 1:A:199:GLY:HA3  | 1:A:230:TRP:HB3  | 1.82                     | 0.62              |
| 3:C:9:LEU:HA     | 3:C:12:ILE:HD13  | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:ALA:HA   | 1:A:152:PHE:HA   | 1.81                     | 0.62              |
| 1:A:262:ASP:N    | 1:A:263:PRO:HD2  | 2.14                     | 0.62              |
| 2:B:131:GLU:HG3  | 2:B:132:VAL:N    | 2.14                     | 0.62              |
| 1:A:28:GLY:N     | 1:A:83:LEU:HD13  | 2.15                     | 0.62              |
| 1:A:442:ALA:O    | 1:A:445:LEU:HB2  | 2.00                     | 0.62              |
| 1:A:189:PHE:CE1  | 1:A:242:PRO:HD3  | 2.34                     | 0.62              |
| 1:A:233:HIS:O    | 1:A:236:VAL:HG22 | 1.99                     | 0.62              |
| 1:A:407:ASN:ND2  | 1:A:506:LEU:HD23 | 2.15                     | 0.62              |
| 1:A:472:LEU:C    | 1:A:472:LEU:CD2  | 2.73                     | 0.62              |
| 1:A:56:LYS:O     | 1:A:59:LEU:O     | 2.18                     | 0.62              |
| 2:B:90:TYR:CZ    | 2:B:147:ILE:HG22 | 2.34                     | 0.62              |
| 1:A:133:TYR:OH   | 6:A:801:HAS:O1A  | 2.17                     | 0.61              |
| 1:A:357:ILE:HG22 | 1:A:358:PRO:N    | 2.14                     | 0.61              |
| 1:A:390:ALA:HA   | 5:A:800:HEM:HBC2 | 1.81                     | 0.61              |
| 1:A:267:LEU:O    | 1:A:268:ALA:C    | 2.41                     | 0.61              |
| 1:A:347:VAL:CG1  | 1:A:351:LEU:HD11 | 2.29                     | 0.61              |
| 1:A:453:ILE:HD13 | 1:A:453:ILE:C    | 2.26                     | 0.61              |
| 1:A:94:ALA:O     | 1:A:97:LEU:N     | 2.30                     | 0.60              |
| 1:A:239:TRP:HE3  | 6:A:801:HAS:HBC2 | 1.65                     | 0.60              |
| 2:B:147:ILE:O    | 2:B:161:PHE:HA   | 2.01                     | 0.60              |
| 1:A:54:LEU:HD22  | 1:A:54:LEU:O     | 2.00                     | 0.60              |
| 1:A:385:PHE:CB   | 6:A:801:HAS:HMA3 | 2.22                     | 0.60              |
| 1:A:544:PRO:O    | 1:A:548:GLN:CG   | 2.49                     | 0.60              |
| 2:B:102:GLU:HA   | 2:B:138:THR:HG23 | 1.84                     | 0.60              |
| 1:A:196:ALA:O    | 1:A:198:LEU:N    | 2.34                     | 0.60              |
| 1:A:59:LEU:HB3   | 1:A:61:PHE:CE1   | 2.36                     | 0.60              |
| 1:A:38:PHE:HA    | 1:A:41:PHE:HD1   | 1.66                     | 0.60              |
| 1:A:44:LEU:C     | 1:A:47:GLY:H     | 2.10                     | 0.60              |
| 1:A:154:LEU:O    | 1:A:157:TRP:N    | 2.35                     | 0.60              |
| 1:A:187:VAL:HG11 | 1:A:527:ILE:HD12 | 1.83                     | 0.60              |
| 1:A:189:PHE:O    | 1:A:191:LEU:N    | 2.35                     | 0.59              |
| 1:A:277:THR:N    | 1:A:278:PRO:HD3  | 2.11                     | 0.59              |
| 1:A:432:MET:O    | 1:A:436:ALA:N    | 2.27                     | 0.59              |
| 1:A:108:LEU:O    | 1:A:112:MET:HG3  | 2.01                     | 0.59              |
| 1:A:282:HIS:CD2  | 1:A:283:HIS:CD2  | 2.90                     | 0.59              |
| 1:A:355:GLY:O    | 1:A:358:PRO:HG2  | 2.02                     | 0.59              |
| 2:B:30:ILE:HA    | 2:B:33:ILE:HD12  | 1.82                     | 0.59              |
| 1:A:550:PHE:HA   | 1:A:553:LEU:HD21 | 1.83                     | 0.59              |
| 2:B:11:ILE:O     | 2:B:12:LEU:C     | 2.46                     | 0.59              |
| 1:A:244:TYR:O    | 1:A:248:TYR:HB2  | 2.02                     | 0.59              |
| 1:A:81:THR:OG1   | 1:A:239:TRP:CD1  | 2.54                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:335:TRP:O    | 1:A:339:LEU:HD22 | 2.03                     | 0.59              |
| 2:B:142:PRO:HA   | 2:B:166:VAL:O    | 2.02                     | 0.59              |
| 1:A:334:GLY:O    | 1:A:336:ILE:N    | 2.35                     | 0.58              |
| 1:A:546:LEU:O    | 1:A:550:PHE:HD1  | 1.86                     | 0.58              |
| 2:B:110:PRO:O    | 2:B:111:ASP:HB3  | 2.02                     | 0.58              |
| 1:A:153:VAL:O    | 1:A:154:LEU:C    | 2.44                     | 0.58              |
| 1:A:134:THR:O    | 1:A:135:PHE:CD1  | 2.56                     | 0.58              |
| 1:A:536:ILE:HG22 | 1:A:537:LEU:HD23 | 1.85                     | 0.58              |
| 1:A:64:SER:O     | 1:A:65:TYR:C     | 2.44                     | 0.58              |
| 1:A:184:TYR:CE2  | 1:A:266:ARG:HG2  | 2.38                     | 0.58              |
| 2:B:70:ALA:O     | 2:B:81:VAL:HA    | 2.04                     | 0.58              |
| 2:B:90:TYR:CE1   | 2:B:147:ILE:HG22 | 2.39                     | 0.58              |
| 2:B:157:HIS:ND1  | 2:B:157:HIS:C    | 2.59                     | 0.58              |
| 1:A:74:VAL:O     | 1:A:78:ILE:HB    | 2.04                     | 0.58              |
| 1:A:52:TYR:O     | 1:A:56:LYS:N     | 2.36                     | 0.58              |
| 1:A:554:ASN:HD22 | 2:B:52:ARG:HG3   | 1.68                     | 0.58              |
| 1:A:449:ARG:HH12 | 6:A:801:HAS:CGA  | 2.16                     | 0.58              |
| 2:B:157:HIS:O    | 2:B:160:MET:HB3  | 2.04                     | 0.58              |
| 1:A:135:PHE:CZ   | 1:A:228:PHE:CE1  | 2.90                     | 0.58              |
| 1:A:382:PRO:HA   | 1:A:385:PHE:CE2  | 2.39                     | 0.57              |
| 1:A:451:ALA:O    | 1:A:453:ILE:N    | 2.34                     | 0.57              |
| 1:A:140:LYS:HE3  | 1:A:211:TRP:CE2  | 2.38                     | 0.57              |
| 2:B:63:PRO:HG2   | 2:B:82:TYR:CE2   | 2.39                     | 0.57              |
| 2:B:101:ALA:O    | 2:B:103:ILE:HD12 | 2.04                     | 0.57              |
| 1:A:235:ILE:O    | 1:A:235:ILE:HG12 | 2.03                     | 0.57              |
| 2:B:71:VAL:O     | 2:B:72:VAL:HG12  | 2.03                     | 0.57              |
| 2:B:149:CYS:SG   | 2:B:160:MET:HG2  | 2.44                     | 0.57              |
| 1:A:97:LEU:HD22  | 1:A:170:TRP:CD1  | 2.40                     | 0.57              |
| 1:A:24:PHE:CE1   | 1:A:110:TRP:HA   | 2.31                     | 0.57              |
| 1:A:515:PRO:HD2  | 2:B:8:HIS:CD2    | 2.39                     | 0.57              |
| 1:A:35:GLY:CA    | 1:A:75:LEU:HD12  | 2.34                     | 0.57              |
| 1:A:375:VAL:O    | 1:A:376:HIS:C    | 2.47                     | 0.56              |
| 1:A:381:VAL:HB   | 1:A:382:PRO:CD   | 2.35                     | 0.56              |
| 1:A:45:ASN:ND2   | 1:A:65:TYR:CZ    | 2.73                     | 0.56              |
| 1:A:52:TYR:H     | 1:A:53:PRO:CD    | 2.18                     | 0.56              |
| 1:A:260:VAL:HA   | 1:A:512:ILE:HD13 | 1.87                     | 0.56              |
| 1:A:297:ILE:C    | 1:A:299:SER:N    | 2.59                     | 0.56              |
| 1:A:351:LEU:HA   | 1:A:354:LEU:CD2  | 2.33                     | 0.56              |
| 1:A:381:VAL:O    | 1:A:384:HIS:HB3  | 2.05                     | 0.56              |
| 2:B:83:VAL:HG12  | 2:B:84:LEU:N     | 2.19                     | 0.56              |
| 1:A:91:TYR:OH    | 1:A:407:ASN:OD1  | 2.22                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:24:ALA:O     | 2:B:25:MET:C     | 2.49                     | 0.56              |
| 1:A:405:LEU:O    | 1:A:408:LEU:N    | 2.38                     | 0.56              |
| 1:A:24:PHE:CD2   | 1:A:86:GLN:HB3   | 2.40                     | 0.56              |
| 1:A:41:PHE:CE2   | 1:A:55:LEU:HB2   | 2.41                     | 0.56              |
| 1:A:44:LEU:HD12  | 1:A:51:ALA:HB2   | 1.88                     | 0.56              |
| 1:A:151:VAL:O    | 1:A:152:PHE:C    | 2.48                     | 0.56              |
| 1:A:395:LEU:HD21 | 1:A:428:TRP:CD1  | 2.40                     | 0.56              |
| 2:B:90:TYR:OH    | 2:B:149:CYS:CB   | 2.52                     | 0.56              |
| 1:A:23:TYR:CD1   | 1:A:107:TRP:HH2  | 2.23                     | 0.55              |
| 1:A:157:TRP:CZ2  | 1:A:194:PHE:CE2  | 2.91                     | 0.55              |
| 1:A:344:PRO:HG3  | 1:A:422:LEU:CD2  | 2.36                     | 0.55              |
| 2:B:56:THR:O     | 2:B:60:GLN:NE2   | 2.39                     | 0.55              |
| 1:A:226:THR:HG23 | 1:A:281:PHE:HE2  | 1.70                     | 0.55              |
| 1:A:428:TRP:CD1  | 1:A:428:TRP:C    | 2.84                     | 0.55              |
| 1:A:467:MET:HA   | 1:A:470:ASN:HD22 | 1.71                     | 0.55              |
| 2:B:54:ASP:OD1   | 2:B:54:ASP:C     | 2.49                     | 0.55              |
| 1:A:340:PRO:C    | 1:A:342:ASP:H    | 2.15                     | 0.55              |
| 1:A:442:ALA:O    | 1:A:447:VAL:HG23 | 2.06                     | 0.55              |
| 1:A:365:VAL:O    | 1:A:367:ALA:N    | 2.39                     | 0.55              |
| 1:A:481:LEU:HD12 | 1:A:481:LEU:O    | 2.05                     | 0.55              |
| 1:A:515:PRO:CD   | 2:B:8:HIS:HD2    | 2.18                     | 0.55              |
| 1:A:277:THR:H    | 1:A:278:PRO:CD   | 2.07                     | 0.55              |
| 1:A:465:VAL:O    | 1:A:466:PRO:C    | 2.50                     | 0.55              |
| 2:B:35:TYR:C     | 2:B:35:TYR:CD1   | 2.76                     | 0.55              |
| 1:A:135:PHE:CE1  | 1:A:228:PHE:CE1  | 2.95                     | 0.55              |
| 1:A:106:MET:O    | 1:A:109:SER:HB3  | 2.07                     | 0.55              |
| 2:B:88:PHE:HE2   | 2:B:153:CYS:SG   | 2.30                     | 0.55              |
| 1:A:184:TYR:CE2  | 1:A:266:ARG:HB3  | 2.42                     | 0.55              |
| 2:B:82:TYR:H     | 2:B:82:TYR:HD1   | 1.51                     | 0.54              |
| 3:C:10:ALA:O     | 3:C:14:VAL:HG23  | 2.07                     | 0.54              |
| 1:A:192:MET:HB2  | 1:A:273:LEU:CB   | 2.36                     | 0.54              |
| 1:A:191:LEU:HB3  | 1:A:531:PHE:CD2  | 2.42                     | 0.54              |
| 1:A:282:HIS:NE2  | 1:A:283:HIS:CD2  | 2.76                     | 0.54              |
| 1:A:386:HIS:HA   | 1:A:390:ALA:CB   | 2.37                     | 0.54              |
| 1:A:497:ARG:HH21 | 1:A:499:PRO:CG   | 2.20                     | 0.54              |
| 2:B:27:PHE:O     | 2:B:31:ALA:N     | 2.29                     | 0.54              |
| 3:C:10:ALA:O     | 3:C:13:LEU:HB3   | 2.07                     | 0.54              |
| 1:A:52:TYR:N     | 1:A:53:PRO:HD2   | 2.21                     | 0.54              |
| 1:A:89:MET:O     | 1:A:93:PRO:HG2   | 2.06                     | 0.54              |
| 1:A:406:PRO:HD3  | 1:A:413:ILE:HD12 | 1.88                     | 0.54              |
| 2:B:116:PHE:O    | 2:B:116:PHE:CD2  | 2.61                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:465:VAL:O    | 1:A:468:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:135:PHE:O    | 1:A:137:PRO:CD   | 2.52                     | 0.54              |
| 1:A:234:PRO:HG3  | 1:A:277:THR:HA   | 1.90                     | 0.54              |
| 1:A:532:ALA:O    | 1:A:536:ILE:N    | 2.38                     | 0.54              |
| 1:A:547:VAL:HG13 | 1:A:548:GLN:H    | 1.71                     | 0.54              |
| 1:A:89:MET:HB3   | 1:A:190:TRP:NE1  | 2.23                     | 0.54              |
| 1:A:122:LEU:HA   | 1:A:125:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:267:LEU:HD12 | 1:A:270:LEU:HB3  | 1.89                     | 0.54              |
| 1:A:398:MET:O    | 1:A:401:LEU:HB2  | 2.08                     | 0.54              |
| 2:B:157:HIS:C    | 2:B:159:ASN:H    | 2.15                     | 0.54              |
| 1:A:233:HIS:CD2  | 1:A:233:HIS:C    | 2.86                     | 0.54              |
| 1:A:285:PHE:CE1  | 1:A:369:PHE:HA   | 2.43                     | 0.54              |
| 1:A:23:TYR:O     | 1:A:24:PHE:C     | 2.51                     | 0.54              |
| 1:A:41:PHE:HE2   | 1:A:54:LEU:HD11  | 1.72                     | 0.54              |
| 1:A:124:LEU:CD2  | 1:A:129:ALA:HB3  | 2.34                     | 0.54              |
| 1:A:346:PHE:O    | 1:A:349:PRO:HD2  | 2.08                     | 0.54              |
| 1:A:371:LEU:HD23 | 3:C:26:VAL:HG12  | 1.89                     | 0.54              |
| 1:A:511:VAL:HG12 | 1:A:512:ILE:O    | 2.06                     | 0.54              |
| 6:A:801:HAS:HHA  | 6:A:801:HAS:CBA  | 2.38                     | 0.54              |
| 2:B:58:VAL:HG13  | 2:B:59:ARG:N     | 2.23                     | 0.54              |
| 1:A:498:LYS:N    | 1:A:499:PRO:CD   | 2.71                     | 0.54              |
| 2:B:158:GLN:HG2  | 2:B:158:GLN:O    | 2.07                     | 0.54              |
| 1:A:23:TYR:C     | 1:A:25:LEU:N     | 2.63                     | 0.53              |
| 1:A:160:ILE:HD13 | 1:A:194:PHE:HB2  | 1.89                     | 0.53              |
| 2:B:88:PHE:CE2   | 2:B:153:CYS:SG   | 3.01                     | 0.53              |
| 1:A:559:TRP:CB   | 1:A:561:LEU:CD2  | 2.74                     | 0.53              |
| 2:B:3:ASP:N      | 2:B:6:LYS:HB3    | 2.22                     | 0.53              |
| 2:B:40:HIS:CD2   | 2:B:41:THR:CG2   | 2.91                     | 0.53              |
| 1:A:21:THR:O     | 1:A:25:LEU:HB2   | 2.08                     | 0.53              |
| 1:A:50:ASP:O     | 1:A:53:PRO:CD    | 2.56                     | 0.53              |
| 1:A:170:TRP:HE3  | 1:A:171:LYS:HA   | 1.74                     | 0.53              |
| 1:A:222:LEU:HD12 | 1:A:222:LEU:O    | 2.08                     | 0.53              |
| 1:A:410:GLY:HA3  | 1:A:499:PRO:HB3  | 1.90                     | 0.53              |
| 3:C:9:LEU:O      | 3:C:10:ALA:C     | 2.51                     | 0.53              |
| 1:A:206:LEU:HB2  | 1:A:207:PHE:CD2  | 2.44                     | 0.53              |
| 2:B:32:LEU:O     | 2:B:33:ILE:C     | 2.52                     | 0.53              |
| 2:B:86:PHE:CD1   | 2:B:86:PHE:C     | 2.86                     | 0.53              |
| 1:A:27:LEU:O     | 1:A:28:GLY:C     | 2.50                     | 0.53              |
| 1:A:41:PHE:CE1   | 1:A:55:LEU:HD13  | 2.44                     | 0.53              |
| 1:A:313:ALA:HB2  | 6:A:801:HAS:C19  | 2.39                     | 0.53              |
| 1:A:324:GLY:O    | 1:A:329:GLY:N    | 2.40                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:506:LEU:O   | 1:A:508:PHE:N    | 2.42                     | 0.53              |
| 2:B:11:ILE:HG22 | 2:B:12:LEU:H     | 1.72                     | 0.53              |
| 1:A:97:LEU:O    | 1:A:99:MET:HG3   | 2.08                     | 0.53              |
| 1:A:351:LEU:HB3 | 1:A:429:PHE:CD2  | 2.43                     | 0.53              |
| 2:B:28:VAL:O    | 2:B:31:ALA:HB3   | 2.09                     | 0.53              |
| 1:A:220:ASP:CB  | 1:A:554:ASN:H    | 2.22                     | 0.53              |
| 1:A:236:VAL:HA  | 1:A:239:TRP:CD2  | 2.43                     | 0.53              |
| 2:B:24:ALA:O    | 2:B:28:VAL:HG23  | 2.09                     | 0.53              |
| 1:A:184:TYR:CG  | 1:A:184:TYR:O    | 2.61                     | 0.52              |
| 1:A:63:GLN:NE2  | 1:A:63:GLN:CA    | 2.72                     | 0.52              |
| 1:A:32:LEU:HB2  | 1:A:80:PHE:CD1   | 2.44                     | 0.52              |
| 1:A:352:GLY:HA2 | 1:A:395:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:199:GLY:CA  | 1:A:230:TRP:CG   | 2.92                     | 0.52              |
| 1:A:375:VAL:O   | 1:A:377:ASN:N    | 2.42                     | 0.52              |
| 1:A:111:TRP:O   | 1:A:115:ILE:HD13 | 2.09                     | 0.52              |
| 1:A:329:GLY:HA3 | 1:A:335:TRP:HA   | 1.91                     | 0.52              |
| 1:A:41:PHE:O    | 1:A:43:ALA:N     | 2.43                     | 0.52              |
| 1:A:314:PHE:HD2 | 3:C:12:ILE:HD12  | 1.75                     | 0.52              |
| 1:A:374:VAL:CG2 | 3:C:30:PHE:HA    | 2.38                     | 0.52              |
| 1:A:189:PHE:O   | 1:A:190:TRP:C    | 2.52                     | 0.52              |
| 1:A:262:ASP:HB3 | 1:A:263:PRO:CD   | 2.40                     | 0.52              |
| 1:A:41:PHE:C    | 1:A:43:ALA:N     | 2.66                     | 0.52              |
| 1:A:410:GLY:HA3 | 1:A:499:PRO:HG3  | 1.92                     | 0.52              |
| 2:B:10:ALA:O    | 2:B:11:ILE:C     | 2.53                     | 0.52              |
| 2:B:64:TRP:CH2  | 2:B:132:VAL:HG21 | 2.45                     | 0.52              |
| 2:B:74:THR:O    | 2:B:74:THR:OG1   | 2.26                     | 0.52              |
| 2:B:109:SER:HB3 | 2:B:129:PRO:CG   | 2.38                     | 0.52              |
| 1:A:74:VAL:O    | 1:A:79:VAL:HG23  | 2.09                     | 0.51              |
| 1:A:294:TRP:CH2 | 1:A:544:PRO:HD2  | 2.45                     | 0.51              |
| 1:A:302:THR:O   | 1:A:305:VAL:N    | 2.42                     | 0.51              |
| 1:A:316:VAL:O   | 1:A:317:ALA:C    | 2.52                     | 0.51              |
| 1:A:27:LEU:HD23 | 1:A:83:LEU:HD22  | 1.91                     | 0.51              |
| 1:A:218:GLY:O   | 1:A:555:PRO:HB3  | 2.09                     | 0.51              |
| 1:A:356:PHE:HE2 | 6:A:801:HAS:H162 | 1.74                     | 0.51              |
| 1:A:439:LEU:O   | 1:A:440:HIS:C    | 2.52                     | 0.51              |
| 1:A:161:TYR:O   | 1:A:165:ASP:N    | 2.33                     | 0.51              |
| 1:A:406:PRO:CD  | 1:A:413:ILE:CD1  | 2.88                     | 0.51              |
| 1:A:487:GLY:O   | 1:A:488:LEU:C    | 2.52                     | 0.51              |
| 2:B:84:LEU:HG   | 2:B:110:PRO:HD3  | 1.93                     | 0.51              |
| 1:A:459:ALA:O   | 2:B:146:ARG:NH1  | 2.37                     | 0.51              |
| 1:A:52:TYR:H    | 1:A:53:PRO:HD3   | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:82:GLN:CD    | 1:A:152:PHE:HE2  | 2.19                     | 0.51              |
| 1:A:21:THR:HG21  | 1:A:91:TYR:CB    | 2.40                     | 0.51              |
| 1:A:223:VAL:HG12 | 1:A:549:LEU:HD12 | 1.93                     | 0.51              |
| 1:A:412:PRO:CB   | 1:A:501:LEU:HD13 | 2.35                     | 0.51              |
| 1:A:23:TYR:C     | 1:A:110:TRP:HE1  | 2.19                     | 0.51              |
| 2:B:55:PRO:HB3   | 2:B:109:SER:O    | 2.11                     | 0.51              |
| 1:A:402:TYR:HE1  | 1:A:413:ILE:HG21 | 1.75                     | 0.51              |
| 1:A:18:LYS:NZ    | 1:A:504:ALA:HB2  | 2.26                     | 0.50              |
| 1:A:113:ALA:O    | 1:A:117:LEU:N    | 2.34                     | 0.50              |
| 2:B:72:VAL:CG2   | 2:B:72:VAL:O     | 2.59                     | 0.50              |
| 1:A:134:THR:HG22 | 1:A:228:PHE:CE2  | 2.46                     | 0.50              |
| 1:A:348:ALA:O    | 1:A:349:PRO:C    | 2.50                     | 0.50              |
| 1:A:129:ALA:O    | 1:A:131:VAL:HG22 | 2.11                     | 0.50              |
| 1:A:18:LYS:HZ1   | 1:A:504:ALA:CB   | 2.24                     | 0.50              |
| 1:A:18:LYS:HZ1   | 1:A:504:ALA:HB3  | 1.77                     | 0.50              |
| 1:A:70:THR:HG23  | 1:A:132:LEU:CA   | 2.38                     | 0.50              |
| 1:A:211:TRP:HZ2  | 1:A:558:GLY:HA3  | 1.76                     | 0.50              |
| 2:B:158:GLN:OE1  | 2:B:158:GLN:N    | 2.41                     | 0.50              |
| 1:A:162:ILE:O    | 1:A:166:LEU:HD12 | 2.11                     | 0.50              |
| 1:A:417:GLN:HA   | 1:A:420:LEU:HB3  | 1.92                     | 0.50              |
| 2:B:16:LYS:O     | 2:B:17:GLY:C     | 2.54                     | 0.50              |
| 1:A:520:LEU:HG   | 1:A:521:VAL:N    | 2.25                     | 0.50              |
| 2:B:11:ILE:HG23  | 2:B:12:LEU:H     | 1.68                     | 0.50              |
| 2:B:111:ASP:OD2  | 2:B:112:VAL:N    | 2.38                     | 0.50              |
| 3:C:5:PRO:O      | 3:C:9:LEU:HD12   | 2.12                     | 0.50              |
| 1:A:389:VAL:HB   | 6:A:801:HAS:HBC2 | 1.94                     | 0.50              |
| 1:A:409:THR:C    | 1:A:411:LYS:H    | 2.20                     | 0.50              |
| 2:B:116:PHE:O    | 2:B:116:PHE:HD2  | 1.94                     | 0.50              |
| 1:A:463:ALA:O    | 1:A:465:VAL:N    | 2.45                     | 0.49              |
| 1:A:512:ILE:N    | 1:A:512:ILE:CD1  | 2.75                     | 0.49              |
| 2:B:116:PHE:CE1  | 2:B:147:ILE:HD13 | 2.46                     | 0.49              |
| 1:A:220:ASP:HB2  | 1:A:554:ASN:N    | 2.27                     | 0.49              |
| 2:B:14:TYR:HE1   | 3:C:5:PRO:HD2    | 1.77                     | 0.49              |
| 1:A:192:MET:SD   | 1:A:192:MET:C    | 2.96                     | 0.49              |
| 1:A:516:GLU:O    | 1:A:518:ARG:N    | 2.41                     | 0.49              |
| 1:A:192:MET:HB2  | 1:A:273:LEU:CD1  | 2.42                     | 0.49              |
| 1:A:91:TYR:O     | 1:A:95:ARG:HG2   | 2.12                     | 0.49              |
| 1:A:228:PHE:C    | 1:A:228:PHE:CD2  | 2.90                     | 0.49              |
| 1:A:357:ILE:HG22 | 1:A:358:PRO:CD   | 2.43                     | 0.49              |
| 1:A:97:LEU:O     | 1:A:98:ASN:C     | 2.56                     | 0.49              |
| 1:A:154:LEU:O    | 1:A:157:TRP:CB   | 2.55                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:201:VAL:O    | 1:A:205:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:253:LYS:O    | 1:A:253:LYS:HG3  | 2.11                     | 0.49              |
| 1:A:386:HIS:CE1  | 5:A:800:HEM:C4D  | 2.98                     | 0.49              |
| 1:A:472:LEU:O    | 1:A:472:LEU:CD2  | 2.55                     | 0.49              |
| 1:A:386:HIS:CA   | 1:A:390:ALA:HB3  | 2.41                     | 0.49              |
| 1:A:89:MET:HB3   | 1:A:190:TRP:CE2  | 2.48                     | 0.49              |
| 1:A:233:HIS:CB   | 1:A:234:PRO:CD   | 2.89                     | 0.49              |
| 1:A:302:THR:O    | 1:A:303:LEU:C    | 2.54                     | 0.49              |
| 2:B:90:TYR:CZ    | 2:B:147:ILE:CG2  | 2.96                     | 0.48              |
| 1:A:135:PHE:CE1  | 1:A:228:PHE:CD1  | 3.02                     | 0.48              |
| 1:A:171:LYS:NZ   | 1:A:177:LYS:O    | 2.25                     | 0.48              |
| 1:A:353:LEU:O    | 1:A:356:PHE:HB3  | 2.13                     | 0.48              |
| 1:A:181:LEU:O    | 1:A:185:MET:N    | 2.46                     | 0.48              |
| 1:A:192:MET:CG   | 1:A:273:LEU:HA   | 2.44                     | 0.48              |
| 1:A:233:HIS:CD2  | 1:A:237:TYR:CD2  | 3.01                     | 0.48              |
| 1:A:412:PRO:HG3  | 1:A:501:LEU:HD11 | 1.95                     | 0.48              |
| 2:B:151:GLN:O    | 2:B:153:CYS:N    | 2.46                     | 0.48              |
| 1:A:20:ALA:HB3   | 1:A:106:MET:CE   | 2.32                     | 0.48              |
| 1:A:238:PHE:O    | 1:A:242:PRO:HD2  | 2.13                     | 0.48              |
| 1:A:385:PHE:CD2  | 6:A:801:HAS:HAA2 | 2.48                     | 0.48              |
| 1:A:407:ASN:HD21 | 1:A:506:LEU:HD23 | 1.77                     | 0.48              |
| 1:A:12:TYR:CG    | 1:A:19:LYS:HG3   | 2.49                     | 0.48              |
| 1:A:18:LYS:HZ3   | 1:A:504:ALA:HB2  | 1.77                     | 0.48              |
| 1:A:127:ASN:CG   | 1:A:127:ASN:O    | 2.57                     | 0.48              |
| 1:A:379:ALA:O    | 1:A:380:TRP:C    | 2.55                     | 0.48              |
| 1:A:386:HIS:C    | 1:A:390:ALA:HB3  | 2.38                     | 0.48              |
| 1:A:501:LEU:H    | 1:A:501:LEU:HG   | 1.40                     | 0.48              |
| 2:B:40:HIS:CD2   | 2:B:41:THR:HG22  | 2.49                     | 0.48              |
| 1:A:44:LEU:O     | 1:A:47:GLY:N     | 2.47                     | 0.48              |
| 1:A:300:VAL:CG1  | 2:B:30:ILE:HD11  | 2.29                     | 0.48              |
| 2:B:51:GLU:O     | 2:B:51:GLU:HG2   | 2.12                     | 0.48              |
| 2:B:58:VAL:CG1   | 2:B:59:ARG:N     | 2.76                     | 0.48              |
| 3:C:11:VAL:C     | 3:C:13:LEU:N     | 2.70                     | 0.48              |
| 1:A:555:PRO:O    | 1:A:556:VAL:HG13 | 2.14                     | 0.48              |
| 1:A:54:LEU:HD13  | 1:A:55:LEU:H     | 1.75                     | 0.48              |
| 1:A:119:VAL:HG12 | 1:A:148:GLY:CA   | 2.44                     | 0.48              |
| 1:A:164:LEU:HD23 | 1:A:167:TRP:HB3  | 1.94                     | 0.48              |
| 1:A:405:LEU:HA   | 1:A:405:LEU:HD12 | 1.39                     | 0.48              |
| 2:B:35:TYR:CD1   | 2:B:35:TYR:O     | 2.67                     | 0.48              |
| 2:B:99:GLN:HG3   | 2:B:99:GLN:O     | 2.13                     | 0.48              |
| 2:B:40:HIS:CD2   | 2:B:41:THR:HG23  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:72:VAL:O     | 2:B:72:VAL:HG23  | 2.14                     | 0.48              |
| 1:A:86:GLN:HG3   | 1:A:156:THR:HG22 | 1.95                     | 0.48              |
| 1:A:426:TRP:O    | 1:A:430:LEU:HD13 | 2.14                     | 0.48              |
| 1:A:78:ILE:HG22  | 1:A:79:VAL:H     | 1.72                     | 0.47              |
| 1:A:526:ARG:NH2  | 1:A:529:PHE:CB   | 2.71                     | 0.47              |
| 1:A:197:SER:O    | 1:A:201:VAL:HB   | 2.15                     | 0.47              |
| 1:A:229:TRP:CZ3  | 1:A:283:HIS:ND1  | 2.82                     | 0.47              |
| 1:A:477:LEU:HD13 | 5:A:800:HEM:HMB3 | 1.94                     | 0.47              |
| 1:A:552:HIS:ND1  | 1:A:552:HIS:N    | 2.62                     | 0.47              |
| 1:A:162:ILE:O    | 1:A:165:ASP:HB3  | 2.15                     | 0.47              |
| 1:A:233:HIS:O    | 1:A:234:PRO:C    | 2.55                     | 0.47              |
| 1:A:499:PRO:HB3  | 1:A:502:ALA:HB3  | 1.95                     | 0.47              |
| 1:A:512:ILE:N    | 1:A:512:ILE:HD12 | 2.30                     | 0.47              |
| 2:B:138:THR:O    | 2:B:140:LYS:NZ   | 2.37                     | 0.47              |
| 1:A:437:VAL:O    | 1:A:441:TRP:HB2  | 2.14                     | 0.47              |
| 1:A:27:LEU:HD23  | 1:A:83:LEU:CD2   | 2.44                     | 0.47              |
| 1:A:156:THR:O    | 1:A:160:ILE:HG13 | 2.14                     | 0.47              |
| 1:A:518:ARG:HG3  | 1:A:518:ARG:NH2  | 2.05                     | 0.47              |
| 1:A:23:TYR:HD1   | 1:A:107:TRP:CH2  | 2.25                     | 0.47              |
| 1:A:246:ILE:O    | 1:A:250:ILE:HB   | 2.15                     | 0.47              |
| 1:A:288:PRO:HD2  | 2:B:128:LEU:HD22 | 1.95                     | 0.47              |
| 1:A:356:PHE:CD1  | 1:A:392:LEU:HD23 | 2.50                     | 0.47              |
| 1:A:366:ASN:HB3  | 6:A:801:HAS:HMD  | 1.93                     | 0.47              |
| 1:A:378:THR:OG1  | 1:A:380:TRP:HB2  | 2.14                     | 0.47              |
| 1:A:386:HIS:CE1  | 5:A:800:HEM:C1A  | 3.02                     | 0.47              |
| 2:B:32:LEU:HB3   | 3:C:27:TYR:CZ    | 2.50                     | 0.47              |
| 2:B:137:TYR:CD1  | 2:B:138:THR:N    | 2.82                     | 0.47              |
| 3:C:16:THR:O     | 3:C:20:LEU:HG    | 2.15                     | 0.47              |
| 1:A:300:VAL:HG11 | 2:B:30:ILE:CD1   | 2.43                     | 0.47              |
| 1:A:542:TYR:N    | 1:A:542:TYR:CD2  | 2.83                     | 0.47              |
| 1:A:264:MET:HE2  | 1:A:264:MET:CA   | 2.41                     | 0.47              |
| 1:A:346:PHE:C    | 1:A:349:PRO:HD2  | 2.39                     | 0.47              |
| 2:B:13:ALA:HA    | 2:B:16:LYS:NZ    | 2.30                     | 0.47              |
| 1:A:152:PHE:O    | 1:A:155:SER:HB3  | 2.14                     | 0.47              |
| 1:A:204:ALA:HA   | 1:A:208:LEU:HB2  | 1.96                     | 0.47              |
| 1:A:270:LEU:HD12 | 1:A:270:LEU:HA   | 1.69                     | 0.47              |
| 1:A:297:ILE:C    | 1:A:299:SER:H    | 2.23                     | 0.47              |
| 1:A:381:VAL:HG12 | 1:A:385:PHE:CE2  | 2.50                     | 0.47              |
| 1:A:411:LYS:CG   | 1:A:497:ARG:HB3  | 2.44                     | 0.47              |
| 1:A:497:ARG:HE   | 1:A:499:PRO:HG2  | 1.80                     | 0.47              |
| 1:A:548:GLN:HB3  | 1:A:549:LEU:H    | 1.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:55:PRO:CB    | 2:B:110:PRO:HA   | 2.45                     | 0.47              |
| 1:A:21:THR:HG21  | 1:A:91:TYR:HB3   | 1.97                     | 0.46              |
| 1:A:54:LEU:C     | 1:A:54:LEU:CD2   | 2.76                     | 0.46              |
| 1:A:123:PRO:HG3  | 1:A:144:ALA:HB3  | 1.96                     | 0.46              |
| 1:A:182:VAL:O    | 1:A:182:VAL:HG12 | 2.14                     | 0.46              |
| 1:A:429:PHE:O    | 1:A:433:MET:HG2  | 2.15                     | 0.46              |
| 3:C:17:LEU:HD23  | 3:C:17:LEU:HA    | 1.66                     | 0.46              |
| 1:A:81:THR:CB    | 1:A:239:TRP:CD1  | 2.98                     | 0.46              |
| 1:A:185:MET:CE   | 1:A:265:ALA:HB1  | 2.44                     | 0.46              |
| 1:A:324:GLY:HA3  | 1:A:335:TRP:HB2  | 1.98                     | 0.46              |
| 1:A:406:PRO:O    | 1:A:410:GLY:N    | 2.46                     | 0.46              |
| 1:A:29:PHE:O     | 1:A:32:LEU:HB3   | 2.16                     | 0.46              |
| 1:A:59:LEU:HB3   | 1:A:61:PHE:CD1   | 2.50                     | 0.46              |
| 2:B:32:LEU:HB2   | 3:C:23:TRP:HH2   | 1.80                     | 0.46              |
| 2:B:145:TYR:CE1  | 2:B:166:VAL:CG2  | 2.98                     | 0.46              |
| 3:C:24:LEU:O     | 3:C:25:GLY:C     | 2.58                     | 0.46              |
| 1:A:199:GLY:HA3  | 1:A:230:TRP:CB   | 2.44                     | 0.46              |
| 1:A:258:ARG:HB3  | 1:A:510:GLU:O    | 2.15                     | 0.46              |
| 1:A:325:ARG:NH1  | 1:A:331:GLY:O    | 2.48                     | 0.46              |
| 1:A:425:VAL:HG12 | 1:A:426:TRP:N    | 2.31                     | 0.46              |
| 1:A:427:LEU:O    | 1:A:480:ALA:HB2  | 2.15                     | 0.46              |
| 1:A:518:ARG:CG   | 1:A:518:ARG:NH2  | 2.70                     | 0.46              |
| 1:A:562:TRP:C    | 1:A:562:TRP:CD1  | 2.92                     | 0.46              |
| 2:B:32:LEU:HB2   | 3:C:23:TRP:CH2   | 2.51                     | 0.46              |
| 2:B:18:TRP:CZ2   | 3:C:12:ILE:HB    | 2.50                     | 0.46              |
| 2:B:85:ALA:HB3   | 2:B:127:VAL:HG11 | 1.98                     | 0.46              |
| 1:A:47:GLY:HA2   | 1:A:470:ASN:HB2  | 1.96                     | 0.46              |
| 1:A:135:PHE:CE1  | 1:A:228:PHE:HE1  | 2.34                     | 0.46              |
| 1:A:164:LEU:O    | 1:A:168:ARG:HB2  | 2.16                     | 0.46              |
| 1:A:229:TRP:CZ3  | 1:A:283:HIS:CG   | 3.04                     | 0.46              |
| 2:B:155:LEU:C    | 2:B:157:HIS:H    | 2.24                     | 0.46              |
| 1:A:346:PHE:CZ   | 1:A:350:VAL:HG21 | 2.51                     | 0.46              |
| 2:B:29:PHE:O     | 2:B:30:ILE:C     | 2.58                     | 0.46              |
| 2:B:140:LYS:C    | 2:B:141:ARG:HG3  | 2.41                     | 0.46              |
| 3:C:13:LEU:HD12  | 3:C:17:LEU:HG    | 1.97                     | 0.46              |
| 1:A:179:THR:HG22 | 1:A:183:THR:HB   | 1.97                     | 0.46              |
| 2:B:54:ASP:OD1   | 2:B:54:ASP:O     | 2.33                     | 0.46              |
| 2:B:81:VAL:O     | 2:B:81:VAL:HG12  | 2.15                     | 0.46              |
| 1:A:134:THR:HG22 | 1:A:228:PHE:CZ   | 2.51                     | 0.46              |
| 1:A:300:VAL:HA   | 1:A:303:LEU:HD12 | 1.98                     | 0.46              |
| 1:A:456:VAL:HG23 | 1:A:456:VAL:O    | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:143:TRP:CE3  | 1:A:213:PHE:HE2  | 2.33                     | 0.46              |
| 1:A:365:VAL:C    | 1:A:367:ALA:N    | 2.74                     | 0.46              |
| 3:C:18:THR:C     | 3:C:20:LEU:N     | 2.74                     | 0.46              |
| 1:A:35:GLY:N     | 1:A:75:LEU:HD12  | 2.30                     | 0.45              |
| 1:A:41:PHE:O     | 1:A:42:GLN:C     | 2.59                     | 0.45              |
| 1:A:259:LEU:O    | 1:A:512:ILE:HD13 | 2.15                     | 0.45              |
| 2:B:24:ALA:O     | 2:B:27:PHE:N     | 2.49                     | 0.45              |
| 2:B:83:VAL:HG13  | 2:B:91:GLN:O     | 2.16                     | 0.45              |
| 3:C:13:LEU:O     | 3:C:14:VAL:C     | 2.59                     | 0.45              |
| 1:A:137:PRO:HG3  | 1:A:208:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:184:TYR:CE2  | 1:A:266:ARG:CB   | 2.99                     | 0.45              |
| 1:A:236:VAL:HG12 | 1:A:239:TRP:CZ3  | 2.52                     | 0.45              |
| 1:A:170:TRP:HE3  | 1:A:171:LYS:CA   | 2.28                     | 0.45              |
| 1:A:182:VAL:O    | 1:A:182:VAL:CG1  | 2.64                     | 0.45              |
| 1:A:251:LEU:HA   | 1:A:254:GLN:HG2  | 1.95                     | 0.45              |
| 1:A:282:HIS:CD2  | 1:A:283:HIS:N    | 2.84                     | 0.45              |
| 1:A:410:GLY:HA2  | 1:A:502:ALA:CA   | 2.45                     | 0.45              |
| 1:A:481:LEU:HD12 | 1:A:481:LEU:C    | 2.41                     | 0.45              |
| 2:B:44:VAL:HB    | 2:B:122:ASN:O    | 2.15                     | 0.45              |
| 1:A:195:LEU:HD12 | 1:A:195:LEU:HA   | 1.60                     | 0.45              |
| 1:A:222:LEU:HD12 | 1:A:222:LEU:C    | 2.42                     | 0.45              |
| 1:A:310:LEU:HD23 | 1:A:310:LEU:HA   | 1.68                     | 0.45              |
| 1:A:361:ALA:O    | 1:A:365:VAL:HG23 | 2.17                     | 0.45              |
| 2:B:121:THR:HA   | 3:C:33:ARG:HB3   | 1.98                     | 0.45              |
| 1:A:119:VAL:HG12 | 1:A:148:GLY:HA2  | 1.99                     | 0.45              |
| 1:A:266:ARG:CD   | 1:A:521:VAL:HG13 | 2.47                     | 0.45              |
| 1:A:392:LEU:O    | 1:A:393:VAL:C    | 2.58                     | 0.45              |
| 1:A:405:LEU:HB3  | 1:A:406:PRO:CD   | 2.46                     | 0.45              |
| 1:A:435:MET:O    | 1:A:436:ALA:C    | 2.59                     | 0.45              |
| 3:C:15:LEU:HD12  | 3:C:15:LEU:C     | 2.42                     | 0.45              |
| 3:C:33:ARG:HH21  | 3:C:33:ARG:HD2   | 1.59                     | 0.45              |
| 1:A:69:LEU:HD11  | 5:A:800:HEM:CBA  | 2.46                     | 0.45              |
| 1:A:308:PRO:O    | 1:A:312:THR:N    | 2.50                     | 0.45              |
| 1:A:504:ALA:C    | 1:A:506:LEU:H    | 2.25                     | 0.45              |
| 2:B:96:GLU:HA    | 2:B:165:VAL:HG23 | 1.97                     | 0.45              |
| 1:A:207:PHE:CD1  | 1:A:219:VAL:HG13 | 2.52                     | 0.45              |
| 1:A:382:PRO:O    | 1:A:386:HIS:HB2  | 2.17                     | 0.45              |
| 1:A:398:MET:HE2  | 1:A:484:PHE:CD1  | 2.51                     | 0.45              |
| 1:A:428:TRP:CD1  | 1:A:429:PHE:N    | 2.85                     | 0.45              |
| 2:B:27:PHE:HA    | 2:B:30:ILE:HG13  | 1.99                     | 0.45              |
| 1:A:210:PRO:HB2  | 1:A:216:VAL:HG22 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:418:ARG:HB3  | 1:A:418:ARG:CZ   | 2.46                     | 0.45              |
| 1:A:477:LEU:HA   | 1:A:480:ALA:HB3  | 1.99                     | 0.45              |
| 2:B:110:PRO:O    | 2:B:111:ASP:CB   | 2.65                     | 0.45              |
| 1:A:48:ASN:C     | 1:A:48:ASN:HD22  | 2.24                     | 0.45              |
| 1:A:91:TYR:CE2   | 1:A:408:LEU:CD2  | 2.97                     | 0.45              |
| 1:A:96:GLU:OE1   | 1:A:180:PRO:HB2  | 2.17                     | 0.45              |
| 1:A:235:ILE:HA   | 1:A:238:PHE:HB3  | 1.99                     | 0.45              |
| 1:A:310:LEU:HD22 | 2:B:18:TRP:CZ2   | 2.52                     | 0.45              |
| 1:A:351:LEU:HD21 | 1:A:426:TRP:CH2  | 2.51                     | 0.45              |
| 1:A:225:ARG:HA   | 1:A:228:PHE:CB   | 2.45                     | 0.44              |
| 1:A:306:ALA:O    | 1:A:307:VAL:C    | 2.60                     | 0.44              |
| 1:A:547:VAL:O    | 1:A:548:GLN:C    | 2.60                     | 0.44              |
| 2:B:97:VAL:CG2   | 2:B:166:VAL:CG1  | 2.87                     | 0.44              |
| 1:A:18:LYS:NZ    | 1:A:504:ALA:CB   | 2.79                     | 0.44              |
| 1:A:84:PHE:CE1   | 1:A:397:ALA:HA   | 2.52                     | 0.44              |
| 1:A:191:LEU:HD23 | 1:A:191:LEU:HA   | 1.54                     | 0.44              |
| 3:C:15:LEU:O     | 3:C:19:ILE:HG13  | 2.16                     | 0.44              |
| 1:A:266:ARG:HD2  | 1:A:521:VAL:HG13 | 2.00                     | 0.44              |
| 1:A:308:PRO:O    | 1:A:311:MET:N    | 2.50                     | 0.44              |
| 3:C:9:LEU:C      | 3:C:11:VAL:N     | 2.70                     | 0.44              |
| 1:A:248:TYR:CE1  | 1:A:312:THR:HG23 | 2.52                     | 0.44              |
| 1:A:413:ILE:HG13 | 1:A:491:VAL:HG21 | 2.00                     | 0.44              |
| 2:B:18:TRP:O     | 2:B:19:LEU:C     | 2.61                     | 0.44              |
| 2:B:103:ILE:HD13 | 2:B:139:PHE:HD1  | 1.82                     | 0.44              |
| 1:A:15:TYR:HA    | 1:A:100:ARG:HH11 | 1.82                     | 0.44              |
| 1:A:238:PHE:O    | 1:A:242:PRO:CD   | 2.66                     | 0.44              |
| 1:A:300:VAL:O    | 1:A:301:LEU:C    | 2.58                     | 0.44              |
| 1:A:404:LEU:HD12 | 1:A:404:LEU:HA   | 1.70                     | 0.44              |
| 1:A:67:GLN:CD    | 1:A:127:ASN:HB2  | 2.43                     | 0.44              |
| 1:A:284:GLN:HG3  | 1:A:287:ASP:CG   | 2.43                     | 0.44              |
| 1:A:543:GLY:HA3  | 1:A:544:PRO:HD3  | 1.84                     | 0.44              |
| 2:B:99:GLN:HE21  | 2:B:100:GLY:N    | 2.16                     | 0.44              |
| 1:A:414:SER:OG   | 1:A:416:ALA:HB3  | 2.17                     | 0.44              |
| 1:A:485:ILE:C    | 1:A:487:GLY:N    | 2.74                     | 0.44              |
| 1:A:514:GLY:CA   | 2:B:8:HIS:CD2    | 3.01                     | 0.44              |
| 2:B:67:PRO:HB3   | 2:B:91:GLN:HG2   | 2.00                     | 0.44              |
| 1:A:121:ALA:O    | 1:A:125:LEU:HD11 | 2.18                     | 0.44              |
| 1:A:164:LEU:HD21 | 1:A:167:TRP:HE3  | 1.83                     | 0.44              |
| 1:A:207:PHE:HD1  | 1:A:219:VAL:HG13 | 1.82                     | 0.44              |
| 1:A:344:PRO:C    | 1:A:346:PHE:N    | 2.76                     | 0.44              |
| 1:A:362:GLY:O    | 1:A:363:GLY:C    | 2.61                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:526:ARG:O    | 1:A:527:ILE:C    | 2.61                     | 0.44              |
| 1:A:12:TYR:CD1   | 1:A:19:LYS:HG3   | 2.53                     | 0.43              |
| 1:A:117:LEU:O    | 1:A:120:ALA:HB3  | 2.17                     | 0.43              |
| 1:A:189:PHE:C    | 1:A:191:LEU:N    | 2.75                     | 0.43              |
| 1:A:288:PRO:CD   | 2:B:128:LEU:HD22 | 2.48                     | 0.43              |
| 1:A:292:PRO:HD3  | 2:B:48:GLY:HA3   | 2.00                     | 0.43              |
| 1:A:318:ALA:O    | 1:A:321:GLU:N    | 2.50                     | 0.43              |
| 1:A:220:ASP:HA   | 1:A:221:PRO:HD2  | 1.69                     | 0.43              |
| 1:A:262:ASP:HB3  | 1:A:263:PRO:HD3  | 1.99                     | 0.43              |
| 1:A:354:LEU:HD22 | 1:A:354:LEU:H    | 1.83                     | 0.43              |
| 1:A:377:ASN:HB3  | 2:B:150:ASN:HB2  | 2.00                     | 0.43              |
| 2:B:64:TRP:CD1   | 2:B:83:VAL:O     | 2.71                     | 0.43              |
| 1:A:80:PHE:CD2   | 1:A:80:PHE:C     | 2.95                     | 0.43              |
| 1:A:96:GLU:CD    | 1:A:180:PRO:HB2  | 2.42                     | 0.43              |
| 1:A:161:TYR:O    | 1:A:162:ILE:C    | 2.61                     | 0.43              |
| 1:A:282:HIS:CG   | 6:A:801:HAS:OMD  | 2.72                     | 0.43              |
| 1:A:301:LEU:HD23 | 1:A:301:LEU:HA   | 1.61                     | 0.43              |
| 1:A:309:SER:O    | 6:A:801:HAS:H272 | 2.17                     | 0.43              |
| 2:B:25:MET:O     | 2:B:26:LEU:C     | 2.59                     | 0.43              |
| 2:B:119:GLU:OE2  | 2:B:146:ARG:HD3  | 2.18                     | 0.43              |
| 1:A:26:VAL:O     | 1:A:29:PHE:HB2   | 2.18                     | 0.43              |
| 1:A:95:ARG:HH11  | 1:A:504:ALA:CB   | 2.30                     | 0.43              |
| 1:A:230:TRP:HA   | 1:A:542:TYR:CZ   | 2.53                     | 0.43              |
| 2:B:149:CYS:O    | 2:B:157:HIS:HE1  | 2.01                     | 0.43              |
| 1:A:79:VAL:HA    | 1:A:152:PHE:HZ   | 1.81                     | 0.43              |
| 1:A:109:SER:O    | 1:A:112:MET:HB2  | 2.19                     | 0.43              |
| 1:A:241:LEU:HD11 | 1:A:272:PHE:CE1  | 2.54                     | 0.43              |
| 1:A:248:TYR:OH   | 1:A:312:THR:HA   | 2.18                     | 0.43              |
| 1:A:258:ARG:O    | 1:A:259:LEU:C    | 2.61                     | 0.43              |
| 1:A:22:LEU:HD13  | 1:A:408:LEU:HB3  | 2.01                     | 0.43              |
| 1:A:259:LEU:CD1  | 1:A:261:SER:H    | 2.31                     | 0.43              |
| 1:A:231:THR:O    | 1:A:234:PRO:HG2  | 2.19                     | 0.43              |
| 1:A:353:LEU:HB3  | 6:A:801:HAS:C24  | 2.48                     | 0.43              |
| 1:A:406:PRO:CD   | 1:A:413:ILE:HD13 | 2.49                     | 0.43              |
| 1:A:26:VAL:O     | 1:A:30:LEU:HG    | 2.18                     | 0.43              |
| 1:A:69:LEU:HD11  | 5:A:800:HEM:CGA  | 2.49                     | 0.43              |
| 1:A:334:GLY:C    | 1:A:336:ILE:N    | 2.77                     | 0.43              |
| 1:A:351:LEU:HD21 | 1:A:426:TRP:CZ3  | 2.53                     | 0.43              |
| 1:A:385:PHE:CD2  | 6:A:801:HAS:CAA  | 3.02                     | 0.43              |
| 1:A:390:ALA:O    | 1:A:394:THR:HB   | 2.19                     | 0.43              |
| 1:A:445:LEU:HA   | 1:A:445:LEU:HD23 | 1.62                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:8:HIS:ND1    | 2:B:11:ILE:HG21  | 2.33                     | 0.43              |
| 2:B:83:VAL:CG1   | 2:B:84:LEU:N     | 2.81                     | 0.43              |
| 2:B:92:PRO:HG2   | 2:B:95:ILE:HG12  | 2.00                     | 0.43              |
| 1:A:95:ARG:HH11  | 1:A:504:ALA:HB3  | 1.84                     | 0.43              |
| 1:A:122:LEU:C    | 1:A:124:LEU:N    | 2.77                     | 0.43              |
| 1:A:192:MET:HG3  | 1:A:273:LEU:HA   | 2.01                     | 0.43              |
| 1:A:522:LEU:HD12 | 1:A:522:LEU:HA   | 1.87                     | 0.43              |
| 6:A:801:HAS:H281 | 6:A:801:HAS:H251 | 1.58                     | 0.43              |
| 1:A:184:TYR:O    | 1:A:188:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:192:MET:HB2  | 1:A:273:LEU:HB2  | 2.00                     | 0.42              |
| 2:B:122:ASN:HD21 | 3:C:33:ARG:HB2   | 1.83                     | 0.42              |
| 1:A:546:LEU:HD22 | 1:A:550:PHE:HE1  | 1.83                     | 0.42              |
| 1:A:66:TYR:O     | 1:A:70:THR:N     | 2.48                     | 0.42              |
| 1:A:202:LEU:HB2  | 1:A:227:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:340:PRO:O    | 1:A:343:ASN:N    | 2.49                     | 0.42              |
| 1:A:506:LEU:HD12 | 1:A:508:PHE:CE1  | 2.54                     | 0.42              |
| 1:A:385:PHE:HD2  | 6:A:801:HAS:HAA2 | 1.84                     | 0.42              |
| 1:A:482:LEU:HA   | 1:A:485:ILE:CD1  | 2.50                     | 0.42              |
| 1:A:151:VAL:HB   | 1:A:152:PHE:H    | 1.54                     | 0.42              |
| 1:A:331:GLY:H    | 1:A:334:GLY:HA3  | 1.84                     | 0.42              |
| 1:A:393:VAL:O    | 1:A:396:THR:HB   | 2.20                     | 0.42              |
| 1:A:481:LEU:O    | 1:A:484:PHE:HB3  | 2.19                     | 0.42              |
| 1:A:533:VAL:O    | 1:A:537:LEU:HG   | 2.19                     | 0.42              |
| 1:A:545:THR:HG22 | 1:A:546:LEU:N    | 2.34                     | 0.42              |
| 2:B:55:PRO:HB2   | 2:B:110:PRO:HA   | 2.00                     | 0.42              |
| 2:B:59:ARG:HH21  | 2:B:59:ARG:HD3   | 1.66                     | 0.42              |
| 1:A:16:PRO:HD2   | 1:A:100:ARG:NE   | 2.34                     | 0.42              |
| 1:A:25:LEU:HD22  | 1:A:29:PHE:CE1   | 2.55                     | 0.42              |
| 1:A:439:LEU:C    | 1:A:441:TRP:N    | 2.76                     | 0.42              |
| 1:A:445:LEU:O    | 1:A:446:ASN:HB2  | 2.19                     | 0.42              |
| 1:A:514:GLY:HA2  | 1:A:515:PRO:HD3  | 1.80                     | 0.42              |
| 1:A:546:LEU:HD23 | 1:A:546:LEU:HA   | 1.76                     | 0.42              |
| 1:A:42:GLN:NE2   | 1:A:72:HIS:CD2   | 2.87                     | 0.42              |
| 1:A:220:ASP:N    | 1:A:555:PRO:HA   | 2.34                     | 0.42              |
| 1:A:248:TYR:CD2  | 1:A:265:ALA:HB2  | 2.54                     | 0.42              |
| 1:A:250:ILE:O    | 1:A:251:LEU:C    | 2.62                     | 0.42              |
| 2:B:27:PHE:N     | 2:B:27:PHE:HD2   | 2.18                     | 0.42              |
| 2:B:104:VAL:O    | 2:B:104:VAL:HG12 | 2.18                     | 0.42              |
| 1:A:137:PRO:HA   | 1:A:138:PRO:HA   | 1.77                     | 0.42              |
| 1:A:251:LEU:HD13 | 1:A:349:PRO:HG3  | 2.01                     | 0.42              |
| 1:A:312:THR:C    | 1:A:314:PHE:N    | 2.78                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:381:VAL:HB   | 1:A:382:PRO:HD3  | 2.02                     | 0.42              |
| 1:A:402:TYR:CD1  | 1:A:413:ILE:HG21 | 2.55                     | 0.42              |
| 1:A:441:TRP:CD1  | 1:A:441:TRP:C    | 2.94                     | 0.42              |
| 1:A:562:TRP:HA   | 2:B:155:LEU:CD1  | 2.50                     | 0.42              |
| 2:B:27:PHE:N     | 2:B:27:PHE:CD2   | 2.87                     | 0.42              |
| 3:C:7:GLY:O      | 3:C:8:ALA:C      | 2.63                     | 0.42              |
| 1:A:38:PHE:HA    | 1:A:41:PHE:CD1   | 2.50                     | 0.42              |
| 1:A:229:TRP:CE3  | 1:A:283:HIS:CG   | 3.07                     | 0.42              |
| 1:A:365:VAL:O    | 1:A:366:ASN:C    | 2.63                     | 0.42              |
| 1:A:495:ARG:O    | 1:A:496:GLU:C    | 2.61                     | 0.42              |
| 2:B:109:SER:HB3  | 2:B:129:PRO:CD   | 2.50                     | 0.42              |
| 2:B:167:LYS:H    | 2:B:167:LYS:HG3  | 1.70                     | 0.42              |
| 1:A:229:TRP:CZ3  | 1:A:283:HIS:CE1  | 3.08                     | 0.42              |
| 1:A:295:LYS:O    | 1:A:296:MET:C    | 2.61                     | 0.42              |
| 1:A:379:ALA:HB3  | 1:A:443:GLY:CA   | 2.50                     | 0.42              |
| 1:A:410:GLY:O    | 1:A:501:LEU:HD12 | 2.20                     | 0.42              |
| 1:A:52:TYR:CZ    | 1:A:65:TYR:HD1   | 2.38                     | 0.41              |
| 1:A:236:VAL:O    | 1:A:239:TRP:N    | 2.53                     | 0.41              |
| 1:A:334:GLY:C    | 1:A:336:ILE:H    | 2.28                     | 0.41              |
| 1:A:354:LEU:O    | 1:A:358:PRO:HD2  | 2.19                     | 0.41              |
| 1:A:374:VAL:O    | 1:A:374:VAL:CG1  | 2.68                     | 0.41              |
| 1:A:463:ALA:HB3  | 1:A:467:MET:SD   | 2.60                     | 0.41              |
| 2:B:81:VAL:HG11  | 2:B:95:ILE:HD13  | 2.02                     | 0.41              |
| 1:A:11:VAL:C     | 1:A:13:GLU:N     | 2.77                     | 0.41              |
| 1:A:240:LEU:HB2  | 6:A:801:HAS:HBC1 | 2.01                     | 0.41              |
| 1:A:451:ALA:C    | 1:A:453:ILE:N    | 2.77                     | 0.41              |
| 2:B:93:ASN:HA    | 2:B:94:PRO:HA    | 1.85                     | 0.41              |
| 2:B:114:HIS:CE1  | 2:B:153:CYS:HB2  | 2.54                     | 0.41              |
| 2:B:163:THR:HG22 | 2:B:164:ILE:N    | 2.35                     | 0.41              |
| 1:A:29:PHE:O     | 1:A:30:LEU:C     | 2.61                     | 0.41              |
| 1:A:45:ASN:HD21  | 1:A:452:TYR:HA   | 1.85                     | 0.41              |
| 1:A:181:LEU:HG   | 1:A:185:MET:HE3  | 2.02                     | 0.41              |
| 1:A:387:LEU:C    | 1:A:388:GLN:HE21 | 2.29                     | 0.41              |
| 1:A:537:LEU:O    | 1:A:538:VAL:C    | 2.62                     | 0.41              |
| 1:A:79:VAL:HG13  | 1:A:152:PHE:HE1  | 1.85                     | 0.41              |
| 1:A:371:LEU:HD23 | 3:C:26:VAL:CG1   | 2.50                     | 0.41              |
| 1:A:15:TYR:HD1   | 1:A:100:ARG:HH11 | 1.67                     | 0.41              |
| 1:A:20:ALA:CB    | 1:A:106:MET:HE3  | 2.33                     | 0.41              |
| 1:A:288:PRO:HB3  | 2:B:133:SER:HA   | 2.02                     | 0.41              |
| 1:A:354:LEU:O    | 1:A:355:GLY:C    | 2.63                     | 0.41              |
| 1:A:259:LEU:HG   | 1:A:261:SER:H    | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:271:LEU:O    | 1:A:275:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:320:LEU:H    | 1:A:320:LEU:HG   | 1.63                     | 0.41              |
| 1:A:365:VAL:C    | 1:A:367:ALA:H    | 2.29                     | 0.41              |
| 1:A:514:GLY:O    | 1:A:517:ASP:HB2  | 2.21                     | 0.41              |
| 2:B:44:VAL:HG11  | 2:B:122:ASN:CB   | 2.44                     | 0.41              |
| 3:C:11:VAL:O     | 3:C:12:ILE:C     | 2.60                     | 0.41              |
| 1:A:179:THR:CG2  | 1:A:183:THR:HB   | 2.51                     | 0.41              |
| 1:A:267:LEU:N    | 1:A:524:MET:SD   | 2.93                     | 0.41              |
| 1:A:344:PRO:O    | 1:A:345:ALA:C    | 2.64                     | 0.41              |
| 1:A:81:THR:HG1   | 1:A:239:TRP:HD1  | 1.59                     | 0.41              |
| 1:A:112:MET:HB3  | 1:A:112:MET:HE2  | 1.69                     | 0.41              |
| 1:A:546:LEU:O    | 1:A:550:PHE:CD1  | 2.71                     | 0.41              |
| 2:B:122:ASN:ND2  | 3:C:33:ARG:HB2   | 2.35                     | 0.41              |
| 3:C:18:THR:O     | 3:C:20:LEU:N     | 2.54                     | 0.41              |
| 1:A:21:THR:HB    | 1:A:408:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:22:LEU:HA    | 1:A:22:LEU:HD12  | 1.23                     | 0.41              |
| 1:A:192:MET:SD   | 1:A:193:TRP:N    | 2.94                     | 0.41              |
| 1:A:272:PHE:CZ   | 1:A:308:PRO:HB2  | 2.56                     | 0.41              |
| 1:A:350:VAL:O    | 1:A:354:LEU:CD2  | 2.60                     | 0.41              |
| 1:A:353:LEU:HB3  | 6:A:801:HAS:H22  | 2.03                     | 0.41              |
| 1:A:497:ARG:NH2  | 1:A:499:PRO:HG2  | 2.31                     | 0.41              |
| 1:A:514:GLY:HA3  | 2:B:8:HIS:CD2    | 2.55                     | 0.41              |
| 2:B:41:THR:HG23  | 2:B:41:THR:H     | 1.61                     | 0.41              |
| 2:B:49:LYS:HG3   | 2:B:50:LEU:O     | 2.20                     | 0.41              |
| 2:B:71:VAL:C     | 2:B:72:VAL:CG1   | 2.94                     | 0.41              |
| 2:B:84:LEU:HD12  | 2:B:84:LEU:HA    | 1.75                     | 0.41              |
| 2:B:123:ILE:HG23 | 2:B:135:VAL:HG21 | 2.02                     | 0.41              |
| 2:B:139:PHE:CG   | 2:B:166:VAL:HG11 | 2.55                     | 0.41              |
| 2:B:144:GLU:C    | 2:B:145:TYR:CD1  | 2.99                     | 0.41              |
| 2:B:154:GLY:O    | 2:B:157:HIS:CB   | 2.64                     | 0.41              |
| 3:C:31:PHE:C     | 3:C:33:ARG:N     | 2.78                     | 0.41              |
| 1:A:410:GLY:HA3  | 1:A:499:PRO:CB   | 2.49                     | 0.41              |
| 1:A:514:GLY:HA2  | 2:B:8:HIS:CD2    | 2.56                     | 0.41              |
| 1:A:521:VAL:O    | 1:A:521:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:550:PHE:HA   | 1:A:553:LEU:HD23 | 1.99                     | 0.41              |
| 2:B:145:TYR:CE1  | 2:B:166:VAL:HG22 | 2.55                     | 0.41              |
| 1:A:184:TYR:HE2  | 1:A:266:ARG:CB   | 2.33                     | 0.40              |
| 1:A:314:PHE:CD2  | 3:C:12:ILE:HD12  | 2.54                     | 0.40              |
| 3:C:15:LEU:O     | 3:C:16:THR:C     | 2.64                     | 0.40              |
| 3:C:18:THR:HG22  | 3:C:22:PHE:CD1   | 2.56                     | 0.40              |
| 1:A:187:VAL:O    | 1:A:191:LEU:HB2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:191:LEU:HD22 | 1:A:531:PHE:CE2  | 2.56                     | 0.40              |
| 1:A:264:MET:HA   | 1:A:264:MET:CE   | 2.45                     | 0.40              |
| 2:B:157:HIS:C    | 2:B:159:ASN:N    | 2.77                     | 0.40              |
| 1:A:170:TRP:O    | 1:A:174:ASN:HB2  | 2.21                     | 0.40              |
| 1:A:278:PRO:C    | 1:A:279:VAL:HG13 | 2.47                     | 0.40              |
| 1:A:548:GLN:O    | 1:A:550:PHE:N    | 2.54                     | 0.40              |
| 1:A:16:PRO:C     | 1:A:18:LYS:N     | 2.79                     | 0.40              |
| 2:B:32:LEU:HB3   | 3:C:27:TYR:OH    | 2.19                     | 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     | 555/568 (98%) | 359 (65%) | 126 (23%) | 70 (13%) | 0           | 1 |
| 2   | B     | 164/168 (98%) | 109 (66%) | 40 (24%)  | 15 (9%)  | 0           | 3 |
| 3   | C     | 31/34 (91%)   | 15 (48%)  | 10 (32%)  | 6 (19%)  | 0           | 0 |
| All | All   | 750/770 (97%) | 483 (64%) | 176 (24%) | 91 (12%) | 0           | 1 |

All (91) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | VAL  |
| 1   | A     | 12  | TYR  |
| 1   | A     | 48  | ASN  |
| 1   | A     | 151 | VAL  |
| 1   | A     | 152 | PHE  |
| 1   | A     | 189 | PHE  |
| 1   | A     | 197 | SER  |
| 1   | A     | 335 | TRP  |
| 1   | A     | 340 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 341 | TRP  |
| 1   | A     | 464 | ALA  |
| 1   | A     | 483 | LEU  |
| 1   | A     | 496 | GLU  |
| 1   | A     | 506 | LEU  |
| 1   | A     | 517 | ASP  |
| 1   | A     | 548 | GLN  |
| 2   | B     | 11  | ILE  |
| 2   | B     | 44  | VAL  |
| 2   | B     | 47  | ALA  |
| 2   | B     | 49  | LYS  |
| 2   | B     | 88  | PHE  |
| 2   | B     | 111 | ASP  |
| 2   | B     | 152 | TYR  |
| 3   | C     | 19  | ILE  |
| 1   | A     | 31  | ALA  |
| 1   | A     | 39  | GLY  |
| 1   | A     | 42  | GLN  |
| 1   | A     | 61  | PHE  |
| 1   | A     | 79  | VAL  |
| 1   | A     | 86  | GLN  |
| 1   | A     | 88  | ILE  |
| 1   | A     | 89  | MET  |
| 1   | A     | 94  | ALA  |
| 1   | A     | 130 | THR  |
| 1   | A     | 168 | ARG  |
| 1   | A     | 196 | ALA  |
| 1   | A     | 213 | PHE  |
| 1   | A     | 345 | ALA  |
| 1   | A     | 365 | VAL  |
| 1   | A     | 366 | ASN  |
| 1   | A     | 377 | ASN  |
| 1   | A     | 515 | PRO  |
| 1   | A     | 549 | LEU  |
| 2   | B     | 119 | GLU  |
| 2   | B     | 124 | ASN  |
| 3   | C     | 14  | VAL  |
| 3   | C     | 27  | TYR  |
| 1   | A     | 110 | TRP  |
| 1   | A     | 142 | HIS  |
| 1   | A     | 308 | PRO  |
| 1   | A     | 403 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 452 | TYR  |
| 1   | A     | 469 | PHE  |
| 2   | B     | 76  | PRO  |
| 3   | C     | 13  | LEU  |
| 3   | C     | 15  | LEU  |
| 1   | A     | 121 | ALA  |
| 1   | A     | 129 | ALA  |
| 1   | A     | 181 | LEU  |
| 1   | A     | 190 | TRP  |
| 1   | A     | 376 | HIS  |
| 1   | A     | 384 | HIS  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 531 | PHE  |
| 2   | B     | 72  | VAL  |
| 3   | C     | 16  | THR  |
| 1   | A     | 65  | TYR  |
| 1   | A     | 109 | SER  |
| 1   | A     | 355 | GLY  |
| 1   | A     | 499 | PRO  |
| 1   | A     | 526 | ARG  |
| 2   | B     | 31  | ALA  |
| 2   | B     | 87  | ALA  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 155 | SER  |
| 1   | A     | 279 | VAL  |
| 1   | A     | 280 | GLY  |
| 1   | A     | 356 | PHE  |
| 1   | A     | 383 | GLY  |
| 1   | A     | 405 | LEU  |
| 1   | A     | 465 | VAL  |
| 1   | A     | 491 | VAL  |
| 2   | B     | 48  | GLY  |
| 2   | B     | 110 | PRO  |
| 1   | A     | 329 | GLY  |
| 1   | A     | 543 | GLY  |
| 1   | A     | 115 | ILE  |
| 1   | A     | 233 | HIS  |
| 1   | A     | 504 | ALA  |
| 1   | A     | 28  | GLY  |
| 1   | A     | 34  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | A     | 453/462 (98%) | 338 (75%) | 115 (25%) | 0           | 2 |
| 2   | B     | 136/138 (99%) | 99 (73%)  | 37 (27%)  | 0           | 2 |
| 3   | C     | 26/27 (96%)   | 18 (69%)  | 8 (31%)   | 0           | 1 |
| All | All   | 615/627 (98%) | 455 (74%) | 160 (26%) | 0           | 2 |

All (160) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | ILE  |
| 1   | A     | 25  | LEU  |
| 1   | A     | 27  | LEU  |
| 1   | A     | 33  | ILE  |
| 1   | A     | 37  | LEU  |
| 1   | A     | 38  | PHE  |
| 1   | A     | 42  | GLN  |
| 1   | A     | 49  | VAL  |
| 1   | A     | 54  | LEU  |
| 1   | A     | 55  | LEU  |
| 1   | A     | 57  | ARG  |
| 1   | A     | 63  | GLN  |
| 1   | A     | 64  | SER  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 70  | THR  |
| 1   | A     | 75  | LEU  |
| 1   | A     | 78  | ILE  |
| 1   | A     | 82  | GLN  |
| 1   | A     | 89  | MET  |
| 1   | A     | 98  | ASN  |
| 1   | A     | 100 | ARG  |
| 1   | A     | 103 | MET  |
| 1   | A     | 106 | MET  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 125 | LEU  |
| 1   | A     | 133 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 134 | THR  |
| 1   | A     | 155 | SER  |
| 1   | A     | 157 | TRP  |
| 1   | A     | 162 | ILE  |
| 1   | A     | 164 | LEU  |
| 1   | A     | 168 | ARG  |
| 1   | A     | 179 | THR  |
| 1   | A     | 183 | THR  |
| 1   | A     | 188 | VAL  |
| 1   | A     | 192 | MET  |
| 1   | A     | 195 | LEU  |
| 1   | A     | 201 | VAL  |
| 1   | A     | 202 | LEU  |
| 1   | A     | 205 | VAL  |
| 1   | A     | 213 | PHE  |
| 1   | A     | 215 | LEU  |
| 1   | A     | 216 | VAL  |
| 1   | A     | 222 | LEU  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 235 | ILE  |
| 1   | A     | 236 | VAL  |
| 1   | A     | 244 | TYR  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 254 | GLN  |
| 1   | A     | 276 | SER  |
| 1   | A     | 290 | ILE  |
| 1   | A     | 297 | ILE  |
| 1   | A     | 299 | SER  |
| 1   | A     | 300 | VAL  |
| 1   | A     | 309 | SER  |
| 1   | A     | 311 | MET  |
| 1   | A     | 315 | THR  |
| 1   | A     | 320 | LEU  |
| 1   | A     | 321 | GLU  |
| 1   | A     | 325 | ARG  |
| 1   | A     | 327 | ARG  |
| 1   | A     | 330 | ARG  |
| 1   | A     | 339 | LEU  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 357 | ILE  |
| 1   | A     | 364 | ILE  |
| 1   | A     | 368 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 370 | THR  |
| 1   | A     | 371 | LEU  |
| 1   | A     | 388 | GLN  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 394 | THR  |
| 1   | A     | 398 | MET  |
| 1   | A     | 405 | LEU  |
| 1   | A     | 408 | LEU  |
| 1   | A     | 417 | GLN  |
| 1   | A     | 418 | ARG  |
| 1   | A     | 419 | ARG  |
| 1   | A     | 420 | LEU  |
| 1   | A     | 422 | LEU  |
| 1   | A     | 425 | VAL  |
| 1   | A     | 428 | TRP  |
| 1   | A     | 430 | LEU  |
| 1   | A     | 439 | LEU  |
| 1   | A     | 449 | ARG  |
| 1   | A     | 453 | ILE  |
| 1   | A     | 456 | VAL  |
| 1   | A     | 465 | VAL  |
| 1   | A     | 468 | VAL  |
| 1   | A     | 472 | LEU  |
| 1   | A     | 476 | VAL  |
| 1   | A     | 478 | LEU  |
| 1   | A     | 490 | SER  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 494 | SER  |
| 1   | A     | 495 | ARG  |
| 1   | A     | 498 | LYS  |
| 1   | A     | 501 | LEU  |
| 1   | A     | 512 | ILE  |
| 1   | A     | 513 | SER  |
| 1   | A     | 518 | ARG  |
| 1   | A     | 520 | LEU  |
| 1   | A     | 522 | LEU  |
| 1   | A     | 526 | ARG  |
| 1   | A     | 527 | ILE  |
| 1   | A     | 533 | VAL  |
| 1   | A     | 536 | ILE  |
| 1   | A     | 537 | LEU  |
| 1   | A     | 545 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 548 | GLN  |
| 1   | A     | 549 | LEU  |
| 1   | A     | 552 | HIS  |
| 1   | A     | 560 | ARG  |
| 1   | A     | 561 | LEU  |
| 2   | B     | 9   | LYS  |
| 2   | B     | 12  | LEU  |
| 2   | B     | 14  | TYR  |
| 2   | B     | 15  | GLU  |
| 2   | B     | 18  | TRP  |
| 2   | B     | 19  | LEU  |
| 2   | B     | 22  | SER  |
| 2   | B     | 23  | LEU  |
| 2   | B     | 26  | LEU  |
| 2   | B     | 30  | ILE  |
| 2   | B     | 37  | LEU  |
| 2   | B     | 39  | THR  |
| 2   | B     | 54  | ASP  |
| 2   | B     | 61  | GLU  |
| 2   | B     | 71  | VAL  |
| 2   | B     | 72  | VAL  |
| 2   | B     | 74  | THR  |
| 2   | B     | 77  | ASN  |
| 2   | B     | 96  | GLU  |
| 2   | B     | 99  | GLN  |
| 2   | B     | 107 | ILE  |
| 2   | B     | 110 | PRO  |
| 2   | B     | 119 | GLU  |
| 2   | B     | 128 | LEU  |
| 2   | B     | 129 | PRO  |
| 2   | B     | 133 | SER  |
| 2   | B     | 135 | VAL  |
| 2   | B     | 136 | ARG  |
| 2   | B     | 140 | LYS  |
| 2   | B     | 148 | ILE  |
| 2   | B     | 149 | CYS  |
| 2   | B     | 157 | HIS  |
| 2   | B     | 159 | ASN  |
| 2   | B     | 160 | MET  |
| 2   | B     | 165 | VAL  |
| 2   | B     | 166 | VAL  |
| 2   | B     | 167 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 2   | GLU  |
| 3   | C     | 3   | GLU  |
| 3   | C     | 6   | LYS  |
| 3   | C     | 12  | ILE  |
| 3   | C     | 13  | LEU  |
| 3   | C     | 19  | ILE  |
| 3   | C     | 21  | VAL  |
| 3   | C     | 24  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 48  | ASN  |
| 1   | A     | 63  | GLN  |
| 1   | A     | 76  | ASN  |
| 1   | A     | 98  | ASN  |
| 1   | A     | 254 | GLN  |
| 1   | A     | 388 | GLN  |
| 1   | A     | 446 | ASN  |
| 1   | A     | 470 | ASN  |
| 1   | A     | 554 | ASN  |
| 2   | B     | 8   | HIS  |
| 2   | B     | 40  | HIS  |
| 2   | B     | 60  | GLN  |
| 2   | B     | 77  | ASN  |
| 2   | B     | 99  | GLN  |
| 2   | B     | 117 | HIS  |
| 2   | B     | 122 | ASN  |
| 2   | B     | 159 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 7   | CUA  | B     | 802 | 2    | 0,1,1        | -    | -           | -           |      |             |
| 5   | HEM  | A     | 800 | 1    | 50,50,50     | 2.14 | 13 (26%)    | 67,82,82    | 1.83 | 16 (23%)    |
| 6   | HAS  | A     | 801 | 1    | 72,72,72     | 2.82 | 31 (43%)    | 87,109,109  | 4.43 | 45 (51%)    |

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

| Mol | Type | Chain | Res | Link | Chirals  | Torsions    | Rings |
|-----|------|-------|-----|------|----------|-------------|-------|
| 5   | HEM  | A     | 800 | 1    | -        | 6/14/54/54  | -     |
| 6   | HAS  | A     | 801 | 1    | 1/1/8/18 | 12/42/82/82 | -     |

All (44) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | A     | 800 | HEM  | C3D-C2D | 7.71  | 1.53        | 1.36     |
| 6   | A     | 801 | HAS  | C4A-NA  | -7.65 | 1.25        | 1.39     |
| 6   | A     | 801 | HAS  | C1A-NA  | -6.50 | 1.27        | 1.39     |
| 6   | A     | 801 | HAS  | C2A-C3A | 6.23  | 1.50        | 1.36     |
| 6   | A     | 801 | HAS  | CHC-C4B | 5.92  | 1.50        | 1.38     |
| 6   | A     | 801 | HAS  | CHD-C4A | 5.75  | 1.49        | 1.38     |
| 6   | A     | 801 | HAS  | FE-ND   | 5.28  | 2.11        | 1.94     |
| 5   | A     | 800 | HEM  | FE-ND   | 5.17  | 2.10        | 1.94     |
| 6   | A     | 801 | HAS  | CHB-C1D | 5.16  | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | A     | 801 | HAS  | CAC-C3C | -5.15 | 1.33        | 1.47     |
| 5   | A     | 800 | HEM  | FE-NC   | 5.13  | 2.12        | 1.95     |
| 6   | A     | 801 | HAS  | FE-NB   | 4.42  | 2.08        | 1.94     |
| 6   | A     | 801 | HAS  | C1D-ND  | -4.32 | 1.32        | 1.40     |
| 6   | A     | 801 | HAS  | CHB-C1B | 4.07  | 1.48        | 1.39     |
| 6   | A     | 801 | HAS  | C1C-NC  | -3.99 | 1.32        | 1.39     |
| 6   | A     | 801 | HAS  | CHC-C1C | 3.93  | 1.48        | 1.39     |
| 5   | A     | 800 | HEM  | CAC-C3C | 3.79  | 1.57        | 1.47     |
| 6   | A     | 801 | HAS  | C4A-C3A | 3.79  | 1.52        | 1.45     |
| 6   | A     | 801 | HAS  | C4C-NC  | -3.65 | 1.32        | 1.39     |
| 6   | A     | 801 | HAS  | CHA-C1A | 3.57  | 1.45        | 1.38     |
| 5   | A     | 800 | HEM  | CMA-C3A | 3.55  | 1.58        | 1.50     |
| 6   | A     | 801 | HAS  | O1D-CGD | 3.36  | 1.33        | 1.22     |
| 6   | A     | 801 | HAS  | C2D-C3D | 3.34  | 1.44        | 1.37     |
| 5   | A     | 800 | HEM  | CAB-C3B | 3.22  | 1.56        | 1.47     |
| 6   | A     | 801 | HAS  | C4D-C3D | -3.13 | 1.39        | 1.45     |
| 5   | A     | 800 | HEM  | O1D-CGD | 3.09  | 1.32        | 1.22     |
| 6   | A     | 801 | HAS  | FE-NC   | 2.97  | 2.05        | 1.95     |
| 6   | A     | 801 | HAS  | C1A-C2A | 2.90  | 1.50        | 1.45     |
| 6   | A     | 801 | HAS  | C4B-NB  | -2.88 | 1.35        | 1.40     |
| 6   | A     | 801 | HAS  | C16-C15 | 2.81  | 1.57        | 1.51     |
| 6   | A     | 801 | HAS  | CHD-C4C | 2.79  | 1.45        | 1.39     |
| 6   | A     | 801 | HAS  | C3B-C2B | 2.74  | 1.41        | 1.34     |
| 5   | A     | 800 | HEM  | FE-NB   | 2.65  | 2.03        | 1.94     |
| 6   | A     | 801 | HAS  | C1C-C2C | 2.63  | 1.49        | 1.43     |
| 5   | A     | 800 | HEM  | O1A-CGA | 2.61  | 1.30        | 1.22     |
| 6   | A     | 801 | HAS  | C14-C15 | 2.60  | 1.39        | 1.33     |
| 5   | A     | 800 | HEM  | FE-NA   | 2.57  | 2.03        | 1.95     |
| 6   | A     | 801 | HAS  | CHA-C4D | 2.53  | 1.44        | 1.39     |
| 6   | A     | 801 | HAS  | CBA-CGA | 2.46  | 1.56        | 1.50     |
| 6   | A     | 801 | HAS  | C4D-ND  | -2.38 | 1.34        | 1.38     |
| 6   | A     | 801 | HAS  | C1B-C2B | -2.13 | 1.40        | 1.44     |
| 5   | A     | 800 | HEM  | CMB-C2B | 2.13  | 1.55        | 1.50     |
| 5   | A     | 800 | HEM  | CMD-C2D | 2.11  | 1.55        | 1.50     |
| 5   | A     | 800 | HEM  | CAD-C3D | 2.11  | 1.56        | 1.51     |

All (61) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 6   | A     | 801 | HAS  | C3C-C2C-C1C | -14.49 | 90.09       | 107.17   |
| 6   | A     | 801 | HAS  | CHA-C1A-C2A | -12.12 | 105.73      | 124.86   |
| 6   | A     | 801 | HAS  | C2D-C3D-C4D | -11.90 | 97.82       | 106.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | A     | 801 | HAS  | C2A-C1A-NA  | 11.37 | 121.29      | 110.32   |
| 6   | A     | 801 | HAS  | CBC-CAC-C3C | 9.07  | 172.82      | 127.53   |
| 6   | A     | 801 | HAS  | C4C-C3C-C2C | 8.72  | 118.14      | 107.30   |
| 6   | A     | 801 | HAS  | C1A-C2A-C3A | -8.33 | 96.14       | 107.11   |
| 6   | A     | 801 | HAS  | C3D-C4D-ND  | 7.91  | 117.99      | 110.35   |
| 6   | A     | 801 | HAS  | CHA-C1A-NA  | 7.59  | 132.72      | 124.45   |
| 6   | A     | 801 | HAS  | CHB-C1B-NB  | 6.44  | 131.36      | 124.42   |
| 6   | A     | 801 | HAS  | CHA-C4D-C3D | -6.31 | 115.58      | 124.77   |
| 6   | A     | 801 | HAS  | CHB-C1D-ND  | 6.20  | 132.03      | 124.37   |
| 6   | A     | 801 | HAS  | CHD-C4A-C3A | -5.99 | 113.03      | 125.49   |
| 6   | A     | 801 | HAS  | CHC-C1C-C2C | -5.90 | 110.29      | 127.43   |
| 6   | A     | 801 | HAS  | CMC-C2C-C3C | -5.58 | 113.44      | 126.55   |
| 6   | A     | 801 | HAS  | C2C-C1C-NC  | 5.54  | 119.02      | 110.14   |
| 6   | A     | 801 | HAS  | C1B-CHB-C1D | -5.46 | 113.88      | 125.69   |
| 6   | A     | 801 | HAS  | OMD-CMD-C2D | -5.24 | 113.80      | 125.62   |
| 5   | A     | 800 | HEM  | C4D-ND-C1D  | 5.20  | 111.37      | 105.21   |
| 6   | A     | 801 | HAS  | CHD-C4A-NA  | 5.06  | 129.97      | 124.45   |
| 6   | A     | 801 | HAS  | C1A-CHA-C4D | -5.01 | 115.37      | 126.02   |
| 6   | A     | 801 | HAS  | C3C-C4C-NC  | -4.94 | 105.64      | 109.80   |
| 6   | A     | 801 | HAS  | CHB-C1B-C2B | -4.87 | 117.34      | 125.03   |
| 5   | A     | 800 | HEM  | CAA-CBA-CGA | -4.78 | 100.99      | 113.67   |
| 6   | A     | 801 | HAS  | CMA-C3A-C4A | -4.62 | 116.59      | 124.73   |
| 6   | A     | 801 | HAS  | CMA-C3A-C2A | -4.60 | 113.70      | 126.15   |
| 6   | A     | 801 | HAS  | CAA-C2A-C1A | -4.55 | 115.60      | 124.85   |
| 6   | A     | 801 | HAS  | C1C-CHC-C4B | -4.51 | 115.64      | 126.25   |
| 5   | A     | 800 | HEM  | C3B-C4B-NB  | -4.26 | 106.41      | 109.47   |
| 6   | A     | 801 | HAS  | CAD-C3D-C4D | 4.17  | 131.97      | 124.70   |
| 6   | A     | 801 | HAS  | C17-C18-C19 | -4.16 | 118.09      | 127.62   |
| 6   | A     | 801 | HAS  | C28-C24-C23 | -3.90 | 100.25      | 113.19   |
| 6   | A     | 801 | HAS  | C3A-C4A-NA  | 3.76  | 116.59      | 109.64   |
| 6   | A     | 801 | HAS  | C21-C22-C23 | -3.73 | 119.09      | 127.62   |
| 6   | A     | 801 | HAS  | CHC-C4B-NB  | 3.60  | 128.82      | 124.37   |
| 6   | A     | 801 | HAS  | C4A-C3A-C2A | -3.52 | 101.75      | 106.97   |
| 5   | A     | 800 | HEM  | CAD-CBD-CGD | -3.41 | 104.63      | 113.67   |
| 6   | A     | 801 | HAS  | C1D-C2D-C3D | 3.40  | 110.41      | 107.28   |
| 6   | A     | 801 | HAS  | CHC-C1C-NC  | 3.36  | 129.95      | 123.86   |
| 5   | A     | 800 | HEM  | C2A-C1A-NA  | -3.33 | 106.46      | 110.15   |
| 6   | A     | 801 | HAS  | CMC-C2C-C1C | -3.11 | 120.69      | 125.42   |
| 5   | A     | 800 | HEM  | C4B-C3B-C2B | 2.99  | 110.03      | 107.28   |
| 5   | A     | 800 | HEM  | C3C-C2C-C1C | 2.95  | 109.84      | 107.05   |
| 6   | A     | 801 | HAS  | O2A-CGA-CBA | 2.84  | 122.97      | 114.00   |
| 6   | A     | 801 | HAS  | C25-C23-C24 | 2.83  | 120.14      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | A     | 800 | HEM  | CMA-C3A-C2A | 2.64  | 131.23      | 125.62   |
| 5   | A     | 800 | HEM  | CAD-C3D-C4D | 2.63  | 129.28      | 124.70   |
| 5   | A     | 800 | HEM  | CHA-C1A-C2A | 2.63  | 131.05      | 125.30   |
| 5   | A     | 800 | HEM  | C1D-C2D-C3D | -2.54 | 104.31      | 106.98   |
| 6   | A     | 801 | HAS  | C27-C19-C20 | 2.51  | 119.59      | 115.23   |
| 6   | A     | 801 | HAS  | C31-C30-C29 | -2.46 | 115.26      | 122.66   |
| 6   | A     | 801 | HAS  | CBD-CAD-C3D | -2.45 | 105.76      | 112.53   |
| 5   | A     | 800 | HEM  | C3D-C4D-ND  | -2.41 | 107.52      | 110.17   |
| 6   | A     | 801 | HAS  | C4C-CHD-C4A | -2.37 | 117.33      | 124.66   |
| 5   | A     | 800 | HEM  | CMD-C2D-C1D | 2.17  | 128.43      | 125.03   |
| 6   | A     | 801 | HAS  | CAA-C2A-C3A | -2.16 | 123.83      | 127.87   |
| 5   | A     | 800 | HEM  | CHC-C4B-NB  | 2.10  | 126.69      | 124.42   |
| 6   | A     | 801 | HAS  | C13-C12-C11 | -2.08 | 111.07      | 114.39   |
| 6   | A     | 801 | HAS  | CHC-C4B-C3B | -2.06 | 120.60      | 125.80   |
| 5   | A     | 800 | HEM  | CBC-CAC-C3C | -2.04 | 117.33      | 127.53   |
| 5   | A     | 800 | HEM  | CAA-C2A-C3A | -2.02 | 122.55      | 127.07   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 6   | A     | 801 | HAS  | NA   |

All (18) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | A     | 800 | HEM  | C2B-C3B-CAB-CBB |
| 5   | A     | 800 | HEM  | C2C-C3C-CAC-CBC |
| 5   | A     | 800 | HEM  | C4C-C3C-CAC-CBC |
| 6   | A     | 801 | HAS  | C1D-C2D-CMD-OMD |
| 6   | A     | 801 | HAS  | C3D-C2D-CMD-OMD |
| 6   | A     | 801 | HAS  | C3A-C2A-CAA-CBA |
| 6   | A     | 801 | HAS  | C2A-CAA-CBA-CGA |
| 5   | A     | 800 | HEM  | C4B-C3B-CAB-CBB |
| 6   | A     | 801 | HAS  | C2D-C3D-CAD-CBD |
| 6   | A     | 801 | HAS  | C4D-C3D-CAD-CBD |
| 6   | A     | 801 | HAS  | C26-C15-C16-C17 |
| 6   | A     | 801 | HAS  | C25-C23-C24-C28 |
| 6   | A     | 801 | HAS  | C27-C19-C20-C21 |
| 5   | A     | 800 | HEM  | C2D-C3D-CAD-CBD |
| 6   | A     | 801 | HAS  | C23-C24-C28-C29 |
| 5   | A     | 800 | HEM  | C4D-C3D-CAD-CBD |
| 6   | A     | 801 | HAS  | C14-C15-C16-C17 |

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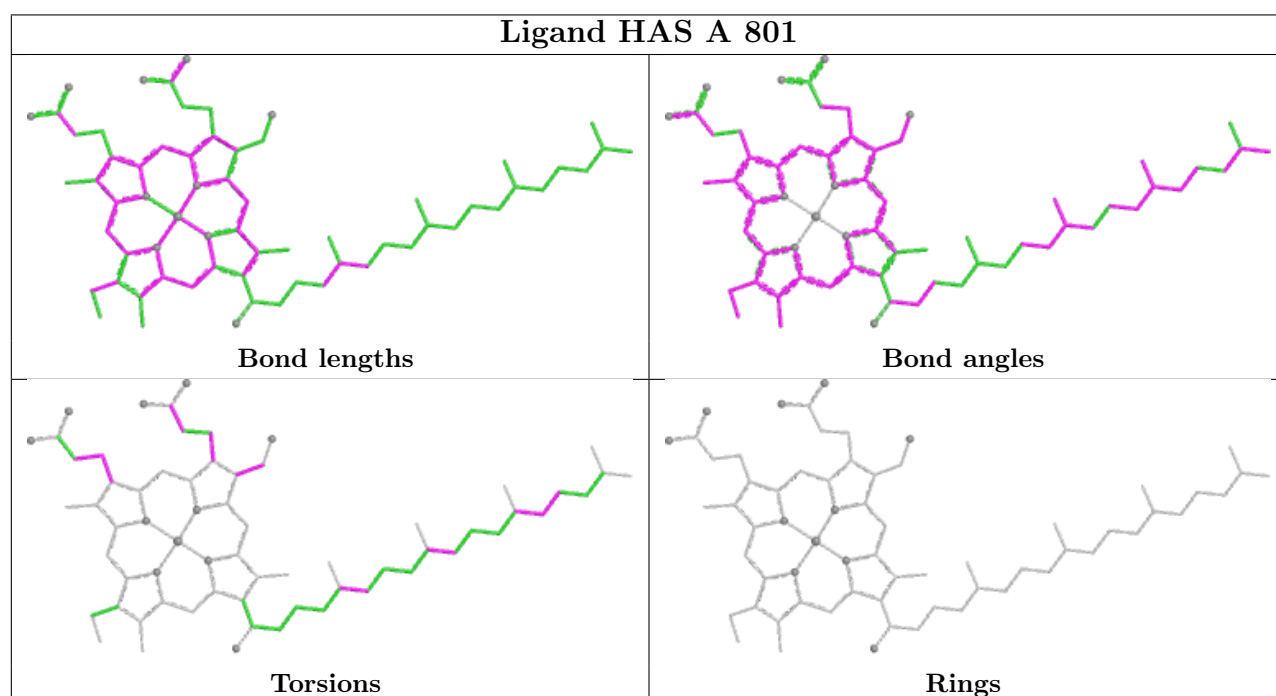
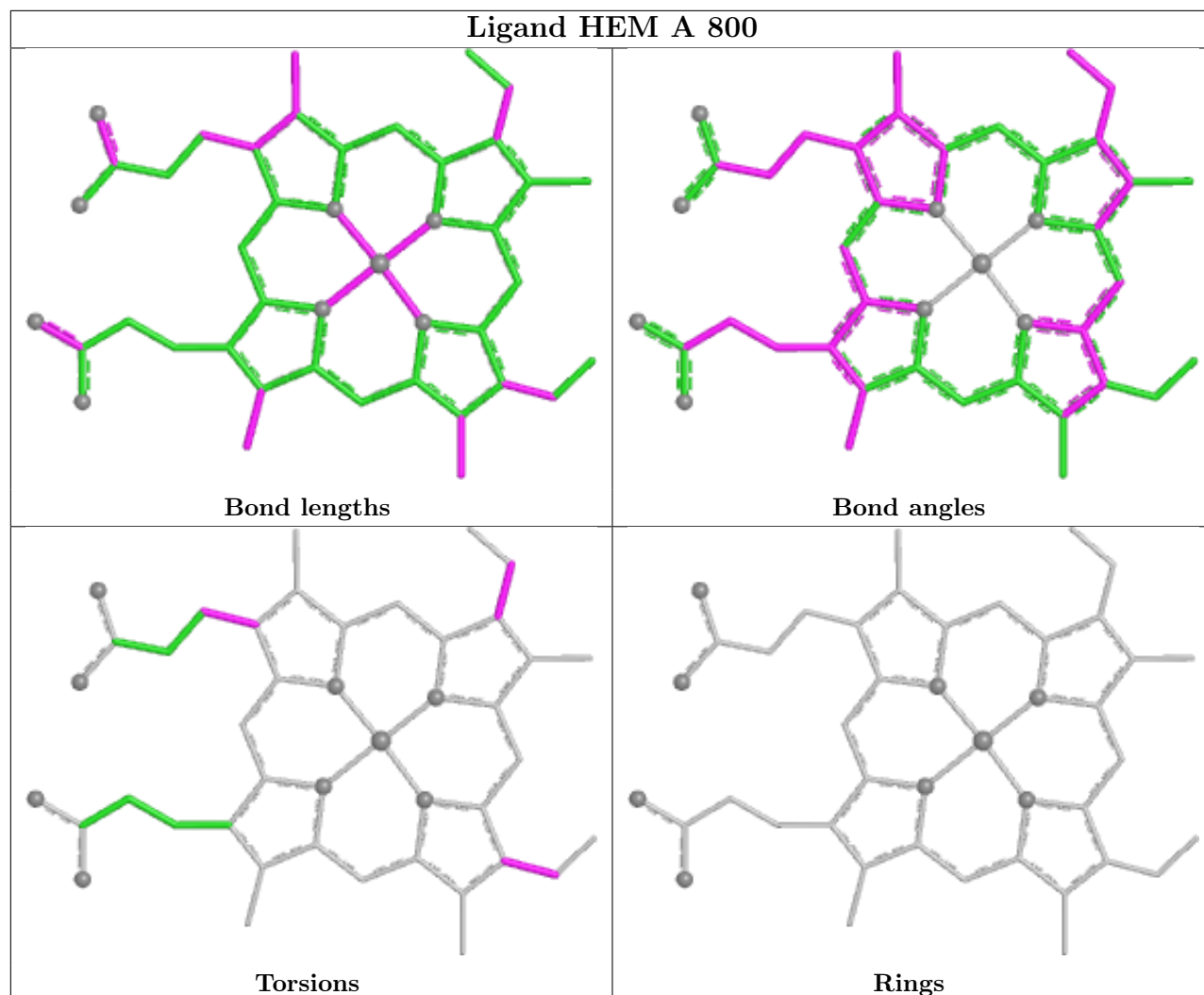
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | A     | 801 | HAS  | CAD-CBD-CGD-O2D |

There are no ring outliers.

2 monomers are involved in 40 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 800 | HEM  | 9       | 0            |
| 6   | A     | 801 | HAS  | 31      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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     | 557/568 (98%) | -0.84  | 0 100 100 | 8, 39, 82, 189        | 0     |
| 2   | B     | 166/168 (98%) | -0.96  | 0 100 100 | 11, 39, 66, 150       | 0     |
| 3   | C     | 33/34 (97%)   | -0.87  | 0 100 100 | 16, 28, 99, 128       | 0     |
| All | All   | 756/770 (98%) | -0.86  | 0 100 100 | 8, 39, 82, 189        | 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 oligosaccharides in this entry.

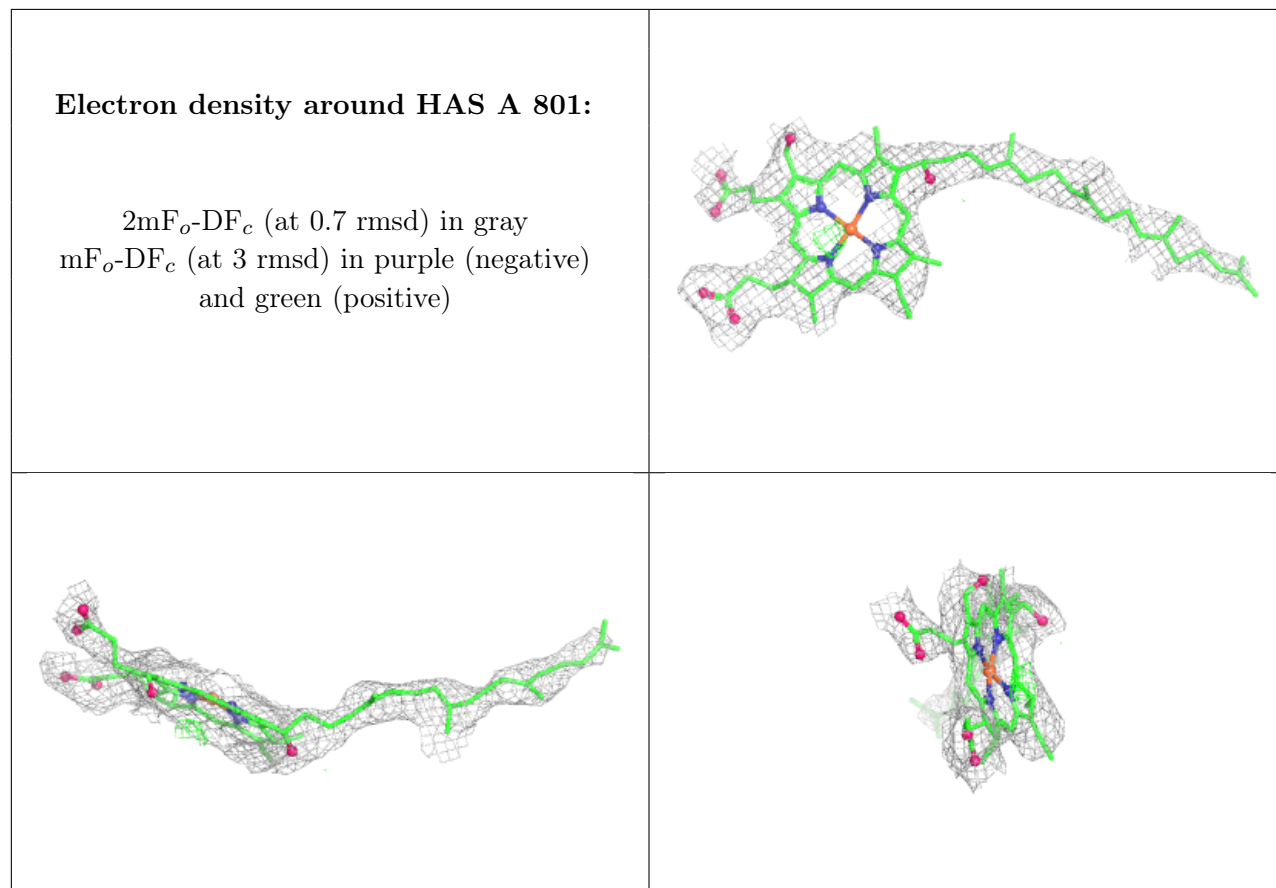
### 6.4 Ligands [i](#)

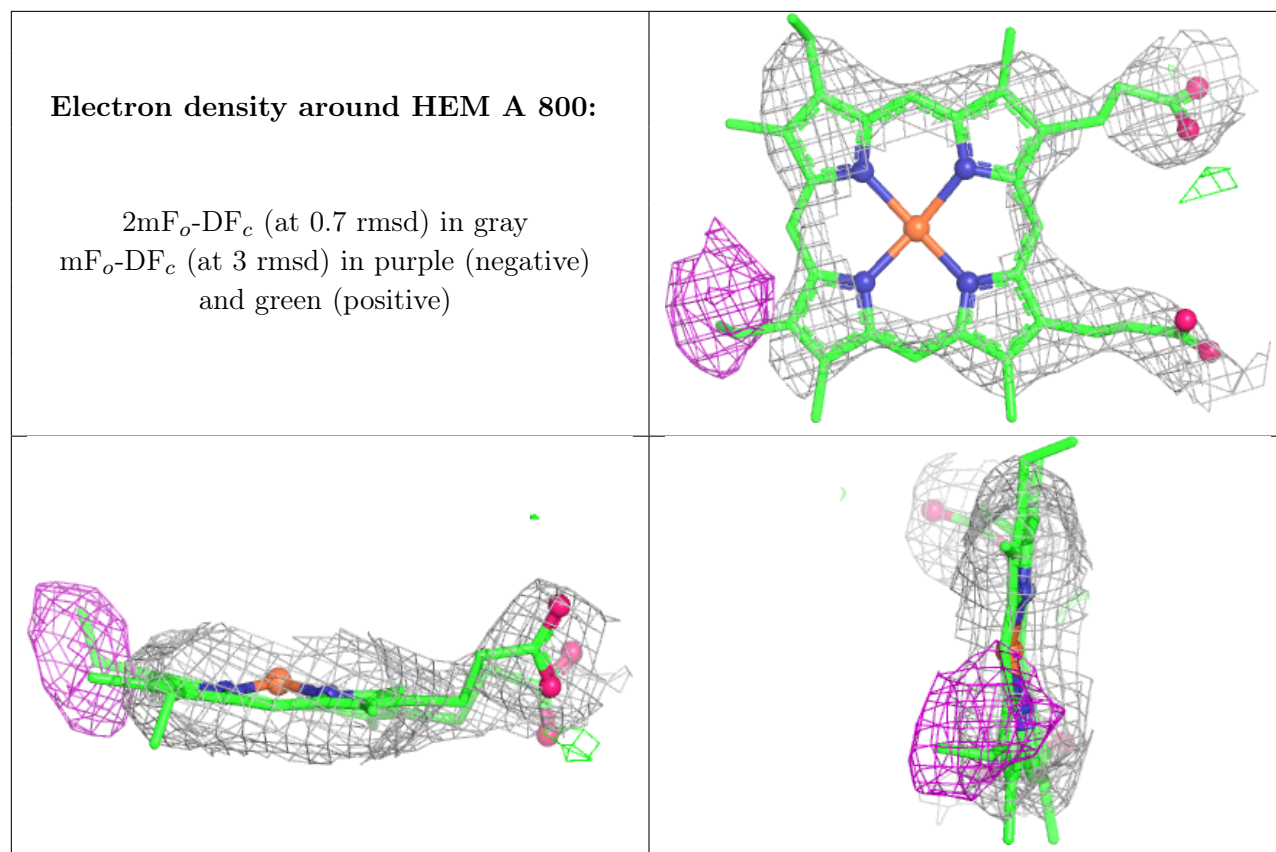
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6   | HAS  | A     | 801 | 65/65 | 0.96 | 0.08 | 17,54,76,85                | 0     |
| 5   | HEM  | A     | 800 | 43/43 | 0.97 | 0.08 | 44,71,84,86                | 0     |
| 4   | CU1  | A     | 803 | 1/1   | 0.97 | 0.03 | 83,83,83,83                | 0     |
| 7   | CUA  | B     | 802 | 2/2   | 0.99 | 0.03 | 49,49,49,52                | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.