



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:44 PM UTC

PDB ID : 1EHA / pdb\_00001eha  
Title : CRYSTAL STRUCTURE OF GLYCOSYLTREHALOSE TREHALOHYDROLASE FROM SULFOLOBUS SOLFATARICUS  
Authors : Feese, M.D.; Kato, Y.; Tamada, T.; Kato, M.; Komeda, T.; Kobayashi, K.; Kuroki, R.  
Deposited on : 2000-02-19  
Resolution : 3.00 Å(reported)

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The types of validation reports are described at

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

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

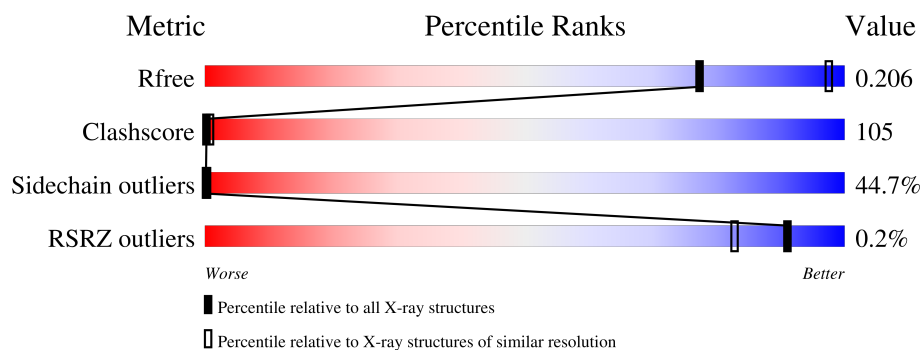
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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                      | 2672 (3.00-3.00)                                      |
| Clashscore         | 190562                      | 2977 (3.00-3.00)                                      |
| Sidechain outliers | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers      | 180081                      | 2671 (3.00-3.00)                                      |

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     | 558    | <div> <div></div> <div>9%</div> <div>53%</div> <div>34%</div> <div>.</div> </div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4572 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 GLYCOSYLTREHALOSE TREHALOHYDROLASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 557      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4542  | 2928 | 741 | 865 | 8 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 298     | VAL      | CYS    | engineered mutation | UNP Q55088 |

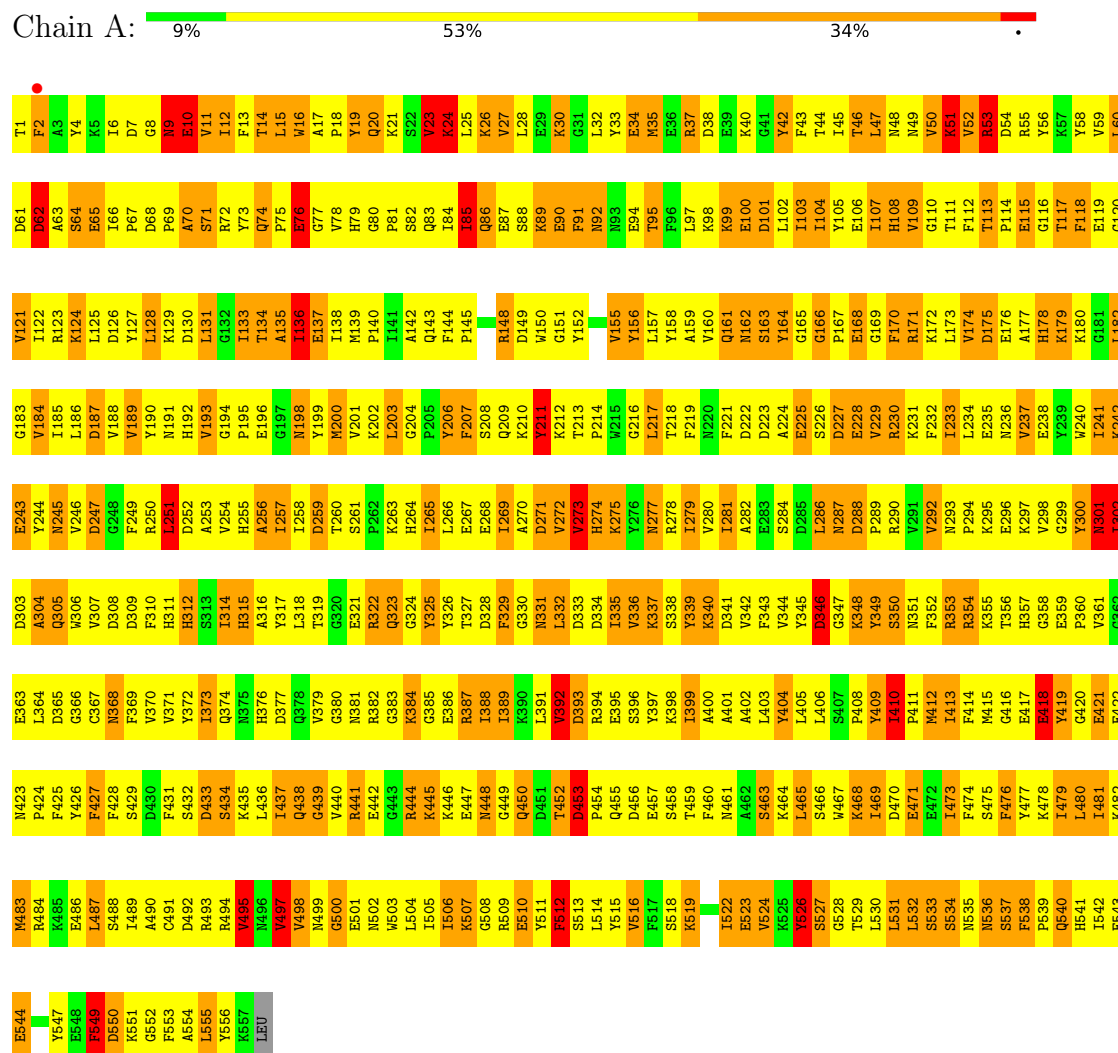
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |

### 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: GLYCOSYLTREHALOSE TREHALOHYDROLASE



## 4 Data and refinement statistics

| Property                                                                | Value                                                        | Source           |
|-------------------------------------------------------------------------|--------------------------------------------------------------|------------------|
| Space group                                                             | P 32 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 80.37Å 80.37Å 282.00Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.00<br>20.00 – 3.00                                 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.0 (20.00-3.00)<br>97.0 (20.00-3.00)                       | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                         | Depositor        |
| $R_{sym}$                                                               | (Not available)                                              | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.71 (at 3.01Å)                                              | Xtriage          |
| Refinement program                                                      | TNT 5E                                                       | Depositor        |
| R, $R_{free}$                                                           | (Not available) , (Not available)<br>(Not available) , 0.206 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1097 reflections (5.10%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 52.9                                                         | Xtriage          |
| Anisotropy                                                              | 0.709                                                        | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 220.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$  | Xtriage          |
| Estimated twinning fraction                                             | 0.042 for -h,-k,l                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                         | EDS              |
| Total number of atoms                                                   | 4572                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 45.0                                                         | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 1.37         | 6/4660 (0.1%) | 1.74        | 92/6307 (1.5%) |

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     | 2                   | 0                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 137 | GLU  | CD-OE2 | 6.51  | 1.37        | 1.25     |
| 1   | A     | 409 | TYR  | C-N    | -6.16 | 1.26        | 1.33     |
| 1   | A     | 410 | ILE  | CA-C   | -6.01 | 1.46        | 1.52     |
| 1   | A     | 71  | SER  | CA-C   | -5.36 | 1.45        | 1.52     |
| 1   | A     | 106 | GLU  | CD-OE2 | 5.26  | 1.35        | 1.25     |
| 1   | A     | 512 | PHE  | CA-C   | -5.00 | 1.46        | 1.52     |

All (92) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 161 | GLN  | N-CA-CB  | 10.43 | 125.30      | 109.34   |
| 1   | A     | 538 | PHE  | CA-C-N   | 9.78  | 132.06      | 119.84   |
| 1   | A     | 538 | PHE  | C-N-CA   | 9.78  | 132.06      | 119.84   |
| 1   | A     | 497 | VAL  | N-CA-C   | 9.43  | 121.70      | 108.12   |
| 1   | A     | 288 | ASP  | CA-C-N   | 9.26  | 129.46      | 119.28   |
| 1   | A     | 288 | ASP  | C-N-CA   | 9.26  | 129.46      | 119.28   |
| 1   | A     | 349 | TYR  | N-CA-C   | 9.14  | 122.83      | 108.67   |
| 1   | A     | 427 | PHE  | CA-CB-CG | -9.11 | 104.69      | 113.80   |
| 1   | A     | 506 | ILE  | N-CA-C   | 8.90  | 119.48      | 106.85   |
| 1   | A     | 76  | GLU  | N-CA-CB  | 8.58  | 122.30      | 109.94   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 346 | ASP  | N-CA-CB  | -8.52 | 97.44       | 110.91   |
| 1   | A     | 200 | MET  | N-CA-C   | -8.04 | 102.46      | 111.14   |
| 1   | A     | 500 | GLY  | N-CA-C   | -7.96 | 103.23      | 112.79   |
| 1   | A     | 373 | ILE  | N-CA-C   | -7.45 | 105.31      | 113.43   |
| 1   | A     | 269 | ILE  | CB-CA-C  | -7.35 | 102.62      | 111.81   |
| 1   | A     | 312 | HIS  | CA-CB-CG | -7.26 | 106.54      | 113.80   |
| 1   | A     | 277 | ASN  | N-CA-CB  | 6.88  | 121.88      | 111.70   |
| 1   | A     | 495 | VAL  | N-CA-CB  | -6.82 | 101.01      | 112.47   |
| 1   | A     | 238 | GLU  | N-CA-CB  | 6.65  | 120.03      | 110.06   |
| 1   | A     | 273 | VAL  | N-CA-CB  | 6.64  | 118.16      | 110.65   |
| 1   | A     | 90  | GLU  | N-CA-C   | 6.54  | 120.94      | 109.96   |
| 1   | A     | 274 | HIS  | CA-CB-CG | -6.50 | 107.30      | 113.80   |
| 1   | A     | 418 | GLU  | N-CA-CB  | 6.49  | 119.80      | 110.06   |
| 1   | A     | 256 | ALA  | N-CA-C   | -6.47 | 103.82      | 112.94   |
| 1   | A     | 506 | ILE  | N-CA-CB  | -6.42 | 103.93      | 111.83   |
| 1   | A     | 251 | LEU  | N-CA-C   | 6.40  | 119.13      | 108.96   |
| 1   | A     | 85  | ILE  | N-CA-CB  | -6.37 | 105.00      | 112.32   |
| 1   | A     | 490 | ALA  | N-CA-C   | 6.33  | 119.66      | 110.28   |
| 1   | A     | 90  | GLU  | N-CA-CB  | 6.31  | 120.46      | 110.23   |
| 1   | A     | 392 | VAL  | N-CA-C   | 6.29  | 117.83      | 108.46   |
| 1   | A     | 287 | ASN  | CA-CB-CG | 6.25  | 118.85      | 112.60   |
| 1   | A     | 287 | ASN  | N-CA-CB  | 6.19  | 120.95      | 110.49   |
| 1   | A     | 237 | VAL  | N-CA-CB  | 6.16  | 119.81      | 110.58   |
| 1   | A     | 225 | GLU  | N-CA-C   | 6.12  | 120.45      | 112.92   |
| 1   | A     | 526 | TYR  | N-CA-C   | 6.07  | 118.08      | 108.79   |
| 1   | A     | 136 | ILE  | N-CA-C   | 6.05  | 116.64      | 108.17   |
| 1   | A     | 135 | ALA  | N-CA-C   | 6.04  | 117.68      | 108.07   |
| 1   | A     | 162 | ASN  | N-CA-CB  | -6.02 | 100.32      | 110.49   |
| 1   | A     | 439 | GLY  | N-CA-C   | -6.00 | 105.38      | 112.64   |
| 1   | A     | 236 | ASN  | CA-C-N   | -5.99 | 111.91      | 120.42   |
| 1   | A     | 236 | ASN  | C-N-CA   | -5.99 | 111.91      | 120.42   |
| 1   | A     | 549 | PHE  | N-CA-CB  | 5.98  | 120.89      | 111.20   |
| 1   | A     | 383 | GLY  | N-CA-C   | -5.93 | 106.90      | 114.37   |
| 1   | A     | 24  | LYS  | N-CA-C   | 5.91  | 118.03      | 108.34   |
| 1   | A     | 363 | GLU  | N-CA-C   | -5.87 | 103.27      | 110.61   |
| 1   | A     | 91  | PHE  | CA-CB-CG | -5.82 | 107.98      | 113.80   |
| 1   | A     | 70  | ALA  | N-CA-C   | -5.79 | 106.11      | 112.72   |
| 1   | A     | 166 | GLY  | CA-C-N   | 5.74  | 127.01      | 119.84   |
| 1   | A     | 166 | GLY  | C-N-CA   | 5.74  | 127.01      | 119.84   |
| 1   | A     | 410 | ILE  | CA-C-N   | 5.72  | 126.01      | 119.83   |
| 1   | A     | 410 | ILE  | C-N-CA   | 5.72  | 126.01      | 119.83   |
| 1   | A     | 23  | VAL  | CB-CA-C  | 5.71  | 119.14      | 110.62   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 10  | GLU  | N-CA-C   | 5.67  | 118.97      | 109.95   |
| 1   | A     | 211 | TYR  | N-CA-C   | 5.61  | 118.76      | 110.46   |
| 1   | A     | 224 | ALA  | CA-C-N   | -5.60 | 113.68      | 122.65   |
| 1   | A     | 224 | ALA  | C-N-CA   | -5.60 | 113.68      | 122.65   |
| 1   | A     | 301 | ASN  | N-CA-CB  | 5.56  | 119.89      | 110.49   |
| 1   | A     | 170 | PHE  | CA-CB-CG | -5.54 | 108.26      | 113.80   |
| 1   | A     | 304 | ALA  | N-CA-C   | 5.47  | 117.38      | 109.07   |
| 1   | A     | 166 | GLY  | O-C-N    | 5.46  | 127.23      | 121.77   |
| 1   | A     | 304 | ALA  | N-CA-CB  | 5.45  | 120.77      | 111.66   |
| 1   | A     | 51  | LYS  | N-CA-C   | -5.45 | 99.19       | 110.80   |
| 1   | A     | 346 | ASP  | N-CA-C   | -5.44 | 106.43      | 112.57   |
| 1   | A     | 53  | ARG  | CA-CB-CG | -5.43 | 103.23      | 114.10   |
| 1   | A     | 247 | ASP  | N-CA-CB  | 5.42  | 118.47      | 110.33   |
| 1   | A     | 23  | VAL  | N-CA-CB  | 5.40  | 120.79      | 111.39   |
| 1   | A     | 178 | HIS  | CA-CB-CG | -5.39 | 108.41      | 113.80   |
| 1   | A     | 331 | ASN  | CA-CB-CG | 5.37  | 117.97      | 112.60   |
| 1   | A     | 507 | LYS  | N-CA-CB  | 5.36  | 117.89      | 110.17   |
| 1   | A     | 62  | ASP  | CA-CB-CG | 5.34  | 117.94      | 112.60   |
| 1   | A     | 206 | TYR  | N-CA-C   | -5.33 | 106.90      | 113.41   |
| 1   | A     | 115 | GLU  | N-CA-C   | -5.33 | 105.39      | 111.14   |
| 1   | A     | 301 | ASN  | CA-CB-CG | -5.32 | 107.28      | 112.60   |
| 1   | A     | 418 | GLU  | N-CA-C   | 5.25  | 117.69      | 111.33   |
| 1   | A     | 118 | PHE  | N-CA-CB  | 5.24  | 117.67      | 110.07   |
| 1   | A     | 189 | VAL  | N-CA-C   | 5.17  | 115.22      | 107.51   |
| 1   | A     | 524 | VAL  | CB-CA-C  | -5.15 | 102.84      | 111.29   |
| 1   | A     | 538 | PHE  | CB-CA-C  | 5.14  | 115.71      | 109.85   |
| 1   | A     | 200 | MET  | O-C-N    | 5.11  | 127.61      | 122.09   |
| 1   | A     | 241 | ILE  | N-CA-C   | 5.11  | 115.83      | 110.62   |
| 1   | A     | 10  | GLU  | CB-CA-C  | 5.11  | 118.72      | 109.37   |
| 1   | A     | 368 | ASN  | CA-C-O   | 5.11  | 125.40      | 119.32   |
| 1   | A     | 368 | ASN  | CA-CB-CG | -5.09 | 107.51      | 112.60   |
| 1   | A     | 469 | ILE  | CA-C-N   | 5.08  | 130.27      | 122.95   |
| 1   | A     | 469 | ILE  | C-N-CA   | 5.08  | 130.27      | 122.95   |
| 1   | A     | 156 | TYR  | N-CA-C   | 5.08  | 117.32      | 110.06   |
| 1   | A     | 9   | ASN  | N-CA-C   | -5.06 | 106.52      | 113.30   |
| 1   | A     | 166 | GLY  | C-N-CD   | -5.03 | 104.37      | 125.00   |
| 1   | A     | 302 | ILE  | CB-CA-C  | -5.03 | 103.05      | 111.29   |
| 1   | A     | 453 | ASP  | CA-C-N   | 5.03  | 125.30      | 119.47   |
| 1   | A     | 453 | ASP  | C-N-CA   | 5.03  | 125.30      | 119.47   |
| 1   | A     | 42  | TYR  | N-CA-C   | 5.02  | 116.82      | 107.99   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 90  | GLU  | CA   |
| 1   | A     | 304 | ALA  | CA   |

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4542  | 0        | 4353     | 930     | 0            |
| 2   | A     | 30    | 0        | 0        | 7       | 0            |
| All | All   | 4572  | 0        | 4353     | 930     | 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 105.

All (930) 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:113:THR:HG21 | 1:A:120:GLY:HA3  | 1.29                     | 1.14              |
| 1:A:35:MET:HB2   | 1:A:43:PHE:HB3   | 1.27                     | 1.11              |
| 1:A:337:LYS:HD2  | 1:A:344:VAL:HA   | 1.18                     | 1.11              |
| 1:A:35:MET:HE3   | 1:A:45:ILE:HG13  | 1.18                     | 1.10              |
| 1:A:273:VAL:HG21 | 1:A:280:VAL:HG13 | 1.31                     | 1.10              |
| 1:A:139:MET:HE1  | 1:A:376:HIS:HB3  | 1.28                     | 1.09              |
| 1:A:24:LYS:HD2   | 1:A:32:LEU:HD11  | 1.36                     | 1.07              |
| 1:A:104:ILE:HB   | 1:A:412:MET:HB2  | 1.32                     | 1.07              |
| 1:A:287:ASN:HB2  | 1:A:358:GLY:HA3  | 1.37                     | 1.05              |
| 1:A:483:MET:HE2  | 1:A:531:LEU:HD11 | 1.39                     | 1.02              |
| 1:A:113:THR:HG22 | 1:A:116:GLY:H    | 1.19                     | 1.01              |
| 1:A:131:LEU:HD21 | 1:A:418:GLU:HG2  | 1.40                     | 0.99              |
| 1:A:191:ASN:HB3  | 1:A:257:ILE:HD12 | 1.44                     | 0.99              |
| 1:A:55:ARG:HB3   | 1:A:81:PRO:HB2   | 1.43                     | 0.98              |
| 1:A:69:PRO:HB3   | 1:A:200:MET:HE1  | 1.45                     | 0.98              |
| 1:A:476:PHE:HA   | 1:A:479:ILE:HD12 | 1.45                     | 0.98              |
| 1:A:23:VAL:HG13  | 1:A:60:LEU:HA    | 1.47                     | 0.96              |
| 1:A:476:PHE:HE1  | 1:A:532:LEU:HD11 | 1.27                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:LEU:HB2  | 1:A:300:TYR:HD2  | 1.31                     | 0.96              |
| 1:A:25:LEU:HB2   | 1:A:45:ILE:HD12  | 1.45                     | 0.95              |
| 1:A:24:LYS:HB3   | 1:A:32:LEU:HD11  | 1.46                     | 0.95              |
| 1:A:542:ILE:HD12 | 1:A:543:GLU:H    | 1.33                     | 0.94              |
| 1:A:474:PHE:HE1  | 1:A:478:LYS:HD2  | 1.33                     | 0.92              |
| 1:A:52:VAL:HB    | 1:A:54:ASP:HB2   | 1.52                     | 0.92              |
| 1:A:16:TRP:CE3   | 1:A:18:PRO:HD3   | 2.06                     | 0.91              |
| 1:A:139:MET:HE1  | 1:A:376:HIS:CB   | 2.02                     | 0.90              |
| 1:A:25:LEU:HD13  | 1:A:26:LYS:N     | 1.87                     | 0.90              |
| 1:A:255:HIS:HB3  | 1:A:286:LEU:HD12 | 1.54                     | 0.89              |
| 1:A:186:LEU:HD12 | 1:A:187:ASP:N    | 1.86                     | 0.89              |
| 1:A:35:MET:CE    | 1:A:45:ILE:HG13  | 2.03                     | 0.89              |
| 1:A:266:LEU:HB2  | 1:A:300:TYR:CD2  | 2.06                     | 0.89              |
| 1:A:389:ILE:HG23 | 1:A:397:TYR:CE2  | 2.07                     | 0.89              |
| 1:A:219:PHE:HB2  | 1:A:221:PHE:CE1  | 2.07                     | 0.89              |
| 1:A:530:LEU:HD12 | 1:A:531:LEU:N    | 1.87                     | 0.89              |
| 1:A:131:LEU:CD2  | 1:A:418:GLU:HG2  | 2.03                     | 0.88              |
| 1:A:200:MET:HG3  | 1:A:207:PHE:HZ   | 1.39                     | 0.88              |
| 1:A:6:ILE:HA     | 1:A:11:VAL:HG23  | 1.55                     | 0.88              |
| 1:A:35:MET:CB    | 1:A:43:PHE:HB3   | 2.04                     | 0.87              |
| 1:A:69:PRO:CB    | 1:A:200:MET:HE1  | 2.04                     | 0.87              |
| 1:A:186:LEU:HD12 | 1:A:187:ASP:H    | 1.40                     | 0.86              |
| 1:A:547:TYR:HB2  | 1:A:549:PHE:CE1  | 2.11                     | 0.86              |
| 1:A:530:LEU:HB3  | 1:A:540:GLN:HA   | 1.56                     | 0.86              |
| 1:A:104:ILE:CB   | 1:A:412:MET:HB2  | 2.05                     | 0.86              |
| 1:A:287:ASN:HB2  | 1:A:358:GLY:CA   | 2.04                     | 0.86              |
| 1:A:434:SER:HA   | 1:A:437:ILE:HD12 | 1.57                     | 0.85              |
| 1:A:16:TRP:HA    | 1:A:42:TYR:HD1   | 1.41                     | 0.85              |
| 1:A:27:VAL:HG12  | 1:A:30:LYS:H     | 1.42                     | 0.85              |
| 1:A:103:ILE:H    | 1:A:134:THR:HG1  | 1.23                     | 0.85              |
| 1:A:255:HIS:HB3  | 1:A:286:LEU:CD1  | 2.07                     | 0.85              |
| 1:A:532:LEU:HD12 | 1:A:533:SER:N    | 1.92                     | 0.84              |
| 1:A:91:PHE:CE2   | 1:A:242:LYS:HB3  | 2.12                     | 0.84              |
| 1:A:191:ASN:HB3  | 1:A:257:ILE:CD1  | 2.07                     | 0.84              |
| 1:A:287:ASN:H    | 1:A:357:HIS:HE1  | 1.25                     | 0.84              |
| 1:A:349:TYR:HE1  | 1:A:354:ARG:HA   | 1.42                     | 0.84              |
| 1:A:500:GLY:HA3  | 1:A:503:TRP:NE1  | 1.92                     | 0.83              |
| 1:A:465:LEU:HB2  | 1:A:467:TRP:CZ3  | 2.13                     | 0.83              |
| 1:A:113:THR:HG21 | 1:A:120:GLY:CA   | 2.06                     | 0.83              |
| 1:A:78:VAL:HG22  | 1:A:156:TYR:CE1  | 2.14                     | 0.82              |
| 1:A:254:VAL:HG11 | 1:A:282:ALA:HB1  | 1.62                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:406:LEU:HD22 | 1:A:489:ILE:HD12 | 1.62                     | 0.82              |
| 1:A:452:THR:CG2  | 1:A:459:THR:HG23 | 2.09                     | 0.82              |
| 1:A:349:TYR:CE1  | 1:A:354:ARG:HA   | 2.14                     | 0.82              |
| 1:A:419:TYR:CE1  | 1:A:421:GLU:HG2  | 2.14                     | 0.82              |
| 1:A:32:LEU:HD13  | 1:A:33:TYR:N     | 1.95                     | 0.81              |
| 1:A:190:TYR:CD2  | 1:A:251:LEU:HD21 | 2.16                     | 0.81              |
| 1:A:24:LYS:HD2   | 1:A:32:LEU:CD1   | 2.10                     | 0.80              |
| 1:A:24:LYS:HB2   | 1:A:59:VAL:CG1   | 2.11                     | 0.80              |
| 1:A:371:VAL:HG22 | 1:A:409:TYR:HB2  | 1.62                     | 0.80              |
| 1:A:12:ILE:HD12  | 1:A:14:THR:H     | 1.46                     | 0.80              |
| 1:A:474:PHE:CE1  | 1:A:478:LYS:HD2  | 2.17                     | 0.80              |
| 1:A:24:LYS:HB3   | 1:A:32:LEU:CD1   | 2.11                     | 0.79              |
| 1:A:187:ASP:HB2  | 1:A:250:ARG:HD2  | 1.64                     | 0.79              |
| 1:A:119:GLU:HA   | 1:A:122:ILE:HD12 | 1.64                     | 0.79              |
| 1:A:419:TYR:CZ   | 1:A:421:GLU:HG2  | 2.16                     | 0.79              |
| 1:A:50:VAL:HG22  | 1:A:52:VAL:CG2   | 2.12                     | 0.79              |
| 1:A:113:THR:HG23 | 1:A:115:GLU:OE2  | 1.83                     | 0.79              |
| 1:A:452:THR:HB   | 1:A:459:THR:HG23 | 1.65                     | 0.79              |
| 1:A:483:MET:HE2  | 1:A:531:LEU:CD1  | 2.12                     | 0.79              |
| 1:A:25:LEU:O     | 1:A:32:LEU:HD22  | 1.82                     | 0.78              |
| 1:A:16:TRP:CH2   | 1:A:18:PRO:HG3   | 2.18                     | 0.78              |
| 1:A:131:LEU:HD12 | 1:A:131:LEU:O    | 1.84                     | 0.77              |
| 1:A:503:TRP:CZ3  | 1:A:505:ILE:HG23 | 2.19                     | 0.77              |
| 1:A:140:PRO:HG2  | 1:A:152:TYR:CE1  | 2.19                     | 0.77              |
| 1:A:27:VAL:HG11  | 1:A:30:LYS:HB2   | 1.65                     | 0.77              |
| 1:A:145:PRO:HG2  | 1:A:431:PHE:CE1  | 2.20                     | 0.77              |
| 1:A:200:MET:HG3  | 1:A:207:PHE:CZ   | 2.20                     | 0.77              |
| 1:A:461:ASN:HA   | 1:A:464:LYS:HG3  | 1.65                     | 0.77              |
| 1:A:530:LEU:HD12 | 1:A:531:LEU:H    | 1.48                     | 0.77              |
| 1:A:287:ASN:H    | 1:A:357:HIS:CE1  | 2.03                     | 0.76              |
| 1:A:373:ILE:HG23 | 1:A:404:TYR:CD2  | 2.19                     | 0.76              |
| 1:A:301:ASN:O    | 1:A:302:ILE:C    | 2.28                     | 0.76              |
| 1:A:357:HIS:ND1  | 1:A:358:GLY:N    | 2.33                     | 0.76              |
| 1:A:148:ARG:HD2  | 1:A:460:PHE:HD2  | 1.51                     | 0.76              |
| 1:A:503:TRP:CE3  | 1:A:505:ILE:HG23 | 2.21                     | 0.76              |
| 1:A:503:TRP:CD2  | 1:A:522:ILE:HD13 | 2.21                     | 0.75              |
| 1:A:119:GLU:CA   | 1:A:122:ILE:HD12 | 2.16                     | 0.75              |
| 1:A:16:TRP:HA    | 1:A:42:TYR:CD1   | 2.19                     | 0.75              |
| 1:A:113:THR:CG2  | 1:A:115:GLU:HB2  | 2.16                     | 0.75              |
| 1:A:108:HIS:HE2  | 1:A:428:PHE:HZ   | 1.33                     | 0.75              |
| 1:A:406:LEU:HD22 | 1:A:489:ILE:CD1  | 2.15                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:433:ASP:OD2  | 1:A:436:LEU:HG   | 1.87                     | 0.75              |
| 1:A:373:ILE:O    | 1:A:374:GLN:HG2  | 1.87                     | 0.75              |
| 1:A:83:GLN:HG2   | 1:A:84:ILE:N     | 2.01                     | 0.74              |
| 1:A:527:SER:OG   | 1:A:543:GLU:HA   | 1.88                     | 0.74              |
| 1:A:179:LYS:HB2  | 1:A:179:LYS:NZ   | 2.03                     | 0.74              |
| 1:A:245:ASN:ND2  | 1:A:278:ARG:HH12 | 1.85                     | 0.73              |
| 1:A:432:SER:O    | 1:A:437:ILE:HD11 | 1.89                     | 0.73              |
| 1:A:105:TYR:HB3  | 1:A:136:ILE:CD1  | 2.19                     | 0.73              |
| 1:A:105:TYR:HB3  | 1:A:136:ILE:HD12 | 1.69                     | 0.73              |
| 1:A:73:TYR:CZ    | 1:A:75:PRO:HA    | 2.23                     | 0.73              |
| 1:A:173:LEU:HD12 | 1:A:173:LEU:O    | 1.88                     | 0.73              |
| 1:A:498:VAL:HG12 | 1:A:499:ASN:H    | 1.53                     | 0.73              |
| 1:A:25:LEU:CB    | 1:A:45:ILE:HD12  | 2.17                     | 0.73              |
| 1:A:531:LEU:HB3  | 1:A:555:LEU:CD1  | 2.18                     | 0.73              |
| 1:A:27:VAL:CG1   | 1:A:30:LYS:H     | 2.02                     | 0.73              |
| 1:A:6:ILE:HG13   | 1:A:11:VAL:CG2   | 2.19                     | 0.72              |
| 1:A:12:ILE:CD1   | 1:A:14:THR:H     | 2.02                     | 0.72              |
| 1:A:105:TYR:HB2  | 1:A:133:ILE:HG13 | 1.70                     | 0.72              |
| 1:A:265:ILE:HD12 | 1:A:268:GLU:HB2  | 1.72                     | 0.72              |
| 1:A:294:PRO:HA   | 1:A:301:ASN:ND2  | 2.04                     | 0.72              |
| 1:A:384:LYS:HA   | 1:A:426:TYR:HE1  | 1.53                     | 0.72              |
| 1:A:87:GLU:HB3   | 1:A:89:LYS:HG3   | 1.71                     | 0.72              |
| 1:A:373:ILE:HG23 | 1:A:404:TYR:HD2  | 1.53                     | 0.72              |
| 1:A:381:ASN:HA   | 1:A:444:ARG:NH2  | 2.05                     | 0.72              |
| 1:A:361:VAL:HG21 | 1:A:369:PHE:CE2  | 2.25                     | 0.71              |
| 1:A:307:VAL:CG2  | 1:A:369:PHE:HB3  | 2.19                     | 0.71              |
| 1:A:99:LYS:CD    | 1:A:99:LYS:H     | 2.02                     | 0.71              |
| 1:A:286:LEU:CD1  | 1:A:286:LEU:H    | 2.03                     | 0.71              |
| 1:A:24:LYS:CB    | 1:A:32:LEU:HD11  | 2.21                     | 0.71              |
| 1:A:133:ILE:HD11 | 1:A:413:ILE:CD1  | 2.20                     | 0.71              |
| 1:A:91:PHE:CD2   | 1:A:242:LYS:HA   | 2.26                     | 0.71              |
| 1:A:437:ILE:HG23 | 1:A:455:GLN:HG3  | 1.72                     | 0.71              |
| 1:A:16:TRP:CZ2   | 1:A:18:PRO:HG3   | 2.25                     | 0.71              |
| 1:A:432:SER:C    | 1:A:437:ILE:HD11 | 2.16                     | 0.71              |
| 1:A:133:ILE:HD11 | 1:A:413:ILE:HD12 | 1.73                     | 0.70              |
| 1:A:138:ILE:HG22 | 1:A:139:MET:O    | 1.90                     | 0.70              |
| 1:A:137:GLU:HG3  | 1:A:185:ILE:HG22 | 1.72                     | 0.70              |
| 1:A:53:ARG:HH11  | 1:A:53:ARG:HG2   | 1.56                     | 0.70              |
| 1:A:513:SER:HG   | 1:A:515:TYR:HE1  | 1.35                     | 0.70              |
| 1:A:219:PHE:HB2  | 1:A:221:PHE:CZ   | 2.26                     | 0.70              |
| 1:A:99:LYS:H     | 1:A:99:LYS:CE    | 2.04                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:26:LYS:HB2   | 1:A:32:LEU:CD2   | 2.21                     | 0.70              |
| 1:A:103:ILE:HG12 | 1:A:134:THR:OG1  | 1.91                     | 0.70              |
| 1:A:203:LEU:HB2  | 1:A:206:TYR:HE1  | 1.56                     | 0.70              |
| 1:A:35:MET:HB3   | 1:A:44:THR:N     | 2.07                     | 0.70              |
| 1:A:50:VAL:HG22  | 1:A:52:VAL:HG23  | 1.71                     | 0.70              |
| 1:A:264:HIS:CD2  | 1:A:265:ILE:HG22 | 2.26                     | 0.69              |
| 1:A:542:ILE:CD1  | 1:A:543:GLU:H    | 2.04                     | 0.69              |
| 1:A:304:ALA:HB2  | 1:A:368:ASN:HA   | 1.74                     | 0.69              |
| 1:A:337:LYS:HG3  | 1:A:338:SER:N    | 2.07                     | 0.69              |
| 1:A:507:LYS:HG2  | 1:A:508:GLY:N    | 2.06                     | 0.69              |
| 1:A:527:SER:OG   | 1:A:543:GLU:HG2  | 1.93                     | 0.69              |
| 1:A:314:ILE:HA   | 1:A:335:ILE:CD1  | 2.22                     | 0.69              |
| 1:A:24:LYS:CD    | 1:A:32:LEU:HD11  | 2.20                     | 0.69              |
| 1:A:452:THR:CB   | 1:A:459:THR:HG23 | 2.22                     | 0.69              |
| 1:A:336:VAL:O    | 1:A:340:LYS:HG2  | 1.93                     | 0.69              |
| 1:A:342:VAL:HG23 | 1:A:493:ARG:NH1  | 2.08                     | 0.69              |
| 1:A:371:VAL:CG2  | 1:A:409:TYR:HB2  | 2.23                     | 0.69              |
| 1:A:156:TYR:O    | 1:A:158:TYR:N    | 2.27                     | 0.68              |
| 1:A:312:HIS:N    | 1:A:312:HIS:ND1  | 2.36                     | 0.68              |
| 1:A:542:ILE:HG22 | 1:A:556:TYR:CD2  | 2.29                     | 0.68              |
| 1:A:503:TRP:HZ3  | 1:A:505:ILE:HG12 | 1.58                     | 0.68              |
| 1:A:113:THR:HG22 | 1:A:116:GLY:N    | 2.02                     | 0.68              |
| 1:A:105:TYR:HD1  | 1:A:107:ILE:HD11 | 1.58                     | 0.68              |
| 1:A:148:ARG:NH1  | 1:A:148:ARG:HB2  | 2.09                     | 0.68              |
| 1:A:127:TYR:HE1  | 1:A:474:PHE:HE2  | 1.41                     | 0.68              |
| 1:A:287:ASN:HB3  | 1:A:343:PHE:CD1  | 2.29                     | 0.68              |
| 1:A:99:LYS:O     | 1:A:102:LEU:HB2  | 1.94                     | 0.68              |
| 1:A:273:VAL:CG2  | 1:A:280:VAL:HG13 | 2.17                     | 0.68              |
| 1:A:118:PHE:HB3  | 1:A:173:LEU:HB2  | 1.76                     | 0.67              |
| 1:A:419:TYR:OH   | 1:A:421:GLU:HG2  | 1.93                     | 0.67              |
| 1:A:341:ASP:O    | 1:A:343:PHE:N    | 2.28                     | 0.67              |
| 1:A:200:MET:HE2  | 1:A:200:MET:HA   | 1.76                     | 0.67              |
| 1:A:105:TYR:HD1  | 1:A:107:ILE:CD1  | 2.07                     | 0.67              |
| 1:A:424:PRO:O    | 1:A:463:SER:HA   | 1.95                     | 0.67              |
| 1:A:27:VAL:HG12  | 1:A:30:LYS:N     | 2.08                     | 0.67              |
| 1:A:53:ARG:HG2   | 1:A:53:ARG:NH1   | 2.10                     | 0.67              |
| 1:A:155:VAL:HG23 | 1:A:194:GLY:CA   | 2.24                     | 0.67              |
| 1:A:307:VAL:HG23 | 1:A:369:PHE:HB3  | 1.76                     | 0.67              |
| 1:A:345:TYR:HA   | 1:A:348:LYS:CD   | 2.25                     | 0.67              |
| 1:A:269:ILE:HG22 | 1:A:270:ALA:N    | 2.09                     | 0.67              |
| 1:A:225:GLU:O    | 1:A:227:ASP:N    | 2.27                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:6:ILE:CA     | 1:A:11:VAL:HG23  | 2.24                     | 0.66              |
| 1:A:103:ILE:N    | 1:A:134:THR:OG1  | 2.28                     | 0.66              |
| 1:A:531:LEU:HB3  | 1:A:555:LEU:HD13 | 1.76                     | 0.66              |
| 1:A:24:LYS:HB2   | 1:A:59:VAL:HG13  | 1.78                     | 0.66              |
| 1:A:384:LYS:O    | 1:A:386:GLU:N    | 2.29                     | 0.66              |
| 1:A:387:ARG:NH1  | 2:A:577:HOH:O    | 2.28                     | 0.66              |
| 1:A:84:ILE:N     | 1:A:84:ILE:HD12  | 2.11                     | 0.66              |
| 1:A:539:PRO:O    | 1:A:541:HIS:N    | 2.29                     | 0.66              |
| 1:A:30:LYS:HZ2   | 1:A:52:VAL:HG21  | 1.59                     | 0.66              |
| 1:A:124:LYS:HG2  | 1:A:127:TYR:HD2  | 1.61                     | 0.66              |
| 1:A:389:ILE:HD13 | 1:A:397:TYR:HE2  | 1.61                     | 0.66              |
| 1:A:12:ILE:HD12  | 1:A:14:THR:N     | 2.10                     | 0.66              |
| 1:A:78:VAL:HG22  | 1:A:156:TYR:HE1  | 1.59                     | 0.66              |
| 1:A:112:PHE:HD2  | 1:A:121:VAL:HG12 | 1.61                     | 0.66              |
| 1:A:163:SER:O    | 1:A:165:GLY:N    | 2.29                     | 0.66              |
| 1:A:265:ILE:O    | 1:A:268:GLU:HB2  | 1.95                     | 0.66              |
| 1:A:364:LEU:HD23 | 1:A:364:LEU:N    | 2.09                     | 0.66              |
| 1:A:254:VAL:O    | 1:A:256:ALA:N    | 2.29                     | 0.66              |
| 1:A:399:ILE:HG22 | 1:A:400:ALA:N    | 2.10                     | 0.66              |
| 1:A:314:ILE:HG22 | 1:A:315:HIS:N    | 2.09                     | 0.66              |
| 1:A:389:ILE:HG23 | 1:A:397:TYR:CD2  | 2.31                     | 0.66              |
| 1:A:437:ILE:HG23 | 1:A:455:GLN:CD   | 2.20                     | 0.66              |
| 1:A:4:TYR:CE2    | 1:A:72:ARG:HG3   | 2.31                     | 0.65              |
| 1:A:45:ILE:HG22  | 1:A:46:THR:N     | 2.11                     | 0.65              |
| 1:A:68:ASP:O     | 1:A:71:SER:N     | 2.29                     | 0.65              |
| 1:A:271:ASP:O    | 1:A:275:LYS:HB2  | 1.95                     | 0.65              |
| 1:A:328:ASP:HB3  | 1:A:345:TYR:OH   | 1.95                     | 0.65              |
| 1:A:233:ILE:HG22 | 1:A:234:LEU:N    | 2.10                     | 0.65              |
| 1:A:287:ASN:ND2  | 1:A:345:TYR:O    | 2.30                     | 0.65              |
| 1:A:114:PRO:HD2  | 1:A:115:GLU:OE2  | 1.95                     | 0.65              |
| 1:A:437:ILE:HG23 | 1:A:455:GLN:CG   | 2.25                     | 0.65              |
| 1:A:280:VAL:O    | 1:A:303:ASP:HB2  | 1.96                     | 0.65              |
| 1:A:321:GLU:O    | 1:A:322:ARG:NE   | 2.30                     | 0.65              |
| 1:A:367:CYS:SG   | 1:A:410:ILE:HD11 | 2.35                     | 0.65              |
| 1:A:476:PHE:CE1  | 1:A:532:LEU:HD11 | 2.20                     | 0.65              |
| 1:A:384:LYS:HA   | 1:A:426:TYR:CE1  | 2.31                     | 0.65              |
| 1:A:498:VAL:HG12 | 1:A:499:ASN:N    | 2.10                     | 0.65              |
| 1:A:95:THR:HG23  | 1:A:97:LEU:HB2   | 1.77                     | 0.65              |
| 1:A:319:THR:OG1  | 1:A:321:GLU:HB2  | 1.96                     | 0.65              |
| 1:A:338:SER:HB2  | 1:A:344:VAL:HG23 | 1.78                     | 0.65              |
| 1:A:287:ASN:N    | 1:A:357:HIS:HE1  | 1.94                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:27:VAL:CG1   | 1:A:30:LYS:HB2   | 2.28                     | 0.64              |
| 1:A:245:ASN:ND2  | 1:A:245:ASN:O    | 2.29                     | 0.64              |
| 1:A:418:GLU:OE2  | 1:A:418:GLU:N    | 2.29                     | 0.64              |
| 1:A:24:LYS:HB2   | 1:A:59:VAL:HG12  | 1.79                     | 0.64              |
| 1:A:222:ASP:OD2  | 1:A:260:THR:HG23 | 1.96                     | 0.64              |
| 1:A:328:ASP:OD2  | 1:A:352:PHE:HB3  | 1.97                     | 0.64              |
| 1:A:404:TYR:CZ   | 1:A:405:LEU:HD11 | 2.32                     | 0.64              |
| 1:A:385:GLY:HA3  | 1:A:425:PHE:O    | 1.97                     | 0.64              |
| 1:A:466:SER:O    | 1:A:468:LYS:N    | 2.29                     | 0.64              |
| 1:A:113:THR:HB   | 2:A:575:HOH:O    | 1.97                     | 0.64              |
| 1:A:138:ILE:HD12 | 1:A:138:ILE:N    | 2.12                     | 0.64              |
| 1:A:333:ASP:O    | 1:A:336:VAL:HG13 | 1.97                     | 0.64              |
| 1:A:461:ASN:HA   | 1:A:464:LYS:CG   | 2.28                     | 0.64              |
| 1:A:28:LEU:CD1   | 1:A:56:TYR:HA    | 2.28                     | 0.64              |
| 1:A:127:TYR:HE1  | 1:A:474:PHE:CE2  | 2.15                     | 0.64              |
| 1:A:131:LEU:HD21 | 1:A:418:GLU:CG   | 2.24                     | 0.64              |
| 1:A:19:TYR:CD1   | 1:A:204:GLY:HA2  | 2.32                     | 0.63              |
| 1:A:122:ILE:O    | 1:A:125:LEU:HD13 | 1.98                     | 0.63              |
| 1:A:254:VAL:O    | 1:A:257:ILE:N    | 2.31                     | 0.63              |
| 1:A:318:LEU:N    | 1:A:318:LEU:HD23 | 2.13                     | 0.63              |
| 1:A:42:TYR:OH    | 1:A:228:GLU:HG3  | 1.97                     | 0.63              |
| 1:A:135:ALA:C    | 1:A:136:ILE:HD13 | 2.22                     | 0.63              |
| 1:A:127:TYR:CE1  | 1:A:474:PHE:HE2  | 2.16                     | 0.63              |
| 1:A:161:GLN:HG3  | 1:A:162:ASN:H    | 1.62                     | 0.63              |
| 1:A:200:MET:HE2  | 1:A:200:MET:CA   | 2.28                     | 0.63              |
| 1:A:354:ARG:HB3  | 1:A:354:ARG:CZ   | 2.27                     | 0.63              |
| 1:A:312:HIS:CD2  | 1:A:325:TYR:HD2  | 2.15                     | 0.63              |
| 1:A:420:GLY:N    | 1:A:473:ILE:HG21 | 2.13                     | 0.63              |
| 1:A:17:ALA:O     | 1:A:18:PRO:C     | 2.41                     | 0.63              |
| 1:A:203:LEU:HD23 | 1:A:203:LEU:N    | 2.13                     | 0.63              |
| 1:A:56:TYR:HE1   | 1:A:68:ASP:HB2   | 1.62                     | 0.62              |
| 1:A:145:PRO:HG2  | 1:A:431:PHE:HE1  | 1.64                     | 0.62              |
| 1:A:361:VAL:HG21 | 1:A:369:PHE:HE2  | 1.62                     | 0.62              |
| 1:A:139:MET:HE1  | 1:A:376:HIS:CG   | 2.34                     | 0.62              |
| 1:A:289:PRO:C    | 1:A:293:ASN:HD22 | 2.05                     | 0.62              |
| 1:A:51:LYS:O     | 1:A:53:ARG:NH2   | 2.30                     | 0.62              |
| 1:A:48:ASN:OD1   | 1:A:48:ASN:N     | 2.29                     | 0.62              |
| 1:A:108:HIS:NE2  | 1:A:428:PHE:HZ   | 1.97                     | 0.62              |
| 1:A:287:ASN:ND2  | 1:A:345:TYR:HB2  | 2.14                     | 0.62              |
| 1:A:346:ASP:O    | 1:A:360:PRO:HD3  | 1.98                     | 0.62              |
| 1:A:473:ILE:N    | 1:A:473:ILE:HD13 | 2.15                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:504:LEU:CD2  | 1:A:506:ILE:HG13 | 2.29                     | 0.62              |
| 1:A:396:SER:O    | 1:A:397:TYR:C    | 2.42                     | 0.62              |
| 1:A:387:ARG:NH2  | 1:A:415:MET:O    | 2.28                     | 0.62              |
| 1:A:538:PHE:CD1  | 1:A:554:ALA:HB2  | 2.34                     | 0.62              |
| 1:A:144:PHE:CD2  | 1:A:151:GLY:HA2  | 2.35                     | 0.61              |
| 1:A:269:ILE:O    | 1:A:270:ALA:C    | 2.42                     | 0.61              |
| 1:A:91:PHE:CD2   | 1:A:242:LYS:HB3  | 2.36                     | 0.61              |
| 1:A:136:ILE:HG22 | 1:A:138:ILE:CD1  | 2.30                     | 0.61              |
| 1:A:161:GLN:HG3  | 1:A:162:ASN:N    | 2.15                     | 0.61              |
| 1:A:187:ASP:HB2  | 1:A:250:ARG:HB3  | 1.81                     | 0.61              |
| 1:A:503:TRP:HZ3  | 1:A:505:ILE:CG1  | 2.14                     | 0.61              |
| 1:A:519:LYS:HA   | 1:A:549:PHE:O    | 2.00                     | 0.61              |
| 1:A:176:GLU:O    | 1:A:179:LYS:N    | 2.34                     | 0.61              |
| 1:A:461:ASN:CA   | 1:A:464:LYS:HG3  | 2.30                     | 0.61              |
| 1:A:167:PRO:O    | 1:A:171:ARG:N    | 2.29                     | 0.61              |
| 1:A:342:VAL:HG11 | 1:A:369:PHE:CD2  | 2.34                     | 0.61              |
| 1:A:269:ILE:O    | 1:A:272:VAL:HG23 | 2.01                     | 0.61              |
| 1:A:331:ASN:OD1  | 1:A:332:LEU:N    | 2.33                     | 0.61              |
| 1:A:50:VAL:HG22  | 1:A:52:VAL:HG21  | 1.82                     | 0.61              |
| 1:A:437:ILE:HG23 | 1:A:455:GLN:NE2  | 2.16                     | 0.61              |
| 1:A:55:ARG:HB3   | 1:A:81:PRO:CB    | 2.24                     | 0.61              |
| 1:A:207:PHE:HB3  | 1:A:218:THR:O    | 1.99                     | 0.61              |
| 1:A:532:LEU:HD12 | 1:A:532:LEU:C    | 2.25                     | 0.61              |
| 1:A:136:ILE:HG22 | 1:A:138:ILE:HD12 | 1.82                     | 0.61              |
| 1:A:58:TYR:N     | 1:A:66:ILE:O     | 2.32                     | 0.60              |
| 1:A:23:VAL:HG13  | 1:A:60:LEU:CA    | 2.27                     | 0.60              |
| 1:A:217:LEU:HD12 | 1:A:217:LEU:N    | 2.16                     | 0.60              |
| 1:A:26:LYS:NZ    | 1:A:65:GLU:OE1   | 2.34                     | 0.60              |
| 1:A:406:LEU:CD2  | 1:A:489:ILE:HD12 | 2.31                     | 0.60              |
| 1:A:45:ILE:HG22  | 1:A:46:THR:H     | 1.65                     | 0.60              |
| 1:A:47:LEU:HD12  | 1:A:49:ASN:OD1   | 2.00                     | 0.60              |
| 1:A:148:ARG:HD2  | 1:A:460:PHE:CD2  | 2.35                     | 0.60              |
| 1:A:466:SER:C    | 1:A:468:LYS:H    | 2.09                     | 0.60              |
| 1:A:50:VAL:O     | 1:A:51:LYS:HD3   | 2.01                     | 0.60              |
| 1:A:264:HIS:HD2  | 1:A:265:ILE:HG22 | 1.65                     | 0.60              |
| 1:A:264:HIS:CG   | 1:A:300:TYR:HE2  | 2.19                     | 0.60              |
| 1:A:345:TYR:HA   | 1:A:348:LYS:HD3  | 1.83                     | 0.60              |
| 1:A:353:ARG:NE   | 1:A:357:HIS:HD2  | 1.98                     | 0.60              |
| 1:A:438:GLN:O    | 1:A:439:GLY:C    | 2.44                     | 0.60              |
| 1:A:95:THR:HG23  | 1:A:97:LEU:N     | 2.17                     | 0.60              |
| 1:A:499:ASN:HA   | 1:A:504:LEU:HA   | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:246:VAL:O    | 1:A:278:ARG:NH1  | 2.34                     | 0.60              |
| 1:A:119:GLU:N    | 1:A:122:ILE:HD12 | 2.17                     | 0.60              |
| 1:A:304:ALA:HB1  | 1:A:368:ASN:C    | 2.27                     | 0.60              |
| 1:A:179:LYS:HB2  | 1:A:179:LYS:HZ3  | 1.65                     | 0.60              |
| 1:A:202:LYS:C    | 1:A:203:LEU:HD23 | 2.27                     | 0.60              |
| 1:A:396:SER:O    | 1:A:398:LYS:N    | 2.35                     | 0.60              |
| 1:A:286:LEU:H    | 1:A:286:LEU:HD13 | 1.67                     | 0.59              |
| 1:A:382:ARG:HH11 | 1:A:382:ARG:HB3  | 1.67                     | 0.59              |
| 1:A:395:GLU:OE1  | 1:A:535:ASN:ND2  | 2.35                     | 0.59              |
| 1:A:530:LEU:N    | 1:A:540:GLN:O    | 2.33                     | 0.59              |
| 1:A:144:PHE:CE1  | 1:A:149:ASP:HB2  | 2.37                     | 0.59              |
| 1:A:280:VAL:HG23 | 1:A:303:ASP:H    | 1.66                     | 0.59              |
| 1:A:337:LYS:CG   | 1:A:344:VAL:HG22 | 2.32                     | 0.59              |
| 1:A:476:PHE:HA   | 1:A:479:ILE:CD1  | 2.24                     | 0.59              |
| 1:A:16:TRP:HA    | 1:A:16:TRP:HE3   | 1.67                     | 0.59              |
| 1:A:293:ASN:OD1  | 1:A:294:PRO:HD2  | 2.03                     | 0.59              |
| 1:A:323:GLN:O    | 1:A:324:GLY:C    | 2.44                     | 0.59              |
| 1:A:12:ILE:HD12  | 1:A:13:PHE:N     | 2.17                     | 0.59              |
| 1:A:280:VAL:N    | 1:A:303:ASP:OD2  | 2.28                     | 0.59              |
| 1:A:231:LYS:O    | 1:A:235:GLU:HG3  | 2.03                     | 0.59              |
| 1:A:394:ARG:O    | 1:A:398:LYS:HG3  | 2.02                     | 0.59              |
| 1:A:399:ILE:O    | 1:A:402:ALA:HB3  | 2.03                     | 0.59              |
| 1:A:421:GLU:OE2  | 1:A:422:GLU:N    | 2.34                     | 0.59              |
| 1:A:105:TYR:CD1  | 1:A:107:ILE:HD11 | 2.38                     | 0.59              |
| 1:A:112:PHE:CD2  | 1:A:121:VAL:HG12 | 2.37                     | 0.58              |
| 1:A:135:ALA:HB1  | 1:A:183:GLY:O    | 2.03                     | 0.58              |
| 1:A:388:ILE:HG12 | 1:A:388:ILE:O    | 2.03                     | 0.58              |
| 1:A:441:ARG:NH1  | 1:A:453:ASP:OD1  | 2.29                     | 0.58              |
| 1:A:6:ILE:HG13   | 1:A:11:VAL:HG23  | 1.85                     | 0.58              |
| 1:A:418:GLU:O    | 1:A:473:ILE:HG22 | 2.03                     | 0.58              |
| 1:A:16:TRP:CZ3   | 1:A:18:PRO:HD3   | 2.37                     | 0.58              |
| 1:A:32:LEU:HD21  | 1:A:59:VAL:CG1   | 2.33                     | 0.58              |
| 1:A:315:HIS:NE2  | 1:A:321:GLU:OE1  | 2.27                     | 0.58              |
| 1:A:69:PRO:CG    | 1:A:200:MET:HE1  | 2.32                     | 0.58              |
| 1:A:187:ASP:CG   | 1:A:250:ARG:HH11 | 2.09                     | 0.58              |
| 1:A:555:LEU:C    | 1:A:555:LEU:HD22 | 2.28                     | 0.58              |
| 1:A:35:MET:HB3   | 1:A:44:THR:H     | 1.67                     | 0.58              |
| 1:A:77:GLY:C     | 1:A:79:HIS:H     | 2.11                     | 0.58              |
| 1:A:281:ILE:HA   | 1:A:304:ALA:O    | 2.04                     | 0.58              |
| 1:A:108:HIS:O    | 1:A:110:GLY:N    | 2.36                     | 0.58              |
| 1:A:389:ILE:CD1  | 1:A:397:TYR:HE2  | 2.17                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:23:VAL:O     | 1:A:35:MET:HG2   | 2.04                     | 0.58              |
| 1:A:118:PHE:C    | 1:A:122:ILE:HD12 | 2.28                     | 0.58              |
| 1:A:452:THR:HB   | 1:A:459:THR:CG2  | 2.32                     | 0.58              |
| 1:A:543:GLU:C    | 1:A:547:TYR:HH   | 2.12                     | 0.58              |
| 1:A:2:PHE:HD1    | 1:A:235:GLU:OE2  | 1.87                     | 0.57              |
| 1:A:105:TYR:CZ   | 1:A:415:MET:HA   | 2.39                     | 0.57              |
| 1:A:187:ASP:CB   | 1:A:250:ARG:HD2  | 2.34                     | 0.57              |
| 1:A:448:ASN:OD1  | 1:A:448:ASN:N    | 2.36                     | 0.57              |
| 1:A:122:ILE:HA   | 1:A:125:LEU:CD1  | 2.34                     | 0.57              |
| 1:A:244:TYR:O    | 1:A:245:ASN:C    | 2.46                     | 0.57              |
| 1:A:555:LEU:HD22 | 1:A:556:TYR:N    | 2.20                     | 0.57              |
| 1:A:12:ILE:O     | 1:A:12:ILE:HG13  | 2.04                     | 0.57              |
| 1:A:16:TRP:CD2   | 1:A:18:PRO:HD3   | 2.40                     | 0.57              |
| 1:A:314:ILE:HA   | 1:A:335:ILE:HD13 | 1.84                     | 0.57              |
| 1:A:495:VAL:CG1  | 1:A:497:VAL:HG12 | 2.34                     | 0.57              |
| 1:A:160:VAL:HG21 | 1:A:244:TYR:OH   | 2.04                     | 0.57              |
| 1:A:200:MET:HB3  | 1:A:206:TYR:CD1  | 2.39                     | 0.57              |
| 1:A:264:HIS:HD2  | 1:A:265:ILE:N    | 2.01                     | 0.57              |
| 1:A:304:ALA:HB1  | 1:A:368:ASN:O    | 2.05                     | 0.57              |
| 1:A:150:TRP:CH2  | 1:A:380:GLY:HA3  | 2.39                     | 0.57              |
| 1:A:196:GLU:HG3  | 1:A:436:LEU:CD1  | 2.35                     | 0.57              |
| 1:A:302:ILE:HD13 | 1:A:302:ILE:H    | 1.70                     | 0.57              |
| 1:A:273:VAL:HG21 | 1:A:280:VAL:CG1  | 2.21                     | 0.57              |
| 1:A:104:ILE:CG1  | 1:A:412:MET:HB2  | 2.35                     | 0.57              |
| 1:A:453:ASP:O    | 1:A:456:ASP:HB2  | 2.04                     | 0.57              |
| 1:A:15:LEU:C     | 1:A:15:LEU:HD22  | 2.29                     | 0.57              |
| 1:A:52:VAL:O     | 1:A:54:ASP:N     | 2.36                     | 0.57              |
| 1:A:67:PRO:O     | 1:A:69:PRO:HD3   | 2.05                     | 0.57              |
| 1:A:427:PHE:H    | 1:A:450:GLN:HE22 | 1.53                     | 0.56              |
| 1:A:26:LYS:HB2   | 1:A:32:LEU:HD22  | 1.87                     | 0.56              |
| 1:A:321:GLU:HB3  | 1:A:323:GLN:NE2  | 2.20                     | 0.56              |
| 1:A:60:LEU:HD12  | 1:A:64:SER:H     | 1.71                     | 0.56              |
| 1:A:287:ASN:HD21 | 1:A:345:TYR:HB2  | 1.69                     | 0.56              |
| 1:A:373:ILE:HG12 | 1:A:404:TYR:CE2  | 2.40                     | 0.56              |
| 1:A:155:VAL:HG11 | 1:A:196:GLU:O    | 2.04                     | 0.56              |
| 1:A:387:ARG:HG2  | 2:A:576:HOH:O    | 2.05                     | 0.56              |
| 1:A:461:ASN:O    | 1:A:464:LYS:HG3  | 2.05                     | 0.56              |
| 1:A:337:LYS:CD   | 1:A:344:VAL:HA   | 2.12                     | 0.56              |
| 1:A:408:PRO:HB3  | 1:A:492:ASP:O    | 2.06                     | 0.56              |
| 1:A:469:ILE:HD12 | 1:A:469:ILE:H    | 1.70                     | 0.56              |
| 1:A:46:THR:O     | 1:A:47:LEU:HD22  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:186:LEU:HD11 | 2:A:563:HOH:O    | 2.05                     | 0.56              |
| 1:A:26:LYS:HB2   | 1:A:32:LEU:HD23  | 1.86                     | 0.56              |
| 1:A:15:LEU:HD22  | 1:A:16:TRP:N     | 2.20                     | 0.56              |
| 1:A:62:ASP:OD1   | 1:A:64:SER:HB2   | 2.06                     | 0.56              |
| 1:A:144:PHE:HB2  | 1:A:145:PRO:HD2  | 1.88                     | 0.56              |
| 1:A:416:GLY:O    | 1:A:417:GLU:C    | 2.48                     | 0.56              |
| 1:A:346:ASP:HB2  | 1:A:348:LYS:HZ1  | 1.71                     | 0.56              |
| 1:A:475:SER:O    | 1:A:479:ILE:HG13 | 2.05                     | 0.56              |
| 1:A:118:PHE:O    | 1:A:122:ILE:N    | 2.38                     | 0.56              |
| 1:A:163:SER:C    | 1:A:165:GLY:H    | 2.14                     | 0.56              |
| 1:A:301:ASN:O    | 1:A:302:ILE:O    | 2.23                     | 0.56              |
| 1:A:503:TRP:CZ3  | 1:A:505:ILE:HD13 | 2.41                     | 0.56              |
| 1:A:95:THR:CG2   | 1:A:97:LEU:HB2   | 2.35                     | 0.55              |
| 1:A:310:PHE:O    | 1:A:311:HIS:C    | 2.48                     | 0.55              |
| 1:A:245:ASN:C    | 1:A:245:ASN:HD22 | 2.12                     | 0.55              |
| 1:A:255:HIS:HB3  | 1:A:286:LEU:HD11 | 1.89                     | 0.55              |
| 1:A:437:ILE:CG2  | 1:A:455:GLN:HG3  | 2.35                     | 0.55              |
| 1:A:60:LEU:CD1   | 1:A:64:SER:H     | 2.19                     | 0.55              |
| 1:A:111:THR:HG23 | 1:A:460:PHE:HE1  | 1.71                     | 0.55              |
| 1:A:140:PRO:HD3  | 1:A:187:ASP:OD2  | 2.06                     | 0.55              |
| 1:A:245:ASN:ND2  | 1:A:278:ARG:NH1  | 2.55                     | 0.55              |
| 1:A:286:LEU:O    | 1:A:288:ASP:N    | 2.35                     | 0.55              |
| 1:A:288:ASP:OD2  | 1:A:290:ARG:HD2  | 2.05                     | 0.55              |
| 1:A:353:ARG:C    | 1:A:354:ARG:HG2  | 2.29                     | 0.55              |
| 1:A:498:VAL:O    | 1:A:504:LEU:HA   | 2.07                     | 0.55              |
| 1:A:9:ASN:HA     | 1:A:51:LYS:HE2   | 1.89                     | 0.55              |
| 1:A:50:VAL:HA    | 1:A:52:VAL:CG2   | 2.36                     | 0.55              |
| 1:A:244:TYR:O    | 1:A:246:VAL:N    | 2.40                     | 0.55              |
| 1:A:469:ILE:HG22 | 1:A:470:ASP:N    | 2.20                     | 0.55              |
| 1:A:504:LEU:HD21 | 1:A:506:ILE:HD11 | 1.89                     | 0.55              |
| 1:A:155:VAL:HG23 | 1:A:194:GLY:HA3  | 1.89                     | 0.54              |
| 1:A:10:GLU:HB2   | 1:A:47:LEU:O     | 2.06                     | 0.54              |
| 1:A:345:TYR:HA   | 1:A:348:LYS:HD2  | 1.89                     | 0.54              |
| 1:A:547:TYR:HB2  | 1:A:549:PHE:HE1  | 1.67                     | 0.54              |
| 1:A:13:PHE:CD2   | 1:A:25:LEU:HD21  | 2.43                     | 0.54              |
| 1:A:30:LYS:NZ    | 1:A:52:VAL:HG21  | 2.22                     | 0.54              |
| 1:A:35:MET:CB    | 1:A:44:THR:H     | 2.20                     | 0.54              |
| 1:A:166:GLY:O    | 1:A:169:GLY:N    | 2.39                     | 0.54              |
| 1:A:167:PRO:O    | 1:A:171:ARG:HB2  | 2.08                     | 0.54              |
| 1:A:186:LEU:HG   | 1:A:188:VAL:HG13 | 1.88                     | 0.54              |
| 1:A:23:VAL:HG23  | 1:A:43:PHE:CD2   | 2.42                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:100:GLU:O    | 1:A:102:LEU:N    | 2.41                     | 0.54              |
| 1:A:113:THR:HG21 | 1:A:115:GLU:HB2  | 1.89                     | 0.54              |
| 1:A:384:LYS:O    | 1:A:385:GLY:C    | 2.50                     | 0.54              |
| 1:A:331:ASN:O    | 1:A:334:ASP:HB2  | 2.07                     | 0.54              |
| 1:A:516:VAL:HG22 | 1:A:552:GLY:H    | 1.72                     | 0.54              |
| 1:A:254:VAL:CG1  | 1:A:282:ALA:HB1  | 2.36                     | 0.54              |
| 1:A:398:LYS:HB3  | 1:A:476:PHE:CE2  | 2.42                     | 0.54              |
| 1:A:418:GLU:HB3  | 1:A:477:TYR:CD2  | 2.42                     | 0.54              |
| 1:A:487:LEU:HB3  | 1:A:489:ILE:HG13 | 1.90                     | 0.54              |
| 1:A:550:ASP:O    | 1:A:551:LYS:C    | 2.50                     | 0.54              |
| 1:A:278:ARG:C    | 1:A:279:ILE:HD13 | 2.33                     | 0.54              |
| 1:A:25:LEU:HD13  | 1:A:25:LEU:C     | 2.32                     | 0.54              |
| 1:A:440:VAL:HG13 | 1:A:441:ARG:N    | 2.23                     | 0.54              |
| 1:A:131:LEU:HD12 | 1:A:131:LEU:C    | 2.31                     | 0.54              |
| 1:A:170:PHE:HD2  | 1:A:244:TYR:CD2  | 2.26                     | 0.54              |
| 1:A:477:TYR:O    | 1:A:481:ILE:HD12 | 2.07                     | 0.54              |
| 1:A:498:VAL:O    | 1:A:505:ILE:N    | 2.41                     | 0.54              |
| 1:A:32:LEU:HD21  | 1:A:59:VAL:HG12  | 1.89                     | 0.53              |
| 1:A:389:ILE:HA   | 1:A:397:TYR:HD2  | 1.72                     | 0.53              |
| 1:A:124:LYS:HB3  | 1:A:128:LEU:CD2  | 2.38                     | 0.53              |
| 1:A:346:ASP:HB2  | 1:A:348:LYS:NZ   | 2.23                     | 0.53              |
| 1:A:382:ARG:HH11 | 1:A:382:ARG:CB   | 2.21                     | 0.53              |
| 1:A:418:GLU:O    | 1:A:474:PHE:HA   | 2.07                     | 0.53              |
| 1:A:144:PHE:HB2  | 1:A:145:PRO:CD   | 2.39                     | 0.53              |
| 1:A:254:VAL:HG23 | 1:A:255:HIS:N    | 2.24                     | 0.53              |
| 1:A:61:ASP:O     | 1:A:63:ALA:N     | 2.41                     | 0.53              |
| 1:A:103:ILE:HB   | 1:A:133:ILE:HD12 | 1.88                     | 0.53              |
| 1:A:429:SER:OG   | 1:A:455:GLN:HG2  | 2.07                     | 0.53              |
| 1:A:213:THR:HB   | 1:A:214:PRO:HD2  | 1.89                     | 0.53              |
| 1:A:269:ILE:HA   | 1:A:272:VAL:HG23 | 1.91                     | 0.53              |
| 1:A:100:GLU:H    | 1:A:100:GLU:CD   | 2.15                     | 0.53              |
| 1:A:300:TYR:H    | 1:A:300:TYR:HD1  | 1.57                     | 0.53              |
| 1:A:395:GLU:OE2  | 1:A:552:GLY:HA2  | 2.08                     | 0.53              |
| 1:A:431:PHE:N    | 1:A:455:GLN:OE1  | 2.29                     | 0.53              |
| 1:A:16:TRP:CE3   | 1:A:16:TRP:HA    | 2.43                     | 0.53              |
| 1:A:125:LEU:HD23 | 1:A:177:ALA:HA   | 1.91                     | 0.53              |
| 1:A:369:PHE:CD1  | 1:A:369:PHE:N    | 2.76                     | 0.53              |
| 1:A:20:GLN:O     | 1:A:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:A:254:VAL:C    | 1:A:256:ALA:H    | 2.16                     | 0.53              |
| 1:A:321:GLU:HB3  | 1:A:323:GLN:HE22 | 1.74                     | 0.53              |
| 1:A:434:SER:CA   | 1:A:437:ILE:HD12 | 2.34                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:503:TRP:CE3  | 1:A:522:ILE:HD13 | 2.44                     | 0.53              |
| 1:A:530:LEU:HD12 | 1:A:530:LEU:C    | 2.31                     | 0.52              |
| 1:A:530:LEU:CB   | 1:A:540:GLN:HA   | 2.33                     | 0.52              |
| 1:A:148:ARG:CB   | 1:A:148:ARG:HH11 | 2.22                     | 0.52              |
| 1:A:518:SER:O    | 1:A:519:LYS:C    | 2.51                     | 0.52              |
| 1:A:136:ILE:HD13 | 1:A:136:ILE:N    | 2.24                     | 0.52              |
| 1:A:322:ARG:CZ   | 1:A:330:GLY:HA3  | 2.39                     | 0.52              |
| 1:A:337:LYS:HG3  | 1:A:338:SER:H    | 1.72                     | 0.52              |
| 1:A:337:LYS:HG3  | 1:A:344:VAL:HG22 | 1.89                     | 0.52              |
| 1:A:542:ILE:HD11 | 1:A:547:TYR:CZ   | 2.44                     | 0.52              |
| 1:A:87:GLU:O     | 1:A:88:SER:C     | 2.52                     | 0.52              |
| 1:A:270:ALA:O    | 1:A:274:HIS:HD2  | 1.91                     | 0.52              |
| 1:A:536:ASN:C    | 1:A:538:PHE:H    | 2.18                     | 0.52              |
| 1:A:537:SER:O    | 1:A:539:PRO:HD3  | 2.10                     | 0.52              |
| 1:A:264:HIS:CD2  | 1:A:265:ILE:N    | 2.78                     | 0.52              |
| 1:A:25:LEU:HD12  | 1:A:33:TYR:HD2   | 1.74                     | 0.52              |
| 1:A:274:HIS:CD2  | 1:A:274:HIS:H    | 2.28                     | 0.52              |
| 1:A:324:GLY:O    | 1:A:327:THR:HG22 | 2.09                     | 0.52              |
| 1:A:366:GLY:N    | 1:A:491:CYS:O    | 2.35                     | 0.52              |
| 1:A:75:PRO:HG3   | 1:A:83:GLN:OE1   | 2.09                     | 0.52              |
| 1:A:124:LYS:O    | 1:A:125:LEU:C    | 2.52                     | 0.52              |
| 1:A:164:TYR:HD1  | 1:A:164:TYR:N    | 2.08                     | 0.52              |
| 1:A:207:PHE:HE2  | 1:A:219:PHE:CE1  | 2.27                     | 0.52              |
| 1:A:33:TYR:HB2   | 1:A:45:ILE:HD13  | 1.92                     | 0.52              |
| 1:A:191:ASN:O    | 1:A:192:HIS:HB3  | 2.09                     | 0.52              |
| 1:A:257:ILE:O    | 1:A:257:ILE:HG22 | 2.09                     | 0.52              |
| 1:A:300:TYR:N    | 1:A:300:TYR:CD1  | 2.78                     | 0.52              |
| 1:A:111:THR:HG21 | 1:A:463:SER:HB2  | 1.91                     | 0.52              |
| 1:A:113:THR:HG23 | 1:A:115:GLU:CD   | 2.35                     | 0.52              |
| 1:A:530:LEU:N    | 1:A:556:TYR:CD2  | 2.78                     | 0.52              |
| 1:A:50:VAL:HA    | 1:A:52:VAL:HG22  | 1.91                     | 0.51              |
| 1:A:73:TYR:O     | 1:A:75:PRO:HD3   | 2.11                     | 0.51              |
| 1:A:76:GLU:O     | 1:A:77:GLY:O     | 2.28                     | 0.51              |
| 1:A:13:PHE:CE2   | 1:A:25:LEU:HD21  | 2.45                     | 0.51              |
| 1:A:173:LEU:HD12 | 1:A:173:LEU:C    | 2.35                     | 0.51              |
| 1:A:193:VAL:HG13 | 1:A:194:GLY:N    | 2.25                     | 0.51              |
| 1:A:240:TRP:HA   | 1:A:240:TRP:CE3  | 2.45                     | 0.51              |
| 1:A:148:ARG:HB2  | 1:A:148:ARG:HH11 | 1.75                     | 0.51              |
| 1:A:311:HIS:CD2  | 1:A:312:HIS:N    | 2.78                     | 0.51              |
| 1:A:316:ALA:O    | 1:A:322:ARG:NH2  | 2.43                     | 0.51              |
| 1:A:511:TYR:CD1  | 1:A:512:PHE:N    | 2.79                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:234:LEU:CD2  | 1:A:272:VAL:HG21 | 2.40                     | 0.51              |
| 1:A:504:LEU:C    | 1:A:504:LEU:HD23 | 2.36                     | 0.51              |
| 1:A:6:ILE:HG13   | 1:A:11:VAL:HG21  | 1.91                     | 0.51              |
| 1:A:108:HIS:HE1  | 1:A:164:TYR:OH   | 1.93                     | 0.51              |
| 1:A:68:ASP:O     | 1:A:71:SER:HB2   | 2.10                     | 0.51              |
| 1:A:114:PRO:HD2  | 1:A:123:ARG:HH21 | 1.76                     | 0.51              |
| 1:A:345:TYR:CD1  | 1:A:345:TYR:N    | 2.79                     | 0.51              |
| 1:A:373:ILE:C    | 1:A:374:GLN:HG2  | 2.36                     | 0.51              |
| 1:A:35:MET:HE2   | 1:A:44:THR:CA    | 2.41                     | 0.51              |
| 1:A:186:LEU:O    | 1:A:249:PHE:HA   | 2.11                     | 0.51              |
| 1:A:329:PHE:N    | 1:A:329:PHE:CD1  | 2.77                     | 0.51              |
| 1:A:396:SER:O    | 1:A:399:ILE:N    | 2.43                     | 0.51              |
| 1:A:16:TRP:CE3   | 1:A:42:TYR:CE1   | 2.99                     | 0.51              |
| 1:A:53:ARG:HD2   | 1:A:84:ILE:HG22  | 1.92                     | 0.51              |
| 1:A:102:LEU:O    | 1:A:411:PRO:HD2  | 2.10                     | 0.51              |
| 1:A:269:ILE:CA   | 1:A:272:VAL:HG23 | 2.41                     | 0.51              |
| 1:A:351:ASN:H    | 1:A:351:ASN:HD22 | 1.57                     | 0.51              |
| 1:A:427:PHE:CD2  | 1:A:444:ARG:HG3  | 2.46                     | 0.51              |
| 1:A:108:HIS:HD2  | 1:A:425:PHE:CZ   | 2.28                     | 0.51              |
| 1:A:382:ARG:HH11 | 1:A:382:ARG:CG   | 2.24                     | 0.51              |
| 1:A:32:LEU:HD13  | 1:A:32:LEU:C     | 2.37                     | 0.50              |
| 1:A:319:THR:C    | 1:A:321:GLU:H    | 2.18                     | 0.50              |
| 1:A:409:TYR:N    | 1:A:409:TYR:CD1  | 2.78                     | 0.50              |
| 1:A:125:LEU:HB3  | 1:A:180:LYS:HG3  | 1.93                     | 0.50              |
| 1:A:259:ASP:OD2  | 1:A:265:ILE:N    | 2.40                     | 0.50              |
| 1:A:344:VAL:HG12 | 1:A:345:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:483:MET:CE   | 1:A:531:LEU:HD11 | 2.27                     | 0.50              |
| 1:A:528:GLY:O    | 1:A:542:ILE:HG22 | 2.11                     | 0.50              |
| 1:A:4:TYR:CE1    | 1:A:72:ARG:NH1   | 2.80                     | 0.50              |
| 1:A:99:LYS:HZ3   | 1:A:99:LYS:N     | 2.08                     | 0.50              |
| 1:A:542:ILE:HG22 | 1:A:556:TYR:CE2  | 2.47                     | 0.50              |
| 1:A:92:ASN:C     | 1:A:94:GLU:H     | 2.19                     | 0.50              |
| 1:A:95:THR:HG23  | 1:A:97:LEU:CB    | 2.42                     | 0.50              |
| 1:A:503:TRP:CE3  | 1:A:504:LEU:N    | 2.79                     | 0.50              |
| 1:A:168:GLU:O    | 1:A:171:ARG:HB3  | 2.12                     | 0.50              |
| 1:A:373:ILE:CG2  | 1:A:404:TYR:HD2  | 2.23                     | 0.50              |
| 1:A:92:ASN:O     | 1:A:278:ARG:NH2  | 2.45                     | 0.50              |
| 1:A:101:ASP:OD1  | 1:A:101:ASP:N    | 2.43                     | 0.50              |
| 1:A:355:LYS:HG2  | 1:A:356:THR:N    | 2.26                     | 0.50              |
| 1:A:427:PHE:O    | 1:A:454:PRO:HB3  | 2.11                     | 0.50              |
| 1:A:43:PHE:O     | 1:A:44:THR:OG1   | 2.28                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:98:LYS:HA    | 1:A:99:LYS:NZ    | 2.27                     | 0.50              |
| 1:A:118:PHE:CD2  | 1:A:170:PHE:N    | 2.80                     | 0.50              |
| 1:A:171:ARG:O    | 1:A:175:ASP:OD1  | 2.29                     | 0.50              |
| 1:A:245:ASN:HD22 | 1:A:278:ARG:HH12 | 1.58                     | 0.50              |
| 1:A:289:PRO:O    | 1:A:290:ARG:C    | 2.55                     | 0.50              |
| 1:A:477:TYR:C    | 1:A:481:ILE:HD12 | 2.37                     | 0.50              |
| 1:A:526:TYR:N    | 1:A:526:TYR:CD1  | 2.79                     | 0.50              |
| 1:A:20:GLN:HG2   | 1:A:23:VAL:HG22  | 1.93                     | 0.50              |
| 1:A:108:HIS:O    | 1:A:109:VAL:C    | 2.55                     | 0.50              |
| 1:A:389:ILE:HA   | 1:A:397:TYR:CD2  | 2.47                     | 0.50              |
| 1:A:170:PHE:CD2  | 1:A:244:TYR:CD2  | 3.00                     | 0.50              |
| 1:A:311:HIS:CD2  | 1:A:312:HIS:ND1  | 2.80                     | 0.50              |
| 1:A:371:VAL:HG22 | 1:A:409:TYR:CB   | 2.37                     | 0.50              |
| 1:A:414:PHE:CD1  | 1:A:415:MET:N    | 2.79                     | 0.50              |
| 1:A:269:ILE:HA   | 1:A:272:VAL:CG2  | 2.42                     | 0.49              |
| 1:A:434:SER:O    | 1:A:438:GLN:HB2  | 2.11                     | 0.49              |
| 1:A:4:TYR:HE1    | 1:A:6:ILE:HD12   | 1.77                     | 0.49              |
| 1:A:221:PHE:CD1  | 1:A:221:PHE:N    | 2.79                     | 0.49              |
| 1:A:312:HIS:NE2  | 1:A:325:TYR:CD2  | 2.80                     | 0.49              |
| 1:A:533:SER:OG   | 1:A:535:ASN:O    | 2.30                     | 0.49              |
| 1:A:84:ILE:C     | 1:A:85:ILE:HD12  | 2.37                     | 0.49              |
| 1:A:207:PHE:HA   | 1:A:219:PHE:HA   | 1.95                     | 0.49              |
| 1:A:426:TYR:HB3  | 1:A:459:THR:HG22 | 1.94                     | 0.49              |
| 1:A:250:ARG:HD3  | 1:A:250:ARG:C    | 2.37                     | 0.49              |
| 1:A:24:LYS:HB2   | 1:A:32:LEU:HD21  | 1.94                     | 0.49              |
| 1:A:25:LEU:HD12  | 1:A:33:TYR:CD2   | 2.47                     | 0.49              |
| 1:A:73:TYR:HB3   | 1:A:85:ILE:HD11  | 1.95                     | 0.49              |
| 1:A:83:GLN:HG2   | 1:A:84:ILE:H     | 1.75                     | 0.49              |
| 1:A:506:ILE:HG22 | 1:A:506:ILE:O    | 2.12                     | 0.49              |
| 1:A:113:THR:HG23 | 1:A:115:GLU:H    | 1.77                     | 0.49              |
| 1:A:191:ASN:ND2  | 1:A:252:ASP:O    | 2.46                     | 0.49              |
| 1:A:411:PRO:HG3  | 1:A:484:ARG:CZ   | 2.43                     | 0.49              |
| 1:A:523:GLU:O    | 1:A:524:VAL:C    | 2.55                     | 0.49              |
| 1:A:67:PRO:HG2   | 1:A:156:TYR:OH   | 2.13                     | 0.49              |
| 1:A:213:THR:HB   | 1:A:214:PRO:CD   | 2.43                     | 0.49              |
| 1:A:367:CYS:CB   | 1:A:410:ILE:HD11 | 2.43                     | 0.49              |
| 1:A:164:TYR:N    | 1:A:164:TYR:CD1  | 2.79                     | 0.49              |
| 1:A:474:PHE:HE1  | 1:A:478:LYS:CD   | 2.15                     | 0.49              |
| 1:A:503:TRP:CB   | 1:A:522:ILE:HD11 | 2.43                     | 0.49              |
| 1:A:107:ILE:O    | 1:A:139:MET:HG3  | 2.13                     | 0.49              |
| 1:A:207:PHE:CE2  | 1:A:219:PHE:CE1  | 3.01                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:254:VAL:O    | 1:A:257:ILE:HB   | 2.13                     | 0.49              |
| 1:A:20:GLN:O     | 1:A:43:PHE:HZ    | 1.96                     | 0.48              |
| 1:A:72:ARG:O     | 1:A:159:ALA:HA   | 2.13                     | 0.48              |
| 1:A:161:GLN:CG   | 1:A:162:ASN:N    | 2.76                     | 0.48              |
| 1:A:324:GLY:O    | 1:A:325:TYR:C    | 2.53                     | 0.48              |
| 1:A:51:LYS:H     | 1:A:52:VAL:CG2   | 2.26                     | 0.48              |
| 1:A:74:GLN:OE1   | 1:A:80:GLY:O     | 2.30                     | 0.48              |
| 1:A:257:ILE:HG21 | 1:A:266:LEU:HD21 | 1.94                     | 0.48              |
| 1:A:312:HIS:CD2  | 1:A:325:TYR:CD2  | 2.99                     | 0.48              |
| 1:A:441:ARG:HH11 | 1:A:453:ASP:CG   | 2.19                     | 0.48              |
| 1:A:530:LEU:HD12 | 1:A:532:LEU:H    | 1.77                     | 0.48              |
| 1:A:140:PRO:HD3  | 1:A:187:ASP:CG   | 2.38                     | 0.48              |
| 1:A:117:THR:O    | 1:A:121:VAL:HG13 | 2.14                     | 0.48              |
| 1:A:457:GLU:O    | 1:A:460:PHE:HB3  | 2.14                     | 0.48              |
| 1:A:73:TYR:OH    | 1:A:75:PRO:HA    | 2.13                     | 0.48              |
| 1:A:351:ASN:H    | 1:A:351:ASN:ND2  | 2.11                     | 0.48              |
| 1:A:467:TRP:O    | 1:A:469:ILE:HD12 | 2.14                     | 0.48              |
| 1:A:234:LEU:HD22 | 1:A:272:VAL:HG21 | 1.94                     | 0.48              |
| 1:A:298:VAL:HG12 | 1:A:298:VAL:O    | 2.13                     | 0.48              |
| 1:A:315:HIS:C    | 1:A:315:HIS:CD2  | 2.92                     | 0.48              |
| 1:A:487:LEU:HD12 | 1:A:487:LEU:HA   | 1.67                     | 0.48              |
| 1:A:23:VAL:HG23  | 1:A:43:PHE:CE2   | 2.48                     | 0.48              |
| 1:A:70:ALA:O     | 1:A:71:SER:C     | 2.56                     | 0.48              |
| 1:A:423:ASN:ND2  | 1:A:466:SER:HB3  | 2.28                     | 0.48              |
| 1:A:19:TYR:CE1   | 1:A:204:GLY:HA2  | 2.48                     | 0.48              |
| 1:A:304:ALA:CB   | 1:A:368:ASN:C    | 2.87                     | 0.48              |
| 1:A:409:TYR:O    | 1:A:484:ARG:NH2  | 2.45                     | 0.48              |
| 1:A:71:SER:HB3   | 1:A:159:ALA:HB2  | 1.96                     | 0.47              |
| 1:A:216:GLY:C    | 1:A:217:LEU:HG   | 2.39                     | 0.47              |
| 1:A:306:TRP:CD1  | 1:A:370:VAL:HG22 | 2.49                     | 0.47              |
| 1:A:323:GLN:O    | 1:A:326:TYR:N    | 2.46                     | 0.47              |
| 1:A:325:TYR:CD1  | 1:A:325:TYR:N    | 2.81                     | 0.47              |
| 1:A:539:PRO:O    | 1:A:540:GLN:C    | 2.57                     | 0.47              |
| 1:A:145:PRO:HG2  | 1:A:431:PHE:CD1  | 2.48                     | 0.47              |
| 1:A:155:VAL:HG13 | 1:A:155:VAL:O    | 2.13                     | 0.47              |
| 1:A:185:ILE:HG22 | 1:A:185:ILE:O    | 2.13                     | 0.47              |
| 1:A:254:VAL:HA   | 1:A:257:ILE:HD13 | 1.96                     | 0.47              |
| 1:A:531:LEU:CB   | 1:A:555:LEU:HD13 | 2.43                     | 0.47              |
| 1:A:274:HIS:CD2  | 1:A:274:HIS:N    | 2.80                     | 0.47              |
| 1:A:336:VAL:HG22 | 1:A:337:LYS:N    | 2.28                     | 0.47              |
| 1:A:355:LYS:CG   | 1:A:356:THR:N    | 2.78                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:139:MET:HE2  | 1:A:376:HIS:ND1  | 2.29                     | 0.47              |
| 1:A:511:TYR:HD1  | 1:A:512:PHE:C    | 2.22                     | 0.47              |
| 1:A:542:ILE:HD12 | 1:A:543:GLU:N    | 2.15                     | 0.47              |
| 1:A:105:TYR:CD1  | 1:A:107:ILE:HG13 | 2.49                     | 0.47              |
| 1:A:250:ARG:HD3  | 1:A:250:ARG:O    | 2.14                     | 0.47              |
| 1:A:368:ASN:HB2  | 1:A:369:PHE:CE1  | 2.48                     | 0.47              |
| 1:A:395:GLU:CD   | 1:A:535:ASN:HD21 | 2.22                     | 0.47              |
| 1:A:444:ARG:HH12 | 1:A:450:GLN:HB2  | 1.80                     | 0.47              |
| 1:A:27:VAL:HG11  | 1:A:30:LYS:HD3   | 1.97                     | 0.47              |
| 1:A:92:ASN:O     | 1:A:94:GLU:N     | 2.44                     | 0.47              |
| 1:A:365:ASP:O    | 1:A:369:PHE:HE1  | 1.98                     | 0.47              |
| 1:A:389:ILE:HD11 | 2:A:576:HOH:O    | 2.15                     | 0.47              |
| 1:A:471:GLU:O    | 1:A:475:SER:HB2  | 2.13                     | 0.47              |
| 1:A:28:LEU:HD12  | 1:A:56:TYR:HA    | 1.96                     | 0.47              |
| 1:A:211:TYR:OH   | 1:A:222:ASP:OD2  | 2.28                     | 0.47              |
| 1:A:341:ASP:O    | 1:A:342:VAL:C    | 2.58                     | 0.47              |
| 1:A:359:GLU:O    | 1:A:359:GLU:HG3  | 2.03                     | 0.47              |
| 1:A:542:ILE:CG1  | 1:A:543:GLU:N    | 2.78                     | 0.47              |
| 1:A:542:ILE:CG2  | 1:A:556:TYR:CD2  | 2.97                     | 0.47              |
| 1:A:105:TYR:HD1  | 1:A:107:ILE:CG1  | 2.28                     | 0.47              |
| 1:A:302:ILE:HD13 | 1:A:302:ILE:N    | 2.29                     | 0.47              |
| 1:A:43:PHE:CD1   | 1:A:43:PHE:N     | 2.82                     | 0.47              |
| 1:A:145:PRO:HG3  | 2:A:586:HOH:O    | 2.14                     | 0.47              |
| 1:A:469:ILE:CG2  | 1:A:470:ASP:N    | 2.78                     | 0.47              |
| 1:A:18:PRO:HD2   | 1:A:203:LEU:O    | 2.15                     | 0.46              |
| 1:A:269:ILE:C    | 1:A:272:VAL:HG23 | 2.40                     | 0.46              |
| 1:A:305:GLN:O    | 1:A:369:PHE:HA   | 2.13                     | 0.46              |
| 1:A:444:ARG:HD2  | 1:A:444:ARG:HA   | 1.46                     | 0.46              |
| 1:A:452:THR:HG21 | 1:A:459:THR:HG23 | 1.94                     | 0.46              |
| 1:A:531:LEU:HB3  | 1:A:555:LEU:HD12 | 1.95                     | 0.46              |
| 1:A:56:TYR:CZ    | 1:A:82:SER:HB2   | 2.50                     | 0.46              |
| 1:A:507:LYS:CG   | 1:A:508:GLY:N    | 2.77                     | 0.46              |
| 1:A:51:LYS:O     | 1:A:53:ARG:NE    | 2.48                     | 0.46              |
| 1:A:477:TYR:O    | 1:A:480:LEU:HB2  | 2.14                     | 0.46              |
| 1:A:46:THR:C     | 1:A:47:LEU:HD22  | 2.41                     | 0.46              |
| 1:A:35:MET:HB3   | 1:A:35:MET:HE2   | 1.69                     | 0.46              |
| 1:A:102:LEU:HB3  | 1:A:410:ILE:HG23 | 1.97                     | 0.46              |
| 1:A:217:LEU:HD12 | 1:A:217:LEU:H    | 1.79                     | 0.46              |
| 1:A:119:GLU:HA   | 1:A:122:ILE:CD1  | 2.38                     | 0.46              |
| 1:A:125:LEU:O    | 1:A:128:LEU:HB2  | 2.16                     | 0.46              |
| 1:A:127:TYR:O    | 1:A:130:ASP:HB3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:294:PRO:HA   | 1:A:301:ASN:HD22 | 1.78                     | 0.46              |
| 1:A:350:SER:OG   | 1:A:353:ARG:N    | 2.39                     | 0.46              |
| 1:A:495:VAL:HG13 | 1:A:497:VAL:HG12 | 1.97                     | 0.46              |
| 1:A:35:MET:HE3   | 1:A:44:THR:C     | 2.40                     | 0.46              |
| 1:A:198:ASN:OD1  | 1:A:200:MET:HG2  | 2.15                     | 0.46              |
| 1:A:243:GLU:HB3  | 1:A:244:TYR:CD1  | 2.51                     | 0.46              |
| 1:A:289:PRO:CB   | 1:A:293:ASN:ND2  | 2.79                     | 0.46              |
| 1:A:289:PRO:HB2  | 1:A:293:ASN:ND2  | 2.31                     | 0.46              |
| 1:A:500:GLY:HA3  | 1:A:503:TRP:CD1  | 2.48                     | 0.46              |
| 1:A:542:ILE:HD11 | 1:A:547:TYR:CE1  | 2.51                     | 0.46              |
| 1:A:4:TYR:CE1    | 1:A:6:ILE:CD1    | 2.99                     | 0.46              |
| 1:A:94:GLU:HG2   | 1:A:95:THR:H     | 1.81                     | 0.46              |
| 1:A:170:PHE:O    | 1:A:174:VAL:HG13 | 2.16                     | 0.46              |
| 1:A:253:ALA:HA   | 1:A:255:HIS:CE1  | 2.51                     | 0.46              |
| 1:A:267:GLU:O    | 1:A:271:ASP:OD1  | 2.34                     | 0.46              |
| 1:A:308:ASP:O    | 1:A:312:HIS:ND1  | 2.48                     | 0.46              |
| 1:A:4:TYR:CZ     | 1:A:72:ARG:NH1   | 2.83                     | 0.46              |
| 1:A:11:VAL:HG13  | 1:A:13:PHE:CE1   | 2.51                     | 0.46              |
| 1:A:53:ARG:CD    | 1:A:84:ILE:HG22  | 2.46                     | 0.46              |
| 1:A:207:PHE:CD2  | 1:A:219:PHE:CD1  | 3.04                     | 0.46              |
| 1:A:240:TRP:HB2  | 1:A:249:PHE:HZ   | 1.81                     | 0.46              |
| 1:A:240:TRP:CD1  | 1:A:249:PHE:HE2  | 2.34                     | 0.46              |
| 1:A:332:LEU:HA   | 1:A:335:ILE:HG13 | 1.98                     | 0.46              |
| 1:A:393:ASP:OD1  | 1:A:396:SER:N    | 2.36                     | 0.46              |
| 1:A:473:ILE:HD12 | 1:A:473:ILE:HA   | 1.61                     | 0.46              |
| 1:A:108:HIS:HD2  | 1:A:425:PHE:CE1  | 2.33                     | 0.46              |
| 1:A:176:GLU:O    | 1:A:177:ALA:C    | 2.59                     | 0.46              |
| 1:A:187:ASP:CG   | 1:A:250:ARG:HD2  | 2.41                     | 0.46              |
| 1:A:229:VAL:CG2  | 1:A:230:ARG:N    | 2.79                     | 0.46              |
| 1:A:303:ASP:O    | 1:A:304:ALA:HB2  | 2.15                     | 0.46              |
| 1:A:542:ILE:CD1  | 1:A:547:TYR:CZ   | 2.99                     | 0.46              |
| 1:A:53:ARG:HD3   | 1:A:84:ILE:HB    | 1.98                     | 0.45              |
| 1:A:142:ALA:O    | 1:A:143:GLN:C    | 2.58                     | 0.45              |
| 1:A:193:VAL:CG1  | 1:A:194:GLY:N    | 2.79                     | 0.45              |
| 1:A:498:VAL:CG1  | 1:A:499:ASN:N    | 2.79                     | 0.45              |
| 1:A:507:LYS:HE2  | 1:A:508:GLY:O    | 2.16                     | 0.45              |
| 1:A:440:VAL:CG1  | 1:A:441:ARG:N    | 2.79                     | 0.45              |
| 1:A:507:LYS:HG2  | 1:A:508:GLY:O    | 2.15                     | 0.45              |
| 1:A:11:VAL:CG1   | 1:A:13:PHE:CE1   | 3.00                     | 0.45              |
| 1:A:294:PRO:O    | 1:A:299:GLY:N    | 2.43                     | 0.45              |
| 1:A:503:TRP:CZ3  | 1:A:505:ILE:CD1  | 3.00                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:530:LEU:HB2  | 1:A:556:TYR:CE2  | 2.51                     | 0.45              |
| 1:A:11:VAL:CG1   | 1:A:13:PHE:HE1   | 2.29                     | 0.45              |
| 1:A:14:THR:O     | 1:A:15:LEU:HB2   | 2.15                     | 0.45              |
| 1:A:139:MET:CE   | 1:A:376:HIS:ND1  | 2.80                     | 0.45              |
| 1:A:444:ARG:NH1  | 1:A:450:GLN:CB   | 2.80                     | 0.45              |
| 1:A:16:TRP:CE3   | 1:A:16:TRP:CA    | 3.00                     | 0.45              |
| 1:A:59:VAL:HA    | 1:A:64:SER:O     | 2.17                     | 0.45              |
| 1:A:286:LEU:HD12 | 1:A:286:LEU:H    | 1.80                     | 0.45              |
| 1:A:346:ASP:CB   | 1:A:348:LYS:NZ   | 2.79                     | 0.45              |
| 1:A:376:HIS:O    | 1:A:380:GLY:HA3  | 2.17                     | 0.45              |
| 1:A:487:LEU:CB   | 1:A:489:ILE:HG13 | 2.46                     | 0.45              |
| 1:A:85:ILE:CG2   | 1:A:86:GLN:N     | 2.79                     | 0.45              |
| 1:A:138:ILE:N    | 1:A:138:ILE:CD1  | 2.80                     | 0.45              |
| 1:A:4:TYR:HE1    | 1:A:6:ILE:CD1    | 2.29                     | 0.45              |
| 1:A:45:ILE:CG2   | 1:A:46:THR:N     | 2.80                     | 0.45              |
| 1:A:95:THR:HG23  | 1:A:97:LEU:H     | 1.81                     | 0.45              |
| 1:A:194:GLY:HA2  | 1:A:195:PRO:HD2  | 1.70                     | 0.45              |
| 1:A:289:PRO:O    | 1:A:293:ASN:ND2  | 2.39                     | 0.45              |
| 1:A:293:ASN:CB   | 1:A:294:PRO:HD2  | 2.47                     | 0.45              |
| 1:A:400:ALA:O    | 1:A:401:ALA:C    | 2.60                     | 0.45              |
| 1:A:444:ARG:HD2  | 1:A:448:ASN:OD1  | 2.17                     | 0.45              |
| 1:A:65:GLU:H     | 1:A:65:GLU:HG2   | 1.60                     | 0.45              |
| 1:A:376:HIS:CG   | 1:A:377:ASP:N    | 2.84                     | 0.45              |
| 1:A:404:TYR:CZ   | 1:A:405:LEU:CD1  | 3.00                     | 0.45              |
| 1:A:419:TYR:C    | 1:A:419:TYR:CD1  | 2.95                     | 0.45              |
| 1:A:479:ILE:HG13 | 1:A:479:ILE:H    | 1.51                     | 0.45              |
| 1:A:512:PHE:N    | 1:A:512:PHE:CD1  | 2.85                     | 0.45              |
| 1:A:35:MET:HE2   | 1:A:44:THR:HA    | 1.99                     | 0.44              |
| 1:A:118:PHE:CE2  | 1:A:170:PHE:HB2  | 2.51                     | 0.44              |
| 1:A:118:PHE:HE2  | 1:A:166:GLY:H    | 1.65                     | 0.44              |
| 1:A:221:PHE:O    | 1:A:226:SER:HB2  | 2.17                     | 0.44              |
| 1:A:279:ILE:CG2  | 1:A:280:VAL:N    | 2.80                     | 0.44              |
| 1:A:404:TYR:CE1  | 1:A:405:LEU:CD1  | 3.00                     | 0.44              |
| 1:A:410:ILE:HA   | 1:A:411:PRO:HD3  | 1.56                     | 0.44              |
| 1:A:503:TRP:CG   | 1:A:522:ILE:CD1  | 2.99                     | 0.44              |
| 1:A:504:LEU:HB3  | 1:A:515:TYR:HB2  | 1.99                     | 0.44              |
| 1:A:30:LYS:NZ    | 1:A:52:VAL:CG2   | 2.80                     | 0.44              |
| 1:A:174:VAL:HB   | 1:A:184:VAL:HG11 | 1.98                     | 0.44              |
| 1:A:264:HIS:HB3  | 1:A:300:TYR:CE2  | 2.52                     | 0.44              |
| 1:A:339:TYR:CE1  | 1:A:403:LEU:HD22 | 2.51                     | 0.44              |
| 1:A:437:ILE:CG2  | 1:A:455:GLN:NE2  | 2.79                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:4:TYR:CE1    | 1:A:6:ILE:HD11   | 2.52                     | 0.44              |
| 1:A:145:PRO:CG   | 1:A:431:PHE:HE1  | 2.30                     | 0.44              |
| 1:A:480:LEU:O    | 1:A:481:ILE:C    | 2.61                     | 0.44              |
| 1:A:510:GLU:O    | 1:A:511:TYR:HB3  | 2.17                     | 0.44              |
| 1:A:84:ILE:N     | 1:A:84:ILE:CD1   | 2.79                     | 0.44              |
| 1:A:84:ILE:HG22  | 1:A:85:ILE:N     | 2.33                     | 0.44              |
| 1:A:156:TYR:O    | 1:A:159:ALA:N    | 2.48                     | 0.44              |
| 1:A:294:PRO:HA   | 1:A:301:ASN:HD21 | 1.81                     | 0.44              |
| 1:A:423:ASN:HD21 | 1:A:466:SER:HB3  | 1.82                     | 0.44              |
| 1:A:61:ASP:C     | 1:A:63:ALA:H     | 2.25                     | 0.44              |
| 1:A:176:GLU:O    | 1:A:178:HIS:N    | 2.50                     | 0.44              |
| 1:A:187:ASP:OD1  | 1:A:250:ARG:NH1  | 2.43                     | 0.44              |
| 1:A:474:PHE:C    | 1:A:474:PHE:CD1  | 2.96                     | 0.44              |
| 1:A:503:TRP:CG   | 1:A:522:ILE:HD13 | 2.52                     | 0.44              |
| 1:A:19:TYR:CD1   | 1:A:19:TYR:N     | 2.84                     | 0.44              |
| 1:A:122:ILE:HA   | 1:A:125:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:314:ILE:CA   | 1:A:335:ILE:HD13 | 2.47                     | 0.44              |
| 1:A:13:PHE:CD2   | 1:A:25:LEU:CD2   | 3.00                     | 0.44              |
| 1:A:287:ASN:CB   | 1:A:343:PHE:CD1  | 2.99                     | 0.44              |
| 1:A:304:ALA:CB   | 1:A:368:ASN:O    | 2.66                     | 0.44              |
| 1:A:379:VAL:O    | 1:A:382:ARG:HG3  | 2.16                     | 0.44              |
| 1:A:444:ARG:NH1  | 1:A:450:GLN:HB3  | 2.33                     | 0.44              |
| 1:A:530:LEU:CD1  | 1:A:532:LEU:H    | 2.30                     | 0.44              |
| 1:A:534:SER:OG   | 1:A:553:PHE:N    | 2.30                     | 0.44              |
| 1:A:287:ASN:HB3  | 1:A:343:PHE:CE1  | 2.53                     | 0.44              |
| 1:A:293:ASN:O    | 1:A:301:ASN:HA   | 2.18                     | 0.44              |
| 1:A:307:VAL:HG21 | 1:A:342:VAL:CG1  | 2.48                     | 0.44              |
| 1:A:307:VAL:HG21 | 1:A:369:PHE:HB3  | 1.97                     | 0.44              |
| 1:A:6:ILE:CG1    | 1:A:11:VAL:HG23  | 2.48                     | 0.44              |
| 1:A:97:LEU:HD23  | 1:A:97:LEU:HA    | 1.68                     | 0.44              |
| 1:A:163:SER:C    | 1:A:165:GLY:N    | 2.75                     | 0.44              |
| 1:A:312:HIS:HB3  | 1:A:329:PHE:CE1  | 2.53                     | 0.44              |
| 1:A:450:GLN:HB2  | 1:A:450:GLN:HE21 | 1.58                     | 0.44              |
| 1:A:225:GLU:O    | 1:A:226:SER:C    | 2.60                     | 0.43              |
| 1:A:350:SER:OG   | 1:A:350:SER:O    | 2.36                     | 0.43              |
| 1:A:35:MET:HA    | 1:A:44:THR:O     | 2.18                     | 0.43              |
| 1:A:53:ARG:HD2   | 1:A:84:ILE:C     | 2.43                     | 0.43              |
| 1:A:62:ASP:O     | 1:A:63:ALA:HB3   | 2.18                     | 0.43              |
| 1:A:254:VAL:CG2  | 1:A:255:HIS:N    | 2.80                     | 0.43              |
| 1:A:281:ILE:O    | 1:A:281:ILE:HG22 | 2.11                     | 0.43              |
| 1:A:323:GLN:O    | 1:A:324:GLY:O    | 2.36                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:392:VAL:CG2  | 1:A:397:TYR:H    | 2.31                     | 0.43              |
| 1:A:52:VAL:C     | 1:A:54:ASP:N     | 2.76                     | 0.43              |
| 1:A:144:PHE:CE1  | 1:A:149:ASP:CB   | 3.01                     | 0.43              |
| 1:A:513:SER:OG   | 1:A:515:TYR:HE1  | 2.00                     | 0.43              |
| 1:A:532:LEU:O    | 1:A:555:LEU:N    | 2.50                     | 0.43              |
| 1:A:47:LEU:HD13  | 1:A:47:LEU:HA    | 1.52                     | 0.43              |
| 1:A:112:PHE:O    | 1:A:113:THR:C    | 2.62                     | 0.43              |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:N    | 2.33                     | 0.43              |
| 1:A:124:LYS:HG2  | 1:A:127:TYR:CD2  | 2.48                     | 0.43              |
| 1:A:265:ILE:HD12 | 1:A:268:GLU:CB   | 2.45                     | 0.43              |
| 1:A:175:ASP:OD1  | 1:A:175:ASP:N    | 2.50                     | 0.43              |
| 1:A:199:TYR:O    | 1:A:203:LEU:HG   | 2.18                     | 0.43              |
| 1:A:311:HIS:C    | 1:A:311:HIS:CD2  | 2.97                     | 0.43              |
| 1:A:334:ASP:OD1  | 1:A:334:ASP:N    | 2.45                     | 0.43              |
| 1:A:373:ILE:HD13 | 1:A:404:TYR:CD2  | 2.54                     | 0.43              |
| 1:A:398:LYS:HB3  | 1:A:476:PHE:HE2  | 1.84                     | 0.43              |
| 1:A:427:PHE:CD2  | 1:A:444:ARG:CG   | 3.02                     | 0.43              |
| 1:A:19:TYR:N     | 1:A:19:TYR:HD1   | 2.17                     | 0.43              |
| 1:A:24:LYS:HA    | 1:A:33:TYR:O     | 2.19                     | 0.43              |
| 1:A:51:LYS:HA    | 1:A:51:LYS:HD2   | 1.51                     | 0.43              |
| 1:A:84:ILE:CG2   | 1:A:85:ILE:N     | 2.81                     | 0.43              |
| 1:A:104:ILE:HG13 | 1:A:412:MET:CB   | 2.49                     | 0.43              |
| 1:A:200:MET:HE2  | 1:A:200:MET:N    | 2.33                     | 0.43              |
| 1:A:259:ASP:OD2  | 1:A:264:HIS:HA   | 2.19                     | 0.43              |
| 1:A:437:ILE:CG2  | 1:A:455:GLN:HE21 | 2.32                     | 0.43              |
| 1:A:473:ILE:HG22 | 1:A:474:PHE:N    | 2.33                     | 0.43              |
| 1:A:24:LYS:HD3   | 1:A:34:GLU:HG3   | 1.99                     | 0.43              |
| 1:A:292:VAL:HA   | 1:A:302:ILE:O    | 2.18                     | 0.43              |
| 1:A:427:PHE:HB2  | 1:A:444:ARG:NH2  | 2.34                     | 0.43              |
| 1:A:441:ARG:O    | 1:A:445:LYS:HB3  | 2.19                     | 0.43              |
| 1:A:59:VAL:HG23  | 1:A:64:SER:O     | 2.19                     | 0.43              |
| 1:A:213:THR:CB   | 1:A:214:PRO:CD   | 2.97                     | 0.43              |
| 1:A:83:GLN:O     | 1:A:85:ILE:HD12  | 2.19                     | 0.43              |
| 1:A:293:ASN:O    | 1:A:301:ASN:N    | 2.49                     | 0.43              |
| 1:A:324:GLY:O    | 1:A:326:TYR:N    | 2.52                     | 0.43              |
| 1:A:353:ARG:CZ   | 1:A:357:HIS:CD2  | 3.02                     | 0.43              |
| 1:A:102:LEU:HB3  | 1:A:410:ILE:CG2  | 2.49                     | 0.42              |
| 1:A:71:SER:OG    | 1:A:74:GLN:NE2   | 2.52                     | 0.42              |
| 1:A:92:ASN:N     | 1:A:245:ASN:OD1  | 2.53                     | 0.42              |
| 1:A:19:TYR:CG    | 1:A:204:GLY:HA2  | 2.54                     | 0.42              |
| 1:A:104:ILE:HG13 | 1:A:412:MET:HB2  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:553:PHE:CD1  | 1:A:554:ALA:N    | 2.87                     | 0.42              |
| 1:A:7:ASP:HB2    | 1:A:10:GLU:O     | 2.19                     | 0.42              |
| 1:A:246:VAL:CG1  | 1:A:247:ASP:N    | 2.80                     | 0.42              |
| 1:A:287:ASN:HB2  | 1:A:358:GLY:HA2  | 1.97                     | 0.42              |
| 1:A:289:PRO:O    | 1:A:293:ASN:HB2  | 2.20                     | 0.42              |
| 1:A:346:ASP:CB   | 1:A:348:LYS:HZ1  | 2.31                     | 0.42              |
| 1:A:346:ASP:C    | 1:A:360:PRO:HD3  | 2.44                     | 0.42              |
| 1:A:433:ASP:OD2  | 1:A:436:LEU:N    | 2.52                     | 0.42              |
| 1:A:507:LYS:HG2  | 1:A:508:GLY:H    | 1.82                     | 0.42              |
| 1:A:229:VAL:HG22 | 1:A:230:ARG:N    | 2.34                     | 0.42              |
| 1:A:316:ALA:O    | 1:A:319:THR:O    | 2.38                     | 0.42              |
| 1:A:504:LEU:HD21 | 1:A:506:ILE:CD1  | 2.49                     | 0.42              |
| 1:A:15:LEU:HD23  | 1:A:15:LEU:HA    | 1.88                     | 0.42              |
| 1:A:182:LEU:HD22 | 1:A:182:LEU:HA   | 1.80                     | 0.42              |
| 1:A:253:ALA:O    | 1:A:254:VAL:C    | 2.61                     | 0.42              |
| 1:A:408:PRO:O    | 1:A:491:CYS:N    | 2.47                     | 0.42              |
| 1:A:433:ASP:O    | 1:A:434:SER:C    | 2.62                     | 0.42              |
| 1:A:503:TRP:HZ3  | 1:A:505:ILE:HG23 | 1.76                     | 0.42              |
| 1:A:18:PRO:HG2   | 1:A:204:GLY:HA3  | 2.01                     | 0.42              |
| 1:A:71:SER:OG    | 1:A:82:SER:HB3   | 2.19                     | 0.42              |
| 1:A:171:ARG:HA   | 1:A:171:ARG:HD2  | 1.42                     | 0.42              |
| 1:A:200:MET:HB2  | 1:A:207:PHE:CE1  | 2.54                     | 0.42              |
| 1:A:203:LEU:HB2  | 1:A:206:TYR:CE1  | 2.43                     | 0.42              |
| 1:A:231:LYS:O    | 1:A:232:PHE:C    | 2.62                     | 0.42              |
| 1:A:254:VAL:H    | 1:A:254:VAL:HG13 | 1.47                     | 0.42              |
| 1:A:317:TYR:CB   | 1:A:335:ILE:HD11 | 2.50                     | 0.42              |
| 1:A:350:SER:OG   | 1:A:353:ARG:HG3  | 2.19                     | 0.42              |
| 1:A:187:ASP:HA   | 1:A:250:ARG:O    | 2.20                     | 0.42              |
| 1:A:293:ASN:HA   | 1:A:294:PRO:HD3  | 1.75                     | 0.42              |
| 1:A:339:TYR:HE1  | 1:A:403:LEU:HD22 | 1.83                     | 0.42              |
| 1:A:50:VAL:HG13  | 1:A:51:LYS:N     | 2.35                     | 0.42              |
| 1:A:144:PHE:CD1  | 1:A:149:ASP:HB2  | 2.55                     | 0.42              |
| 1:A:240:TRP:HA   | 1:A:240:TRP:HE3  | 1.84                     | 0.42              |
| 1:A:460:PHE:CD1  | 1:A:460:PHE:C    | 2.97                     | 0.42              |
| 1:A:33:TYR:HB2   | 1:A:45:ILE:CD1   | 2.49                     | 0.42              |
| 1:A:69:PRO:HB3   | 1:A:200:MET:CE   | 2.31                     | 0.42              |
| 1:A:127:TYR:CD1  | 1:A:127:TYR:C    | 2.98                     | 0.42              |
| 1:A:442:GLU:O    | 1:A:446:LYS:N    | 2.44                     | 0.42              |
| 1:A:497:VAL:HB   | 1:A:506:ILE:HG12 | 2.02                     | 0.42              |
| 1:A:143:GLN:OE1  | 1:A:161:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:336:VAL:HG22 | 1:A:340:LYS:HZ2  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:371:VAL:C    | 1:A:372:TYR:CD2  | 2.98                     | 0.41              |
| 1:A:544:GLU:OE2  | 1:A:544:GLU:N    | 2.37                     | 0.41              |
| 1:A:140:PRO:CG   | 1:A:152:TYR:CE1  | 2.98                     | 0.41              |
| 1:A:243:GLU:C    | 1:A:244:TYR:CD1  | 2.99                     | 0.41              |
| 1:A:347:GLY:HA2  | 1:A:357:HIS:O    | 2.20                     | 0.41              |
| 1:A:538:PHE:CG   | 1:A:554:ALA:HB2  | 2.55                     | 0.41              |
| 1:A:7:ASP:HB3    | 1:A:8:GLY:H      | 1.31                     | 0.41              |
| 1:A:234:LEU:HD22 | 1:A:272:VAL:CG2  | 2.51                     | 0.41              |
| 1:A:317:TYR:C    | 1:A:318:LEU:HD23 | 2.45                     | 0.41              |
| 1:A:404:TYR:CD1  | 1:A:404:TYR:C    | 2.99                     | 0.41              |
| 1:A:503:TRP:HE3  | 1:A:504:LEU:N    | 2.18                     | 0.41              |
| 1:A:61:ASP:C     | 1:A:63:ALA:N     | 2.78                     | 0.41              |
| 1:A:124:LYS:O    | 1:A:127:TYR:HB3  | 2.20                     | 0.41              |
| 1:A:288:ASP:HA   | 1:A:289:PRO:HD2  | 1.27                     | 0.41              |
| 1:A:307:VAL:C    | 1:A:309:ASP:N    | 2.79                     | 0.41              |
| 1:A:476:PHE:HA   | 1:A:476:PHE:HD1  | 1.68                     | 0.41              |
| 1:A:12:ILE:C     | 1:A:13:PHE:CD1   | 2.99                     | 0.41              |
| 1:A:228:GLU:O    | 1:A:231:LYS:N    | 2.49                     | 0.41              |
| 1:A:396:SER:C    | 1:A:398:LYS:N    | 2.79                     | 0.41              |
| 1:A:538:PHE:CD1  | 1:A:554:ALA:CB   | 3.03                     | 0.41              |
| 1:A:91:PHE:CD1   | 1:A:91:PHE:C     | 2.99                     | 0.41              |
| 1:A:105:TYR:HD1  | 1:A:107:ILE:HG13 | 1.86                     | 0.41              |
| 1:A:66:ILE:HA    | 1:A:67:PRO:HD3   | 1.84                     | 0.41              |
| 1:A:95:THR:HG23  | 1:A:97:LEU:CA    | 2.51                     | 0.41              |
| 1:A:251:LEU:HD23 | 2:A:582:HOH:O    | 2.20                     | 0.41              |
| 1:A:350:SER:C    | 1:A:352:PHE:N    | 2.78                     | 0.41              |
| 1:A:389:ILE:CD1  | 1:A:397:TYR:CE2  | 3.00                     | 0.41              |
| 1:A:92:ASN:C     | 1:A:94:GLU:N     | 2.79                     | 0.41              |
| 1:A:107:ILE:CG2  | 1:A:108:HIS:N    | 2.83                     | 0.41              |
| 1:A:274:HIS:HE1  | 1:A:303:ASP:OD1  | 2.03                     | 0.41              |
| 1:A:297:LYS:O    | 1:A:298:VAL:C    | 2.63                     | 0.41              |
| 1:A:403:LEU:HD23 | 1:A:403:LEU:HA   | 1.58                     | 0.41              |
| 1:A:413:ILE:HG23 | 1:A:417:GLU:OE2  | 2.21                     | 0.41              |
| 1:A:419:TYR:O    | 1:A:419:TYR:HD1  | 2.03                     | 0.41              |
| 1:A:436:LEU:O    | 1:A:438:GLN:N    | 2.54                     | 0.41              |
| 1:A:439:GLY:O    | 1:A:440:VAL:C    | 2.64                     | 0.41              |
| 1:A:4:TYR:CD1    | 1:A:4:TYR:C      | 2.98                     | 0.41              |
| 1:A:91:PHE:CE2   | 1:A:242:LYS:HD2  | 2.55                     | 0.41              |
| 1:A:416:GLY:C    | 1:A:421:GLU:HB2  | 2.46                     | 0.41              |
| 1:A:35:MET:HA    | 1:A:45:ILE:HG12  | 2.03                     | 0.40              |
| 1:A:108:HIS:ND1  | 1:A:108:HIS:C    | 2.79                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:273:VAL:C    | 1:A:275:LYS:N    | 2.78                     | 0.40              |
| 1:A:483:MET:HG3  | 1:A:531:LEU:HD12 | 2.02                     | 0.40              |
| 1:A:449:GLY:O    | 1:A:450:GLN:C    | 2.60                     | 0.40              |
| 1:A:50:VAL:CG1   | 1:A:51:LYS:N     | 2.80                     | 0.40              |
| 1:A:83:GLN:CG    | 1:A:84:ILE:N     | 2.79                     | 0.40              |
| 1:A:503:TRP:CZ3  | 1:A:505:ILE:HG12 | 2.46                     | 0.40              |
| 1:A:504:LEU:HD21 | 1:A:506:ILE:CG1  | 2.51                     | 0.40              |
| 1:A:162:ASN:HB3  | 1:A:163:SER:H    | 1.26                     | 0.40              |
| 1:A:511:TYR:CD1  | 1:A:512:PHE:C    | 2.99                     | 0.40              |
| 1:A:542:ILE:HG13 | 1:A:543:GLU:N    | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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     | 463/494 (94%) | 256 (55%) | 207 (45%) | <b>0</b> <b>0</b> |

All (207) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | THR  |
| 1   | A     | 2   | PHE  |
| 1   | A     | 9   | ASN  |
| 1   | A     | 10  | GLU  |
| 1   | A     | 11  | VAL  |
| 1   | A     | 12  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | THR  |
| 1   | A     | 15  | LEU  |
| 1   | A     | 16  | TRP  |
| 1   | A     | 19  | TYR  |
| 1   | A     | 20  | GLN  |
| 1   | A     | 21  | LYS  |
| 1   | A     | 23  | VAL  |
| 1   | A     | 24  | LYS  |
| 1   | A     | 26  | LYS  |
| 1   | A     | 27  | VAL  |
| 1   | A     | 30  | LYS  |
| 1   | A     | 34  | GLU  |
| 1   | A     | 35  | MET  |
| 1   | A     | 37  | ARG  |
| 1   | A     | 38  | ASP  |
| 1   | A     | 40  | LYS  |
| 1   | A     | 46  | THR  |
| 1   | A     | 47  | LEU  |
| 1   | A     | 50  | VAL  |
| 1   | A     | 51  | LYS  |
| 1   | A     | 52  | VAL  |
| 1   | A     | 53  | ARG  |
| 1   | A     | 60  | LEU  |
| 1   | A     | 62  | ASP  |
| 1   | A     | 64  | SER  |
| 1   | A     | 65  | GLU  |
| 1   | A     | 74  | GLN  |
| 1   | A     | 76  | GLU  |
| 1   | A     | 85  | ILE  |
| 1   | A     | 86  | GLN  |
| 1   | A     | 89  | LYS  |
| 1   | A     | 90  | GLU  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 95  | THR  |
| 1   | A     | 99  | LYS  |
| 1   | A     | 100 | GLU  |
| 1   | A     | 101 | ASP  |
| 1   | A     | 103 | ILE  |
| 1   | A     | 104 | ILE  |
| 1   | A     | 107 | ILE  |
| 1   | A     | 108 | HIS  |
| 1   | A     | 109 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 113 | THR  |
| 1   | A     | 117 | THR  |
| 1   | A     | 121 | VAL  |
| 1   | A     | 124 | LYS  |
| 1   | A     | 126 | ASP  |
| 1   | A     | 128 | LEU  |
| 1   | A     | 129 | LYS  |
| 1   | A     | 131 | LEU  |
| 1   | A     | 133 | ILE  |
| 1   | A     | 134 | THR  |
| 1   | A     | 136 | ILE  |
| 1   | A     | 148 | ARG  |
| 1   | A     | 155 | VAL  |
| 1   | A     | 157 | LEU  |
| 1   | A     | 163 | SER  |
| 1   | A     | 164 | TYR  |
| 1   | A     | 168 | GLU  |
| 1   | A     | 171 | ARG  |
| 1   | A     | 172 | LYS  |
| 1   | A     | 174 | VAL  |
| 1   | A     | 175 | ASP  |
| 1   | A     | 179 | LYS  |
| 1   | A     | 182 | LEU  |
| 1   | A     | 184 | VAL  |
| 1   | A     | 187 | ASP  |
| 1   | A     | 189 | VAL  |
| 1   | A     | 193 | VAL  |
| 1   | A     | 198 | ASN  |
| 1   | A     | 201 | VAL  |
| 1   | A     | 203 | LEU  |
| 1   | A     | 207 | PHE  |
| 1   | A     | 208 | SER  |
| 1   | A     | 209 | GLN  |
| 1   | A     | 210 | LYS  |
| 1   | A     | 211 | TYR  |
| 1   | A     | 212 | LYS  |
| 1   | A     | 217 | LEU  |
| 1   | A     | 223 | ASP  |
| 1   | A     | 227 | ASP  |
| 1   | A     | 228 | GLU  |
| 1   | A     | 229 | VAL  |
| 1   | A     | 230 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 233 | ILE  |
| 1   | A     | 237 | VAL  |
| 1   | A     | 241 | ILE  |
| 1   | A     | 242 | LYS  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 245 | ASN  |
| 1   | A     | 251 | LEU  |
| 1   | A     | 257 | ILE  |
| 1   | A     | 258 | ILE  |
| 1   | A     | 259 | ASP  |
| 1   | A     | 261 | SER  |
| 1   | A     | 263 | LYS  |
| 1   | A     | 265 | ILE  |
| 1   | A     | 271 | ASP  |
| 1   | A     | 272 | VAL  |
| 1   | A     | 273 | VAL  |
| 1   | A     | 275 | LYS  |
| 1   | A     | 277 | ASN  |
| 1   | A     | 279 | ILE  |
| 1   | A     | 281 | ILE  |
| 1   | A     | 284 | SER  |
| 1   | A     | 286 | LEU  |
| 1   | A     | 292 | VAL  |
| 1   | A     | 295 | LYS  |
| 1   | A     | 296 | GLU  |
| 1   | A     | 300 | TYR  |
| 1   | A     | 301 | ASN  |
| 1   | A     | 302 | ILE  |
| 1   | A     | 305 | GLN  |
| 1   | A     | 314 | ILE  |
| 1   | A     | 315 | HIS  |
| 1   | A     | 322 | ARG  |
| 1   | A     | 323 | GLN  |
| 1   | A     | 325 | TYR  |
| 1   | A     | 329 | PHE  |
| 1   | A     | 332 | LEU  |
| 1   | A     | 335 | ILE  |
| 1   | A     | 336 | VAL  |
| 1   | A     | 337 | LYS  |
| 1   | A     | 339 | TYR  |
| 1   | A     | 340 | LYS  |
| 1   | A     | 346 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 348 | LYS  |
| 1   | A     | 350 | SER  |
| 1   | A     | 353 | ARG  |
| 1   | A     | 354 | ARG  |
| 1   | A     | 384 | LYS  |
| 1   | A     | 387 | ARG  |
| 1   | A     | 388 | ILE  |
| 1   | A     | 389 | ILE  |
| 1   | A     | 391 | LEU  |
| 1   | A     | 392 | VAL  |
| 1   | A     | 393 | ASP  |
| 1   | A     | 399 | ILE  |
| 1   | A     | 404 | TYR  |
| 1   | A     | 410 | ILE  |
| 1   | A     | 412 | MET  |
| 1   | A     | 413 | ILE  |
| 1   | A     | 418 | GLU  |
| 1   | A     | 419 | TYR  |
| 1   | A     | 421 | GLU  |
| 1   | A     | 433 | ASP  |
| 1   | A     | 434 | SER  |
| 1   | A     | 435 | LYS  |
| 1   | A     | 437 | ILE  |
| 1   | A     | 438 | GLN  |
| 1   | A     | 441 | ARG  |
| 1   | A     | 444 | ARG  |
| 1   | A     | 445 | LYS  |
| 1   | A     | 447 | GLU  |
| 1   | A     | 448 | ASN  |
| 1   | A     | 450 | GLN  |
| 1   | A     | 452 | THR  |
| 1   | A     | 453 | ASP  |
| 1   | A     | 458 | SER  |
| 1   | A     | 463 | SER  |
| 1   | A     | 465 | LEU  |
| 1   | A     | 468 | LYS  |
| 1   | A     | 471 | GLU  |
| 1   | A     | 473 | ILE  |
| 1   | A     | 476 | PHE  |
| 1   | A     | 479 | ILE  |
| 1   | A     | 480 | LEU  |
| 1   | A     | 481 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 482 | LYS  |
| 1   | A     | 483 | MET  |
| 1   | A     | 486 | GLU  |
| 1   | A     | 487 | LEU  |
| 1   | A     | 488 | SER  |
| 1   | A     | 494 | ARG  |
| 1   | A     | 495 | VAL  |
| 1   | A     | 497 | VAL  |
| 1   | A     | 498 | VAL  |
| 1   | A     | 501 | GLU  |
| 1   | A     | 502 | ASN  |
| 1   | A     | 509 | ARG  |
| 1   | A     | 510 | GLU  |
| 1   | A     | 512 | PHE  |
| 1   | A     | 514 | LEU  |
| 1   | A     | 516 | VAL  |
| 1   | A     | 519 | LYS  |
| 1   | A     | 522 | ILE  |
| 1   | A     | 523 | GLU  |
| 1   | A     | 526 | TYR  |
| 1   | A     | 527 | SER  |
| 1   | A     | 529 | THR  |
| 1   | A     | 531 | LEU  |
| 1   | A     | 532 | LEU  |
| 1   | A     | 533 | SER  |
| 1   | A     | 534 | SER  |
| 1   | A     | 536 | ASN  |
| 1   | A     | 537 | SER  |
| 1   | A     | 540 | GLN  |
| 1   | A     | 544 | GLU  |
| 1   | A     | 549 | PHE  |
| 1   | A     | 550 | ASP  |
| 1   | A     | 555 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 74  | GLN  |
| 1   | A     | 79  | HIS  |
| 1   | A     | 274 | HIS  |
| 1   | A     | 301 | ASN  |
| 1   | A     | 311 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 323 | GLN  |
| 1   | A     | 351 | ASN  |
| 1   | A     | 423 | ASN  |
| 1   | A     | 450 | GLN  |
| 1   | A     | 496 | ASN  |
| 1   | A     | 535 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | A     | 557/558 (99%) | -0.41  | 1 (0%) 91 83 | 4, 42, 85, 100        | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 2   | PHE  | 2.2  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.