



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1U1U / pdb\_00001u1u  
Title : A. thaliana cobalamine independent methionine synthase  
Authors : Ferrer, J.-L.; Ravanel, S.; Robert, M.; Dumas, R.  
Deposited on : 2004-07-16  
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| 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                                                             |

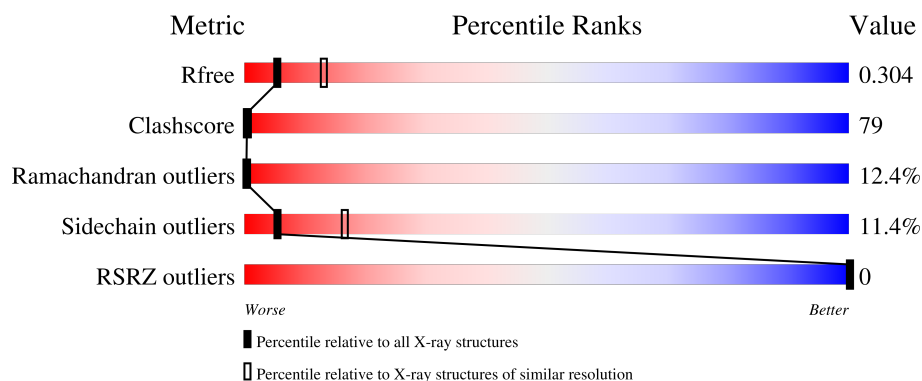
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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                      | 1130 (2.98-2.94)                                      |
| Clashscore            | 190562                      | 1157 (2.98-2.94)                                      |
| Ramachandran outliers | 187476                      | 1101 (2.98-2.94)                                      |
| Sidechain outliers    | 187428                      | 1101 (2.98-2.94)                                      |
| RSRZ outliers         | 180081                      | 1130 (2.98-2.94)                                      |

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     | 765    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | SO4  | A     | 771 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6093 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 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase.

| Mol | Chain | Residues | Atoms |      |     |      |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|---|----|---------|---------|-------|
| 1   | A     | 746      | Total | C    | N   | O    | S | Se | 0       | 0       | 0     |
|     |       |          | 5783  | 3686 | 974 | 1099 | 6 | 18 |         |         |       |

There are 19 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | MSE      | MET    | modified residue | UNP O50008 |
| A     | 11      | MSE      | MET    | modified residue | UNP O50008 |
| A     | 49      | MSE      | MET    | modified residue | UNP O50008 |
| A     | 74      | MSE      | MET    | modified residue | UNP O50008 |
| A     | 97      | MSE      | MET    | modified residue | UNP O50008 |
| A     | 107     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 109     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 212     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 351     | MSE      | LEU    | modified residue | UNP O50008 |
| A     | 496     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 538     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 545     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 549     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 554     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 557     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 648     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 663     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 718     | MSE      | MET    | modified residue | UNP O50008 |
| A     | 750     | MSE      | MET    | modified residue | UNP O50008 |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

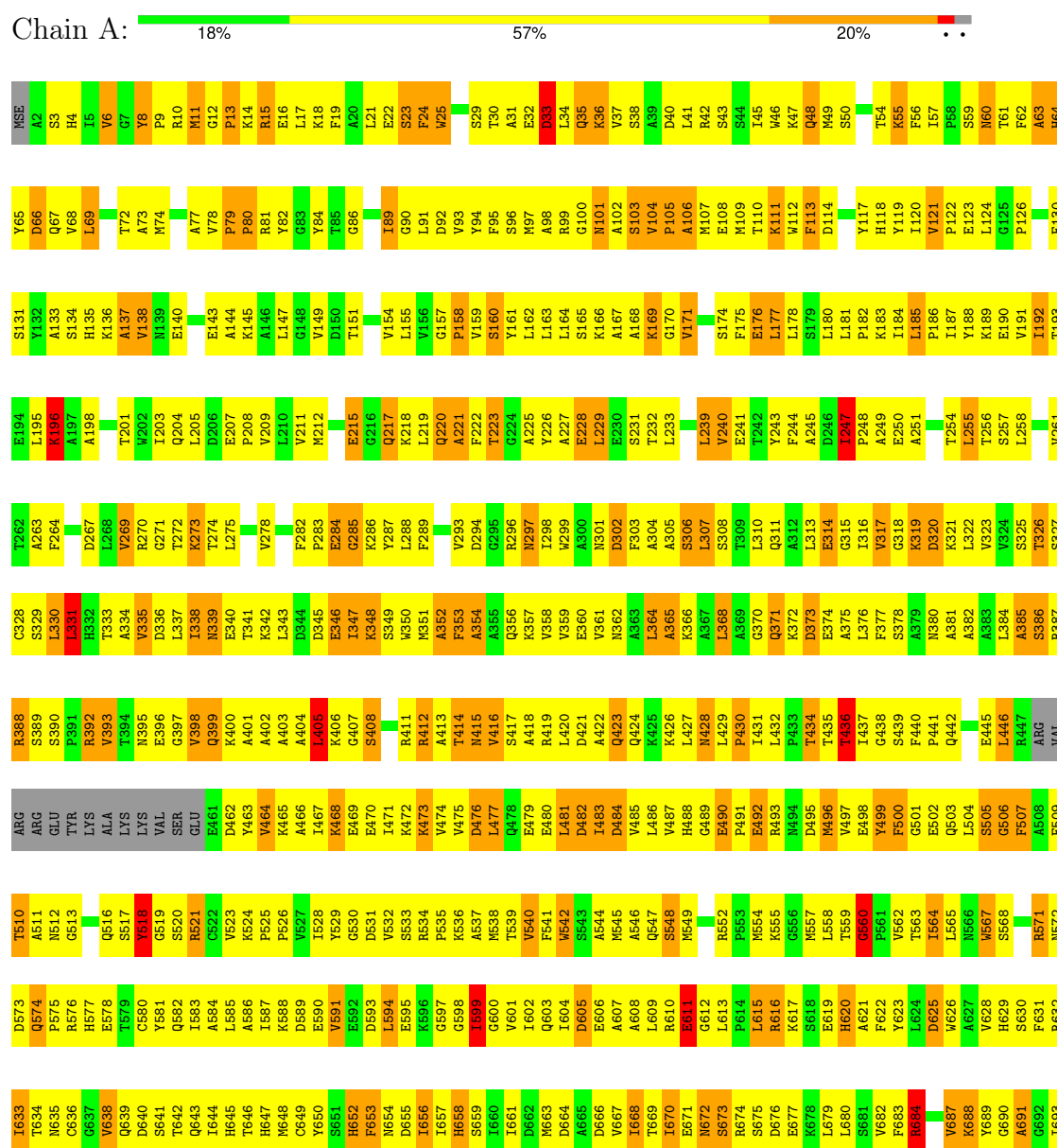
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 288      | Total | O   | 0       | 0       |
|     |       |          | 288   | 288 |         |         |

### 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: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 65                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 123.17Å 123.17Å 132.90Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 45.17 – 2.95<br>45.17 – 2.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (45.17-2.95)<br>100.0 (45.17-2.95)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.18                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.09 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.191 , 0.306<br>0.193 , 0.304                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2485 reflections (8.83%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 53.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.282                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 151.5                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$ | Xtriage          |
| Estimated twinning fraction                                             | 0.164 for h,-h-k,-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 6093                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 53.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.51         | 0/5884  | 1.10        | 49/7949 (0.6%) |

There are no bond length outliers.

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 104 | VAL  | CA-C-N  | 8.52  | 128.46      | 120.03   |
| 1   | A     | 104 | VAL  | C-N-CA  | 8.52  | 128.46      | 120.03   |
| 1   | A     | 33  | ASP  | N-CA-C  | -8.32 | 102.16      | 111.07   |
| 1   | A     | 594 | LEU  | N-CA-C  | -7.19 | 104.48      | 113.18   |
| 1   | A     | 269 | VAL  | N-CA-C  | -7.13 | 105.67      | 111.81   |
| 1   | A     | 331 | LEU  | N-CA-C  | -7.05 | 104.31      | 113.12   |
| 1   | A     | 730 | ASN  | CA-C-N  | 7.03  | 127.48      | 120.52   |
| 1   | A     | 730 | ASN  | C-N-CA  | 7.03  | 127.48      | 120.52   |
| 1   | A     | 13  | PRO  | N-CA-C  | -6.84 | 107.57      | 114.68   |
| 1   | A     | 273 | LYS  | N-CA-C  | -6.82 | 105.09      | 113.41   |
| 1   | A     | 196 | LYS  | N-CA-C  | -6.77 | 102.99      | 111.11   |
| 1   | A     | 574 | GLN  | CA-C-N  | 6.63  | 128.13      | 119.84   |
| 1   | A     | 574 | GLN  | C-N-CA  | 6.63  | 128.13      | 119.84   |
| 1   | A     | 378 | SER  | N-CA-C  | -6.58 | 103.59      | 111.69   |
| 1   | A     | 36  | LYS  | N-CA-C  | -6.38 | 104.42      | 111.82   |
| 1   | A     | 326 | THR  | N-CA-C  | -6.33 | 102.37      | 110.53   |
| 1   | A     | 61  | THR  | N-CA-C  | -6.20 | 105.76      | 113.38   |
| 1   | A     | 66  | ASP  | N-CA-C  | 6.19  | 119.22      | 108.76   |
| 1   | A     | 227 | ALA  | N-CA-C  | -6.10 | 105.59      | 113.16   |
| 1   | A     | 365 | ALA  | N-CA-C  | -6.05 | 104.61      | 111.14   |
| 1   | A     | 436 | THR  | CB-CA-C | -6.01 | 107.76      | 116.54   |
| 1   | A     | 247 | ILE  | N-CA-C  | 5.90  | 113.72      | 107.76   |
| 1   | A     | 64  | HIS  | N-CA-C  | -5.86 | 105.39      | 112.54   |
| 1   | A     | 349 | SER  | N-CA-C  | -5.84 | 105.65      | 112.89   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 23  | SER  | N-CA-C | -5.79 | 98.47       | 110.80   |
| 1   | A     | 215 | GLU  | N-CA-C | -5.73 | 103.13      | 110.53   |
| 1   | A     | 402 | ALA  | N-CA-C | -5.73 | 106.13      | 113.01   |
| 1   | A     | 405 | LEU  | N-CA-C | -5.71 | 106.01      | 112.87   |
| 1   | A     | 138 | VAL  | N-CA-C | 5.65  | 117.06      | 110.62   |
| 1   | A     | 560 | GLY  | CA-C-N | 5.62  | 125.24      | 119.56   |
| 1   | A     | 560 | GLY  | C-N-CA | 5.62  | 125.24      | 119.56   |
| 1   | A     | 638 | VAL  | N-CA-C | 5.58  | 116.16      | 108.12   |
| 1   | A     | 392 | ARG  | N-CA-C | -5.57 | 105.74      | 112.54   |
| 1   | A     | 10  | ARG  | N-CA-C | 5.56  | 118.00      | 110.88   |
| 1   | A     | 440 | PHE  | CA-C-N | 5.52  | 126.29      | 120.11   |
| 1   | A     | 440 | PHE  | C-N-CA | 5.52  | 126.29      | 120.11   |
| 1   | A     | 725 | ASN  | N-CA-C | -5.48 | 107.16      | 112.97   |
| 1   | A     | 440 | PHE  | N-CA-C | 5.44  | 117.03      | 108.55   |
| 1   | A     | 285 | GLY  | N-CA-C | -5.37 | 100.46      | 113.18   |
| 1   | A     | 133 | ALA  | N-CA-C | 5.32  | 117.69      | 110.88   |
| 1   | A     | 339 | ASN  | N-CA-C | -5.29 | 104.41      | 111.87   |
| 1   | A     | 473 | LYS  | N-CA-C | -5.18 | 105.75      | 111.71   |
| 1   | A     | 8   | TYR  | CA-C-N | 5.18  | 125.11      | 119.78   |
| 1   | A     | 8   | TYR  | C-N-CA | 5.18  | 125.11      | 119.78   |
| 1   | A     | 105 | PRO  | N-CA-C | 5.11  | 119.07      | 111.41   |
| 1   | A     | 464 | VAL  | N-CA-C | -5.04 | 106.21      | 113.07   |
| 1   | A     | 718 | MSE  | N-CA-C | -5.04 | 107.26      | 113.41   |
| 1   | A     | 544 | ALA  | N-CA-C | -5.03 | 107.09      | 113.18   |
| 1   | A     | 364 | LEU  | N-CA-C | -5.01 | 105.92      | 112.23   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5783  | 0        | 5795     | 911     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 20    | 0        | 0        | 2       | 0            |
| 4   | A     | 288   | 0        | 0        | 48      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 6093  | 0        | 5795     | 911     | 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 79.

All (911) 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:703:PRO:HA   | 1:A:738:ARG:HE   | 1.11                     | 1.08              |
| 1:A:111:LYS:HZ2  | 1:A:111:LYS:N    | 1.50                     | 1.07              |
| 1:A:477:LEU:HD22 | 1:A:486:LEU:HD22 | 1.36                     | 1.07              |
| 1:A:534:ARG:HH21 | 1:A:537:ALA:HA   | 1.25                     | 1.02              |
| 1:A:628:VAL:HG13 | 1:A:663:MSE:HG2  | 1.42                     | 1.00              |
| 1:A:599:ILE:HD12 | 1:A:599:ILE:H    | 1.25                     | 0.99              |
| 1:A:646:THR:HG22 | 1:A:668:ILE:HG22 | 1.45                     | 0.98              |
| 1:A:670:ILE:HD11 | 1:A:695:PRO:HA   | 1.49                     | 0.94              |
| 1:A:521:ARG:HA   | 1:A:521:ARG:NE   | 1.82                     | 0.94              |
| 1:A:546:ALA:HB3  | 1:A:554:MSE:HE2  | 1.52                     | 0.92              |
| 1:A:693:ILE:HG12 | 1:A:695:PRO:HD3  | 1.51                     | 0.91              |
| 1:A:707:SER:HB2  | 1:A:710:GLU:HG3  | 1.51                     | 0.91              |
| 1:A:703:PRO:CA   | 1:A:738:ARG:HE   | 1.83                     | 0.90              |
| 1:A:565:LEU:HD22 | 1:A:580:CYS:HB2  | 1.52                     | 0.90              |
| 1:A:604:ILE:O    | 1:A:646:THR:HA   | 1.71                     | 0.90              |
| 1:A:645:HIS:HA   | 1:A:667:VAL:O    | 1.71                     | 0.90              |
| 1:A:107:MSE:HE3  | 1:A:120:ILE:HG21 | 1.50                     | 0.90              |
| 1:A:534:ARG:HG2  | 1:A:586:ALA:HB1  | 1.54                     | 0.90              |
| 1:A:716:ASN:HA   | 1:A:719:LEU:HG   | 1.53                     | 0.90              |
| 1:A:97:MSE:HB3   | 1:A:107:MSE:HE2  | 1.54                     | 0.89              |
| 1:A:191:VAL:HG12 | 1:A:195:LEU:HD11 | 1.53                     | 0.88              |
| 1:A:497:VAL:HG21 | 1:A:567:TRP:HE3  | 1.37                     | 0.88              |
| 1:A:357:LYS:HA   | 1:A:360:GLU:HG3  | 1.56                     | 0.88              |
| 1:A:397:GLY:C    | 1:A:399:GLN:H    | 1.82                     | 0.87              |
| 1:A:558:LEU:HD11 | 1:A:591:VAL:HG13 | 1.54                     | 0.87              |
| 1:A:343:LEU:O    | 1:A:348:LYS:HE2  | 1.75                     | 0.87              |
| 1:A:699:ASP:HA   | 1:A:732:ASP:HB2  | 1.57                     | 0.85              |
| 1:A:185:LEU:HD23 | 1:A:228:GLU:HG2  | 1.57                     | 0.85              |
| 1:A:575:PRO:HB3  | 1:A:577:HIS:CE1  | 2.11                     | 0.85              |
| 1:A:273:LYS:NZ   | 1:A:273:LYS:HB3  | 1.92                     | 0.85              |
| 1:A:609:LEU:HD23 | 1:A:650:TYR:HE2  | 1.41                     | 0.83              |
| 1:A:343:LEU:O    | 1:A:348:LYS:CE   | 2.27                     | 0.83              |
| 1:A:700:ILE:HD11 | 1:A:733:CYS:HB2  | 1.61                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:212:MSE:HE1  | 1:A:615:LEU:HB3  | 1.60                     | 0.83              |
| 1:A:263:ALA:CB   | 1:A:287:TYR:HB2  | 2.07                     | 0.83              |
| 1:A:676:ASP:OD2  | 1:A:679:LEU:HD12 | 1.79                     | 0.82              |
| 1:A:703:PRO:HA   | 1:A:738:ARG:NE   | 1.92                     | 0.81              |
| 1:A:608:ALA:HA   | 1:A:611:GLU:OE2  | 1.81                     | 0.81              |
| 1:A:247:ILE:HD12 | 1:A:247:ILE:H    | 1.44                     | 0.80              |
| 1:A:343:LEU:HD21 | 1:A:509:PHE:O    | 1.81                     | 0.80              |
| 1:A:436:THR:HG22 | 1:A:731:PRO:HG2  | 1.62                     | 0.79              |
| 1:A:521:ARG:HA   | 1:A:521:ARG:HE   | 1.43                     | 0.79              |
| 1:A:191:VAL:O    | 1:A:195:LEU:HD12 | 1.83                     | 0.79              |
| 1:A:208:PRO:O    | 1:A:211:VAL:HG22 | 1.82                     | 0.79              |
| 1:A:432:LEU:HD11 | 1:A:727:LEU:HD23 | 1.64                     | 0.78              |
| 1:A:517:SER:O    | 1:A:518:TYR:HB3  | 1.83                     | 0.78              |
| 1:A:747:LEU:C    | 1:A:749:ASN:H    | 1.90                     | 0.78              |
| 1:A:415:ASN:O    | 1:A:417:SER:N    | 2.16                     | 0.78              |
| 1:A:586:ALA:O    | 1:A:589:ASP:HB2  | 1.83                     | 0.78              |
| 1:A:462:ASP:O    | 1:A:466:ALA:HB2  | 1.83                     | 0.78              |
| 1:A:45:ILE:HG22  | 1:A:49:MSE:HE2   | 1.67                     | 0.77              |
| 1:A:610:ARG:HH22 | 1:A:653:PHE:HA   | 1.49                     | 0.77              |
| 1:A:752:ASP:O    | 1:A:756:LEU:HD13 | 1.84                     | 0.77              |
| 1:A:534:ARG:HH21 | 1:A:537:ALA:CA   | 1.96                     | 0.77              |
| 1:A:263:ALA:HB2  | 1:A:287:TYR:HB2  | 1.65                     | 0.77              |
| 1:A:581:TYR:OH   | 1:A:626:TRP:HA   | 1.84                     | 0.77              |
| 1:A:111:LYS:HZ2  | 1:A:111:LYS:H    | 1.28                     | 0.77              |
| 1:A:646:THR:HG22 | 1:A:668:ILE:CG2  | 2.13                     | 0.77              |
| 1:A:35:GLN:HA    | 1:A:35:GLN:HE21  | 1.49                     | 0.76              |
| 1:A:700:ILE:HD12 | 1:A:701:HIS:N    | 2.00                     | 0.76              |
| 1:A:523:VAL:HG23 | 1:A:525:PRO:HD3  | 1.66                     | 0.76              |
| 1:A:581:TYR:CE1  | 1:A:630:SER:HB2  | 2.21                     | 0.76              |
| 1:A:33:ASP:O     | 1:A:37:VAL:HG23  | 1.85                     | 0.76              |
| 1:A:481:LEU:HD22 | 1:A:751:VAL:HG12 | 1.68                     | 0.76              |
| 1:A:188:TYR:O    | 1:A:192:ILE:HG12 | 1.87                     | 0.75              |
| 1:A:470:GLU:O    | 1:A:474:VAL:HG23 | 1.86                     | 0.75              |
| 1:A:231:SER:HB3  | 4:A:963:HOH:O    | 1.85                     | 0.75              |
| 1:A:384:LEU:HD13 | 1:A:388:ARG:NH2  | 2.00                     | 0.75              |
| 1:A:697:VAL:O    | 1:A:698:TYR:HB3  | 1.84                     | 0.75              |
| 1:A:18:LYS:HG3   | 1:A:520:SER:HB2  | 1.69                     | 0.75              |
| 1:A:488:HIS:HB3  | 1:A:554:MSE:HE1  | 1.68                     | 0.75              |
| 1:A:757:ILE:HD13 | 1:A:757:ILE:H    | 1.52                     | 0.75              |
| 1:A:178:LEU:HD21 | 1:A:221:ALA:CB   | 2.17                     | 0.75              |
| 1:A:477:LEU:HD11 | 1:A:487:VAL:HG22 | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:160:SER:HB2  | 1:A:207:GLU:OE1  | 1.88                     | 0.74              |
| 1:A:419:ARG:HG3  | 1:A:640:ASP:O    | 1.86                     | 0.74              |
| 1:A:671:GLU:HG3  | 1:A:732:ASP:OD2  | 1.87                     | 0.74              |
| 1:A:82:TYR:CZ    | 1:A:97:MSE:HA    | 2.23                     | 0.74              |
| 1:A:738:ARG:HG2  | 1:A:743:VAL:HG12 | 1.69                     | 0.74              |
| 1:A:718:MSE:HE2  | 1:A:727:LEU:HD11 | 1.68                     | 0.74              |
| 1:A:335:VAL:HG12 | 1:A:336:ASP:N    | 2.02                     | 0.73              |
| 1:A:647:HIS:HB2  | 4:A:885:HOH:O    | 1.87                     | 0.73              |
| 1:A:605:ASP:HB3  | 1:A:647:HIS:HB3  | 1.69                     | 0.73              |
| 1:A:212:MSE:HE1  | 1:A:615:LEU:HD13 | 1.71                     | 0.72              |
| 1:A:107:MSE:HE3  | 1:A:120:ILE:CG2  | 2.19                     | 0.72              |
| 1:A:330:LEU:HD22 | 1:A:357:LYS:HD3  | 1.71                     | 0.72              |
| 1:A:676:ASP:HB2  | 1:A:679:LEU:HB2  | 1.71                     | 0.72              |
| 1:A:672:ASN:O    | 1:A:673:SER:HB3  | 1.87                     | 0.72              |
| 1:A:673:SER:HB2  | 1:A:696:GLY:O    | 1.90                     | 0.72              |
| 1:A:633:ILE:HG22 | 1:A:633:ILE:O    | 1.89                     | 0.72              |
| 1:A:634:THR:HB   | 4:A:986:HOH:O    | 1.90                     | 0.72              |
| 1:A:477:LEU:CD1  | 1:A:487:VAL:H    | 2.02                     | 0.72              |
| 1:A:114:ASP:HB3  | 1:A:615:LEU:HD21 | 1.71                     | 0.72              |
| 1:A:477:LEU:HD13 | 1:A:486:LEU:HB3  | 1.70                     | 0.72              |
| 1:A:463:TYR:HA   | 1:A:466:ALA:HB3  | 1.72                     | 0.71              |
| 1:A:632:ARG:C    | 1:A:634:THR:H    | 1.95                     | 0.71              |
| 1:A:314:GLU:OE1  | 1:A:322:LEU:HG   | 1.89                     | 0.71              |
| 1:A:497:VAL:HG21 | 1:A:567:TRP:CE3  | 2.23                     | 0.71              |
| 1:A:670:ILE:HD11 | 1:A:695:PRO:CA   | 2.20                     | 0.71              |
| 1:A:62:PHE:HB2   | 4:A:983:HOH:O    | 1.91                     | 0.71              |
| 1:A:689:TYR:CE2  | 1:A:691:ALA:HB3  | 2.26                     | 0.71              |
| 1:A:578:GLU:O    | 1:A:582:GLN:HG3  | 1.90                     | 0.70              |
| 1:A:611:GLU:CD   | 1:A:611:GLU:H    | 1.99                     | 0.70              |
| 1:A:441:PRO:HB2  | 1:A:740:TYR:CE2  | 2.25                     | 0.70              |
| 1:A:65:TYR:CE2   | 1:A:519:GLY:HA2  | 2.25                     | 0.70              |
| 1:A:303:PHE:HB2  | 1:A:380:ASN:OD1  | 1.90                     | 0.70              |
| 1:A:670:ILE:CD1  | 1:A:695:PRO:HA   | 2.21                     | 0.70              |
| 1:A:350:TRP:CH2  | 1:A:387:ARG:HA   | 2.27                     | 0.70              |
| 1:A:565:LEU:CD2  | 1:A:580:CYS:HB2  | 2.20                     | 0.70              |
| 1:A:740:TYR:HA   | 1:A:743:VAL:HG22 | 1.72                     | 0.70              |
| 1:A:84:TYR:CZ    | 1:A:86:GLY:HA2   | 2.26                     | 0.70              |
| 1:A:310:LEU:HB3  | 1:A:368:LEU:HD11 | 1.74                     | 0.70              |
| 1:A:16:GLU:OE1   | 1:A:16:GLU:N     | 2.21                     | 0.70              |
| 1:A:670:ILE:HD13 | 1:A:670:ILE:N    | 2.07                     | 0.70              |
| 1:A:143:GLU:O    | 1:A:147:LEU:HD13 | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:644:ILE:HD12 | 1:A:644:ILE:N    | 2.07                     | 0.69              |
| 1:A:504:LEU:CD2  | 1:A:534:ARG:HB3  | 2.22                     | 0.69              |
| 1:A:384:LEU:HD11 | 4:A:792:HOH:O    | 1.91                     | 0.69              |
| 1:A:191:VAL:HG12 | 1:A:195:LEU:CD1  | 2.22                     | 0.69              |
| 1:A:162:LEU:H    | 1:A:162:LEU:HD12 | 1.55                     | 0.69              |
| 1:A:247:ILE:HD12 | 1:A:247:ILE:N    | 2.07                     | 0.69              |
| 1:A:477:LEU:O    | 1:A:483:ILE:HD12 | 1.93                     | 0.69              |
| 1:A:74:MSE:HE1   | 1:A:155:LEU:HD22 | 1.75                     | 0.69              |
| 1:A:725:ASN:O    | 1:A:726:ILE:HG23 | 1.93                     | 0.69              |
| 1:A:318:GLY:C    | 1:A:320:ASP:H    | 2.01                     | 0.68              |
| 1:A:178:LEU:HD21 | 1:A:221:ALA:HB2  | 1.74                     | 0.68              |
| 1:A:401:ALA:O    | 1:A:405:LEU:HD22 | 1.93                     | 0.68              |
| 1:A:165:SER:O    | 1:A:166:LYS:HD3  | 1.92                     | 0.68              |
| 1:A:723:GLU:HB3  | 1:A:726:ILE:HG13 | 1.75                     | 0.68              |
| 1:A:467:ILE:O    | 1:A:471:ILE:HG22 | 1.94                     | 0.68              |
| 1:A:480:GLU:O    | 1:A:483:ILE:HG13 | 1.94                     | 0.68              |
| 1:A:112:TRP:O    | 1:A:113:PHE:HB2  | 1.93                     | 0.68              |
| 1:A:395:ASN:C    | 1:A:397:GLY:H    | 2.02                     | 0.68              |
| 1:A:504:LEU:HD23 | 1:A:534:ARG:HB3  | 1.76                     | 0.68              |
| 1:A:414:THR:O    | 1:A:416:VAL:N    | 2.27                     | 0.67              |
| 1:A:477:LEU:HD11 | 1:A:487:VAL:H    | 1.59                     | 0.67              |
| 1:A:506:GLY:HA3  | 1:A:530:GLY:O    | 1.94                     | 0.67              |
| 1:A:647:HIS:HE2  | 1:A:649:CYS:HG   | 1.41                     | 0.67              |
| 1:A:565:LEU:HD22 | 1:A:580:CYS:CB   | 2.24                     | 0.67              |
| 1:A:749:ASN:HA   | 1:A:752:ASP:OD2  | 1.94                     | 0.67              |
| 1:A:130:PHE:HD2  | 1:A:183:LYS:HG2  | 1.59                     | 0.67              |
| 1:A:338:ILE:C    | 1:A:339:ASN:HD22 | 2.03                     | 0.67              |
| 1:A:399:GLN:HE21 | 1:A:399:GLN:C    | 2.03                     | 0.67              |
| 1:A:435:THR:O    | 1:A:750:MSE:HE1  | 1.95                     | 0.67              |
| 1:A:411:ARG:O    | 1:A:413:ALA:N    | 2.28                     | 0.67              |
| 1:A:533:SER:O    | 1:A:535:PRO:HD3  | 1.95                     | 0.67              |
| 1:A:3:SER:O      | 1:A:55:LYS:HB3   | 1.95                     | 0.66              |
| 1:A:92:ASP:O     | 1:A:96:SER:HB3   | 1.95                     | 0.66              |
| 1:A:228:GLU:O    | 1:A:228:GLU:HG3  | 1.95                     | 0.66              |
| 1:A:464:VAL:HG13 | 1:A:465:LYS:HG2  | 1.75                     | 0.66              |
| 1:A:154:VAL:HA   | 1:A:204:GLN:HB3  | 1.78                     | 0.66              |
| 1:A:505:SER:O    | 1:A:507:PHE:N    | 2.28                     | 0.66              |
| 1:A:422:ALA:C    | 1:A:424:GLN:H    | 2.02                     | 0.66              |
| 1:A:542:TRP:HA   | 1:A:542:TRP:CE3  | 2.30                     | 0.66              |
| 1:A:329:SER:C    | 1:A:331:LEU:H    | 2.02                     | 0.66              |
| 1:A:353:PHE:N    | 1:A:353:PHE:HD1  | 1.94                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:45:ILE:CG2   | 1:A:49:MSE:HE2   | 2.25                     | 0.66              |
| 1:A:539:THR:HG23 | 4:A:1006:HOH:O   | 1.95                     | 0.65              |
| 1:A:547:GLN:NE2  | 1:A:554:MSE:HB2  | 2.10                     | 0.65              |
| 1:A:157:GLY:HA2  | 1:A:205:LEU:HD22 | 1.76                     | 0.65              |
| 1:A:225:ALA:O    | 1:A:229:LEU:HD13 | 1.97                     | 0.65              |
| 1:A:18:LYS:O     | 1:A:22:GLU:HG3   | 1.96                     | 0.65              |
| 1:A:495:ASP:HB3  | 1:A:498:GLU:CG   | 2.26                     | 0.65              |
| 1:A:496:MSE:HA   | 4:A:974:HOH:O    | 1.95                     | 0.65              |
| 1:A:632:ARG:O    | 1:A:634:THR:N    | 2.29                     | 0.65              |
| 1:A:680:LEU:HB3  | 1:A:722:LEU:HD21 | 1.76                     | 0.65              |
| 1:A:572:ASN:HB3  | 4:A:896:HOH:O    | 1.97                     | 0.65              |
| 1:A:136:LYS:HG3  | 4:A:789:HOH:O    | 1.97                     | 0.65              |
| 1:A:723:GLU:HG2  | 1:A:725:ASN:OD1  | 1.97                     | 0.64              |
| 1:A:222:PHE:O    | 1:A:226:TYR:HD1  | 1.79                     | 0.64              |
| 1:A:648:MSE:HE3  | 1:A:670:ILE:HG22 | 1.79                     | 0.64              |
| 1:A:756:LEU:O    | 1:A:758:ARG:N    | 2.31                     | 0.64              |
| 1:A:336:ASP:OD1  | 1:A:338:ILE:HG22 | 1.98                     | 0.64              |
| 1:A:476:ASP:O    | 1:A:480:GLU:HB2  | 1.97                     | 0.64              |
| 1:A:500:PHE:HD1  | 1:A:538:MSE:HE3  | 1.63                     | 0.64              |
| 1:A:137:ALA:HB3  | 4:A:970:HOH:O    | 1.98                     | 0.64              |
| 1:A:674:ARG:CZ   | 1:A:699:ASP:HB3  | 2.27                     | 0.64              |
| 1:A:350:TRP:HZ2  | 1:A:386:SER:HB2  | 1.63                     | 0.64              |
| 1:A:9:PRO:HD3    | 1:A:330:LEU:O    | 1.96                     | 0.64              |
| 1:A:212:MSE:HE1  | 1:A:615:LEU:CB   | 2.28                     | 0.64              |
| 1:A:330:LEU:HD22 | 1:A:357:LYS:CD   | 2.28                     | 0.64              |
| 1:A:167:ALA:N    | 1:A:177:LEU:HD21 | 2.14                     | 0.63              |
| 1:A:437:ILE:HG13 | 1:A:733:CYS:O    | 1.97                     | 0.63              |
| 1:A:273:LYS:HB3  | 1:A:273:LYS:HZ3  | 1.62                     | 0.63              |
| 1:A:337:LEU:HB2  | 1:A:353:PHE:CD1  | 2.33                     | 0.63              |
| 1:A:654:ASN:ND2  | 1:A:682:VAL:HG11 | 2.12                     | 0.63              |
| 1:A:119:TYR:HE1  | 1:A:121:VAL:HA   | 1.63                     | 0.63              |
| 1:A:319:LYS:O    | 1:A:320:ASP:HB2  | 1.97                     | 0.63              |
| 1:A:581:TYR:O    | 1:A:585:LEU:HD23 | 1.99                     | 0.63              |
| 1:A:715:VAL:HG12 | 1:A:719:LEU:HD21 | 1.79                     | 0.63              |
| 1:A:43:SER:HB3   | 4:A:881:HOH:O    | 1.99                     | 0.63              |
| 1:A:606:GLU:OE1  | 1:A:606:GLU:HA   | 1.98                     | 0.63              |
| 1:A:657:ILE:HD11 | 1:A:687:VAL:HG11 | 1.81                     | 0.63              |
| 1:A:212:MSE:CE   | 1:A:615:LEU:HB3  | 2.28                     | 0.62              |
| 1:A:335:VAL:HA   | 1:A:354:ALA:HB3  | 1.81                     | 0.62              |
| 1:A:705:ILE:HD13 | 1:A:705:ILE:H    | 1.64                     | 0.62              |
| 1:A:8:TYR:CE2    | 1:A:45:ILE:HD12  | 2.34                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:423:GLN:NE2  | 1:A:643:GLN:HA   | 2.13                     | 0.62              |
| 1:A:699:ASP:HA   | 1:A:732:ASP:CB   | 2.27                     | 0.62              |
| 1:A:547:GLN:HA   | 1:A:547:GLN:HE21 | 1.65                     | 0.62              |
| 1:A:760:GLN:H    | 1:A:760:GLN:NE2  | 1.98                     | 0.62              |
| 1:A:506:GLY:HA2  | 1:A:529:TYR:CD1  | 2.34                     | 0.62              |
| 1:A:11:MSE:HA    | 1:A:17:LEU:HB3   | 1.80                     | 0.62              |
| 1:A:204:GLN:HG3  | 1:A:239:LEU:HD12 | 1.80                     | 0.62              |
| 1:A:599:ILE:H    | 1:A:599:ILE:CD1  | 2.06                     | 0.62              |
| 1:A:404:ALA:C    | 1:A:406:LYS:H    | 2.07                     | 0.62              |
| 1:A:506:GLY:HA2  | 1:A:529:TYR:CE1  | 2.36                     | 0.61              |
| 1:A:350:TRP:HH2  | 1:A:390:SER:HB3  | 1.65                     | 0.61              |
| 1:A:353:PHE:N    | 1:A:353:PHE:CD1  | 2.65                     | 0.61              |
| 1:A:162:LEU:HD11 | 1:A:184:ILE:HD11 | 1.81                     | 0.61              |
| 1:A:616:ARG:O    | 1:A:619:GLU:HB2  | 2.01                     | 0.61              |
| 1:A:713:ASP:HA   | 1:A:716:ASN:HB2  | 1.81                     | 0.61              |
| 1:A:336:ASP:CG   | 1:A:338:ILE:HG22 | 2.26                     | 0.61              |
| 1:A:387:ARG:O    | 1:A:393:VAL:HG21 | 1.99                     | 0.61              |
| 1:A:628:VAL:CG1  | 1:A:663:MSE:HG2  | 2.25                     | 0.61              |
| 1:A:661:ILE:HG13 | 1:A:689:TYR:HD1  | 1.65                     | 0.61              |
| 1:A:247:ILE:HD13 | 1:A:274:THR:HG21 | 1.83                     | 0.61              |
| 1:A:30:THR:C     | 1:A:32:GLU:H     | 2.06                     | 0.61              |
| 1:A:79:PRO:HB2   | 1:A:82:TYR:CD2   | 2.36                     | 0.61              |
| 1:A:130:PHE:CD2  | 1:A:183:LYS:HG2  | 2.36                     | 0.61              |
| 1:A:698:TYR:OH   | 1:A:700:ILE:HG22 | 1.99                     | 0.61              |
| 1:A:62:PHE:CD1   | 1:A:63:ALA:N     | 2.67                     | 0.60              |
| 1:A:385:ALA:HB3  | 4:A:1047:HOH:O   | 2.00                     | 0.60              |
| 1:A:423:GLN:HE21 | 1:A:643:GLN:HA   | 1.66                     | 0.60              |
| 1:A:560:GLY:HA3  | 1:A:606:GLU:CD   | 2.25                     | 0.60              |
| 1:A:698:TYR:CZ   | 1:A:700:ILE:HG22 | 2.37                     | 0.60              |
| 1:A:4:HIS:O      | 1:A:325:SER:HA   | 2.01                     | 0.60              |
| 1:A:377:PHE:HA   | 1:A:380:ASN:HB3  | 1.84                     | 0.60              |
| 1:A:477:LEU:HD23 | 1:A:483:ILE:CD1  | 2.31                     | 0.60              |
| 1:A:111:LYS:N    | 1:A:111:LYS:NZ   | 2.38                     | 0.60              |
| 1:A:157:GLY:HA3  | 1:A:207:GLU:CD   | 2.26                     | 0.60              |
| 1:A:343:LEU:O    | 1:A:348:LYS:HE3  | 2.02                     | 0.60              |
| 1:A:674:ARG:NE   | 1:A:699:ASP:HB3  | 2.17                     | 0.60              |
| 1:A:298:ILE:HD11 | 1:A:353:PHE:CG   | 2.37                     | 0.60              |
| 1:A:480:GLU:O    | 1:A:482:ASP:N    | 2.35                     | 0.60              |
| 1:A:293:VAL:HB   | 1:A:326:THR:HA   | 1.84                     | 0.60              |
| 1:A:571:ARG:HB2  | 1:A:573:ASP:OD1  | 2.02                     | 0.60              |
| 1:A:605:ASP:CB   | 1:A:647:HIS:HB3  | 2.32                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:240:VAL:CG2  | 1:A:261:VAL:HG11 | 2.32                     | 0.60              |
| 1:A:366:LYS:HB3  | 1:A:371:GLN:O    | 2.01                     | 0.60              |
| 1:A:11:MSE:HG3   | 1:A:17:LEU:HB3   | 1.84                     | 0.60              |
| 1:A:477:LEU:HD23 | 1:A:483:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:220:GLN:HE21 | 1:A:220:GLN:HA   | 1.67                     | 0.59              |
| 1:A:622:PHE:HD2  | 1:A:622:PHE:O    | 1.83                     | 0.59              |
| 1:A:542:TRP:HA   | 1:A:542:TRP:HE3  | 1.67                     | 0.59              |
| 1:A:760:GLN:HA   | 4:A:1003:HOH:O   | 2.02                     | 0.59              |
| 1:A:271:GLY:HA3  | 4:A:804:HOH:O    | 2.03                     | 0.59              |
| 1:A:341:THR:HG23 | 1:A:342:LYS:N    | 2.17                     | 0.59              |
| 1:A:100:GLY:N    | 1:A:106:ALA:HB2  | 2.18                     | 0.59              |
| 1:A:215:GLU:OE1  | 1:A:217:GLN:HB2  | 2.02                     | 0.59              |
| 1:A:124:LEU:O    | 1:A:167:ALA:HA   | 2.03                     | 0.59              |
| 1:A:162:LEU:HD11 | 1:A:184:ILE:CD1  | 2.31                     | 0.59              |
| 1:A:99:ARG:C     | 1:A:106:ALA:HB2  | 2.27                     | 0.59              |
| 1:A:229:LEU:HB3  | 1:A:233:LEU:CD2  | 2.33                     | 0.59              |
| 1:A:471:ILE:O    | 1:A:474:VAL:HB   | 2.02                     | 0.59              |
| 1:A:404:ALA:C    | 1:A:406:LYS:N    | 2.59                     | 0.59              |
| 1:A:554:MSE:O    | 1:A:599:ILE:HG23 | 2.03                     | 0.59              |
| 1:A:611:GLU:N    | 1:A:611:GLU:OE1  | 2.36                     | 0.59              |
| 1:A:446:LEU:N    | 1:A:446:LEU:HD22 | 2.17                     | 0.59              |
| 1:A:620:HIS:O    | 1:A:622:PHE:N    | 2.35                     | 0.59              |
| 1:A:695:PRO:HD2  | 1:A:718:MSE:HE1  | 1.85                     | 0.59              |
| 1:A:62:PHE:O     | 1:A:63:ALA:HB2   | 2.02                     | 0.58              |
| 1:A:534:ARG:O    | 1:A:534:ARG:HG3  | 2.03                     | 0.58              |
| 1:A:655:ASP:HB3  | 4:A:925:HOH:O    | 2.03                     | 0.58              |
| 1:A:599:ILE:HD12 | 1:A:599:ILE:N    | 2.07                     | 0.58              |
| 1:A:658:HIS:O    | 1:A:661:ILE:N    | 2.35                     | 0.58              |
| 1:A:49:MSE:O     | 1:A:54:THR:OG1   | 2.22                     | 0.58              |
| 1:A:187:ILE:O    | 1:A:191:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:302:ASP:OD2  | 1:A:305:ALA:HB2  | 2.03                     | 0.58              |
| 1:A:399:GLN:NE2  | 1:A:400:LYS:HD3  | 2.18                     | 0.58              |
| 1:A:653:PHE:HB2  | 1:A:656:ILE:CG2  | 2.33                     | 0.58              |
| 1:A:744:LYS:C    | 1:A:746:ALA:H    | 2.09                     | 0.58              |
| 1:A:108:GLU:O    | 1:A:121:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:34:LEU:O     | 1:A:37:VAL:N     | 2.35                     | 0.58              |
| 1:A:639:GLN:C    | 1:A:641:SER:H    | 2.11                     | 0.58              |
| 1:A:680:LEU:C    | 1:A:682:VAL:H    | 2.12                     | 0.58              |
| 1:A:483:ILE:HG22 | 1:A:485:VAL:O    | 2.04                     | 0.58              |
| 1:A:32:GLU:HB3   | 4:A:1043:HOH:O   | 2.02                     | 0.58              |
| 1:A:485:VAL:C    | 1:A:486:LEU:HD23 | 2.28                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:229:LEU:HB3  | 1:A:233:LEU:HD23 | 1.85                     | 0.58              |
| 1:A:8:TYR:CD2    | 1:A:9:PRO:HD2    | 2.38                     | 0.57              |
| 1:A:298:ILE:HG23 | 1:A:298:ILE:O    | 2.04                     | 0.57              |
| 1:A:674:ARG:HB2  | 4:A:818:HOH:O    | 2.04                     | 0.57              |
| 1:A:42:ARG:HG2   | 4:A:983:HOH:O    | 2.02                     | 0.57              |
| 1:A:411:ARG:NH2  | 1:A:419:ARG:HD2  | 2.18                     | 0.57              |
| 1:A:548:SER:HA   | 4:A:976:HOH:O    | 2.03                     | 0.57              |
| 1:A:437:ILE:HG21 | 1:A:733:CYS:C    | 2.29                     | 0.57              |
| 1:A:131:SER:HB3  | 4:A:933:HOH:O    | 2.03                     | 0.57              |
| 1:A:540:VAL:HG12 | 1:A:541:PHE:N    | 2.20                     | 0.57              |
| 1:A:598:GLY:O    | 1:A:599:ILE:C    | 2.47                     | 0.57              |
| 1:A:700:ILE:CG1  | 1:A:733:CYS:H    | 2.18                     | 0.57              |
| 1:A:644:ILE:HD12 | 1:A:644:ILE:H    | 1.68                     | 0.57              |
| 1:A:726:ILE:HD11 | 4:A:921:HOH:O    | 2.04                     | 0.57              |
| 1:A:35:GLN:HA    | 1:A:35:GLN:NE2   | 2.19                     | 0.57              |
| 1:A:3:SER:HB2    | 1:A:361:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:490:GLU:HG2  | 1:A:493:ARG:NH1  | 2.20                     | 0.57              |
| 1:A:93:VAL:HA    | 1:A:96:SER:OG    | 2.05                     | 0.56              |
| 1:A:469:GLU:OE1  | 1:A:472:LYS:HD2  | 2.05                     | 0.56              |
| 1:A:673:SER:OG   | 1:A:699:ASP:HB2  | 2.05                     | 0.56              |
| 1:A:534:ARG:NH2  | 1:A:537:ALA:HA   | 2.09                     | 0.56              |
| 1:A:631:PHE:CG   | 1:A:663:MSE:HE2  | 2.40                     | 0.56              |
| 1:A:477:LEU:CD2  | 1:A:483:ILE:HG21 | 2.35                     | 0.56              |
| 1:A:577:HIS:O    | 1:A:580:CYS:HB3  | 2.06                     | 0.56              |
| 1:A:647:HIS:NE2  | 1:A:649:CYS:SG   | 2.69                     | 0.56              |
| 1:A:399:GLN:HE22 | 1:A:400:LYS:HD3  | 1.70                     | 0.56              |
| 1:A:693:ILE:HG12 | 1:A:695:PRO:CD   | 2.30                     | 0.56              |
| 1:A:701:HIS:NE2  | 1:A:733:CYS:SG   | 2.78                     | 0.56              |
| 1:A:333:THR:HG23 | 1:A:334:ALA:N    | 2.20                     | 0.56              |
| 1:A:373:ASP:C    | 1:A:375:ALA:H    | 2.11                     | 0.56              |
| 1:A:558:LEU:HD12 | 1:A:604:ILE:HG12 | 1.88                     | 0.56              |
| 1:A:310:LEU:HD12 | 1:A:364:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:721:VAL:HG23 | 1:A:722:LEU:HG   | 1.87                     | 0.56              |
| 1:A:101:ASN:HB3  | 4:A:857:HOH:O    | 2.06                     | 0.56              |
| 1:A:330:LEU:HD13 | 1:A:357:LYS:HB2  | 1.87                     | 0.56              |
| 1:A:17:LEU:HD12  | 1:A:21:LEU:HG    | 1.88                     | 0.55              |
| 1:A:389:SER:O    | 1:A:390:SER:C    | 2.50                     | 0.55              |
| 1:A:747:LEU:C    | 1:A:749:ASN:N    | 2.59                     | 0.55              |
| 1:A:126:PRO:HD2  | 1:A:171:VAL:HG22 | 1.88                     | 0.55              |
| 1:A:674:ARG:NE   | 1:A:699:ASP:CB   | 2.70                     | 0.55              |
| 1:A:700:ILE:CG2  | 1:A:731:PRO:HB3  | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:646:THR:H    | 1:A:668:ILE:HA   | 1.72                     | 0.55              |
| 1:A:416:VAL:O    | 1:A:420:LEU:HG   | 2.07                     | 0.55              |
| 1:A:445:GLU:C    | 1:A:446:LEU:HD22 | 2.32                     | 0.55              |
| 1:A:467:ILE:O    | 1:A:468:LYS:C    | 2.50                     | 0.55              |
| 1:A:729:VAL:CG1  | 1:A:750:MSE:HG2  | 2.36                     | 0.55              |
| 1:A:322:LEU:HD13 | 1:A:323:VAL:N    | 2.22                     | 0.55              |
| 1:A:658:HIS:O    | 1:A:661:ILE:HG22 | 2.07                     | 0.55              |
| 1:A:620:HIS:O    | 1:A:623:TYR:N    | 2.39                     | 0.55              |
| 1:A:102:ALA:O    | 1:A:103:SER:CB   | 2.55                     | 0.55              |
| 1:A:574:GLN:NE2  | 1:A:578:GLU:HB3  | 2.22                     | 0.55              |
| 1:A:684:ARG:HG2  | 1:A:684:ARG:HH11 | 1.71                     | 0.55              |
| 1:A:352:ALA:C    | 1:A:353:PHE:HD1  | 2.15                     | 0.55              |
| 1:A:610:ARG:HH22 | 1:A:653:PHE:CA   | 2.20                     | 0.55              |
| 1:A:185:LEU:HD23 | 1:A:228:GLU:CG   | 2.35                     | 0.55              |
| 1:A:263:ALA:HB1  | 1:A:287:TYR:HB2  | 1.86                     | 0.55              |
| 1:A:271:GLY:HA2  | 4:A:961:HOH:O    | 2.06                     | 0.54              |
| 1:A:334:ALA:HB3  | 1:A:353:PHE:CD2  | 2.40                     | 0.54              |
| 1:A:278:VAL:CG1  | 1:A:316:ILE:HG21 | 2.38                     | 0.54              |
| 1:A:473:LYS:O    | 1:A:477:LEU:HB2  | 2.07                     | 0.54              |
| 1:A:588:LYS:HA   | 1:A:591:VAL:HG23 | 1.88                     | 0.54              |
| 1:A:4:HIS:CE1    | 1:A:6:VAL:HG12   | 2.42                     | 0.54              |
| 1:A:11:MSE:HE1   | 1:A:516:GLN:NE2  | 2.22                     | 0.54              |
| 1:A:176:GLU:C    | 1:A:178:LEU:H    | 2.16                     | 0.54              |
| 1:A:431:ILE:HG22 | 1:A:432:LEU:HD13 | 1.88                     | 0.54              |
| 1:A:278:VAL:HG12 | 1:A:316:ILE:HG21 | 1.90                     | 0.54              |
| 1:A:616:ARG:HA   | 1:A:616:ARG:NE   | 2.23                     | 0.54              |
| 1:A:69:LEU:HD21  | 1:A:97:MSE:CE    | 2.37                     | 0.54              |
| 1:A:162:LEU:HD21 | 1:A:184:ILE:CD1  | 2.37                     | 0.54              |
| 1:A:510:THR:CG2  | 1:A:511:ALA:N    | 2.71                     | 0.54              |
| 1:A:517:SER:O    | 1:A:518:TYR:CB   | 2.54                     | 0.54              |
| 1:A:563:THR:HA   | 1:A:608:ALA:HB3  | 1.90                     | 0.54              |
| 1:A:659:SER:O    | 1:A:663:MSE:HG3  | 2.07                     | 0.54              |
| 1:A:700:ILE:HG12 | 1:A:733:CYS:C    | 2.32                     | 0.54              |
| 1:A:121:VAL:HG12 | 1:A:166:LYS:HG2  | 1.88                     | 0.54              |
| 1:A:34:LEU:O     | 1:A:37:VAL:HB    | 2.08                     | 0.54              |
| 1:A:353:PHE:O    | 1:A:357:LYS:HG3  | 2.06                     | 0.54              |
| 1:A:376:LEU:O    | 1:A:380:ASN:N    | 2.39                     | 0.54              |
| 1:A:130:PHE:HB3  | 1:A:187:ILE:HD12 | 1.87                     | 0.54              |
| 1:A:66:ASP:OD2   | 1:A:68:VAL:HB    | 2.07                     | 0.54              |
| 1:A:55:LYS:HG2   | 1:A:56:PHE:CE2   | 2.43                     | 0.54              |
| 1:A:301:ASN:O    | 1:A:303:PHE:N    | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:422:ALA:O    | 1:A:424:GLN:N    | 2.41                     | 0.54              |
| 1:A:707:SER:HB3  | 1:A:709:GLU:HG3  | 1.90                     | 0.54              |
| 1:A:243:TYR:HA   | 1:A:267:ASP:HB2  | 1.89                     | 0.53              |
| 1:A:370:GLY:O    | 1:A:371:GLN:C    | 2.51                     | 0.53              |
| 1:A:398:VAL:O    | 1:A:398:VAL:HG12 | 2.08                     | 0.53              |
| 1:A:119:TYR:CE1  | 1:A:121:VAL:HA   | 2.44                     | 0.53              |
| 1:A:167:ALA:H    | 1:A:177:LEU:HD21 | 1.72                     | 0.53              |
| 1:A:428:ASN:O    | 1:A:429:LEU:HB2  | 2.08                     | 0.53              |
| 1:A:610:ARG:NH2  | 1:A:653:PHE:HB3  | 2.23                     | 0.53              |
| 1:A:648:MSE:O    | 1:A:670:ILE:HA   | 2.07                     | 0.53              |
| 1:A:282:PHE:CD1  | 1:A:283:PRO:HD2  | 2.44                     | 0.53              |
| 1:A:338:ILE:HG23 | 1:A:338:ILE:O    | 2.08                     | 0.53              |
| 1:A:477:LEU:HB3  | 1:A:486:LEU:HD13 | 1.90                     | 0.53              |
| 1:A:571:ARG:HD2  | 1:A:573:ASP:OD1  | 2.08                     | 0.53              |
| 1:A:581:TYR:OH   | 1:A:629:HIS:HB3  | 2.08                     | 0.53              |
| 1:A:136:LYS:NZ   | 1:A:140:GLU:OE2  | 2.33                     | 0.53              |
| 1:A:557:MSE:SE   | 1:A:603:GLN:HE21 | 2.41                     | 0.53              |
| 1:A:591:VAL:HG21 | 1:A:634:THR:O    | 2.08                     | 0.53              |
| 1:A:739:LYS:HG2  | 1:A:740:TYR:N    | 2.24                     | 0.53              |
| 1:A:359:VAL:O    | 1:A:360:GLU:C    | 2.51                     | 0.53              |
| 1:A:638:VAL:HG22 | 1:A:642:THR:HB   | 1.90                     | 0.53              |
| 1:A:696:GLY:HA3  | 1:A:731:PRO:O    | 2.09                     | 0.53              |
| 1:A:703:PRO:HD3  | 1:A:738:ARG:HH21 | 1.74                     | 0.53              |
| 1:A:43:SER:O     | 1:A:47:LYS:HD2   | 2.09                     | 0.53              |
| 1:A:646:THR:O    | 1:A:669:THR:HG22 | 2.08                     | 0.53              |
| 1:A:373:ASP:OD2  | 1:A:376:LEU:HG   | 2.09                     | 0.53              |
| 1:A:601:VAL:HG13 | 1:A:643:GLN:O    | 2.08                     | 0.53              |
| 1:A:738:ARG:CG   | 1:A:743:VAL:HG12 | 2.39                     | 0.53              |
| 1:A:754:ALA:O    | 1:A:755:LYS:C    | 2.52                     | 0.53              |
| 1:A:123:GLU:HB3  | 1:A:168:ALA:HB2  | 1.89                     | 0.53              |
| 1:A:422:ALA:C    | 1:A:424:GLN:N    | 2.65                     | 0.53              |
| 1:A:718:MSE:HB3  | 1:A:722:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:729:VAL:HG12 | 1:A:750:MSE:HE3  | 1.91                     | 0.52              |
| 1:A:30:THR:C     | 1:A:32:GLU:N     | 2.67                     | 0.52              |
| 1:A:67:GLN:HG2   | 1:A:68:VAL:N     | 2.23                     | 0.52              |
| 1:A:178:LEU:HD21 | 1:A:221:ALA:HB1  | 1.89                     | 0.52              |
| 1:A:289:PHE:HA   | 1:A:323:VAL:O    | 2.10                     | 0.52              |
| 1:A:672:ASN:CG   | 1:A:673:SER:H    | 2.16                     | 0.52              |
| 1:A:439:SER:OG   | 1:A:736:LYS:HB2  | 2.09                     | 0.52              |
| 1:A:469:GLU:O    | 1:A:473:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:559:THR:HA   | 1:A:605:ASP:OD1  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:180:LEU:O    | 1:A:184:ILE:HG12 | 2.10                     | 0.52              |
| 1:A:481:LEU:O    | 1:A:482:ASP:HB2  | 2.09                     | 0.52              |
| 1:A:562:VAL:HB   | 1:A:606:GLU:OE2  | 2.09                     | 0.52              |
| 1:A:740:TYR:HA   | 1:A:743:VAL:CG2  | 2.39                     | 0.52              |
| 1:A:22:GLU:HA    | 1:A:25:TRP:HB2   | 1.92                     | 0.52              |
| 1:A:67:GLN:HB3   | 4:A:940:HOH:O    | 2.10                     | 0.52              |
| 1:A:73:ALA:O     | 1:A:134:SER:HB2  | 2.10                     | 0.52              |
| 1:A:437:ILE:CG1  | 1:A:731:PRO:HB2  | 2.40                     | 0.52              |
| 1:A:490:GLU:HB3  | 1:A:493:ARG:HD2  | 1.92                     | 0.52              |
| 1:A:495:ASP:HB3  | 1:A:498:GLU:HG2  | 1.91                     | 0.52              |
| 1:A:534:ARG:HG2  | 1:A:586:ALA:CB   | 2.33                     | 0.52              |
| 1:A:163:LEU:HD13 | 1:A:209:VAL:HG11 | 1.92                     | 0.52              |
| 1:A:650:TYR:HB2  | 1:A:653:PHE:CD2  | 2.45                     | 0.52              |
| 1:A:712:ALA:O    | 1:A:716:ASN:ND2  | 2.42                     | 0.52              |
| 1:A:712:ALA:HA   | 1:A:753:ALA:HB1  | 1.91                     | 0.51              |
| 1:A:203:ILE:HG12 | 1:A:204:GLN:N    | 2.26                     | 0.51              |
| 1:A:220:GLN:O    | 1:A:223:THR:N    | 2.43                     | 0.51              |
| 1:A:632:ARG:C    | 1:A:634:THR:N    | 2.63                     | 0.51              |
| 1:A:680:LEU:HB2  | 1:A:721:VAL:HG21 | 1.92                     | 0.51              |
| 1:A:258:LEU:HA   | 4:A:907:HOH:O    | 2.09                     | 0.51              |
| 1:A:322:LEU:HD13 | 1:A:322:LEU:C    | 2.35                     | 0.51              |
| 1:A:414:THR:HG21 | 1:A:419:ARG:HB2  | 1.92                     | 0.51              |
| 1:A:357:LYS:HA   | 1:A:360:GLU:CG   | 2.37                     | 0.51              |
| 1:A:244:PHE:O    | 1:A:245:ALA:HB2  | 2.10                     | 0.51              |
| 1:A:341:THR:C    | 1:A:343:LEU:N    | 2.65                     | 0.51              |
| 1:A:610:ARG:O    | 1:A:612:GLY:N    | 2.44                     | 0.51              |
| 1:A:101:ASN:ND2  | 1:A:104:VAL:O    | 2.44                     | 0.51              |
| 1:A:492:GLU:C    | 1:A:493:ARG:HG3  | 2.35                     | 0.51              |
| 1:A:744:LYS:C    | 1:A:746:ALA:N    | 2.67                     | 0.51              |
| 1:A:84:TYR:CE2   | 1:A:86:GLY:HA2   | 2.45                     | 0.51              |
| 1:A:110:THR:O    | 1:A:118:HIS:HA   | 2.11                     | 0.51              |
| 1:A:399:GLN:C    | 1:A:399:GLN:NE2  | 2.69                     | 0.51              |
| 1:A:500:PHE:HD1  | 1:A:538:MSE:CE   | 2.24                     | 0.51              |
| 1:A:298:ILE:HD11 | 1:A:353:PHE:CD2  | 2.46                     | 0.51              |
| 1:A:477:LEU:CD2  | 1:A:486:LEU:HD22 | 2.25                     | 0.51              |
| 1:A:45:ILE:HG22  | 1:A:49:MSE:CE    | 2.40                     | 0.50              |
| 1:A:162:LEU:HD21 | 1:A:184:ILE:HD11 | 1.93                     | 0.50              |
| 1:A:255:LEU:C    | 1:A:257:SER:H    | 2.18                     | 0.50              |
| 1:A:373:ASP:C    | 1:A:375:ALA:N    | 2.69                     | 0.50              |
| 1:A:712:ALA:CA   | 1:A:753:ALA:HB1  | 2.41                     | 0.50              |
| 1:A:747:LEU:O    | 1:A:749:ASN:N    | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:PHE:HA    | 1:A:98:ALA:HB3   | 1.93                     | 0.50              |
| 1:A:437:ILE:HG12 | 1:A:731:PRO:HD2  | 1.93                     | 0.50              |
| 1:A:55:LYS:HA    | 1:A:55:LYS:HE2   | 1.93                     | 0.50              |
| 1:A:416:VAL:C    | 1:A:418:ALA:H    | 2.18                     | 0.50              |
| 1:A:467:ILE:HA   | 1:A:470:GLU:HB2  | 1.92                     | 0.50              |
| 1:A:700:ILE:HD11 | 1:A:701:HIS:CE1  | 2.47                     | 0.50              |
| 1:A:18:LYS:CG    | 1:A:520:SER:HB2  | 2.41                     | 0.50              |
| 1:A:397:GLY:C    | 1:A:399:GLN:N    | 2.53                     | 0.50              |
| 1:A:645:HIS:CD2  | 1:A:667:VAL:HB   | 2.47                     | 0.50              |
| 1:A:337:LEU:HD12 | 1:A:353:PHE:CE1  | 2.47                     | 0.50              |
| 1:A:341:THR:HG23 | 1:A:342:LYS:HD3  | 1.93                     | 0.50              |
| 1:A:395:ASN:OD1  | 1:A:397:GLY:N    | 2.44                     | 0.50              |
| 1:A:739:LYS:CG   | 1:A:740:TYR:H    | 2.24                     | 0.50              |
| 1:A:17:LEU:CD1   | 1:A:21:LEU:HG    | 2.41                     | 0.50              |
| 1:A:59:SER:HB3   | 1:A:151:THR:OG1  | 2.11                     | 0.50              |
| 1:A:189:LYS:O    | 1:A:190:GLU:C    | 2.55                     | 0.50              |
| 1:A:229:LEU:O    | 1:A:232:THR:N    | 2.44                     | 0.50              |
| 1:A:381:ALA:HA   | 1:A:384:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:426:LYS:O    | 1:A:427:LEU:HG   | 2.11                     | 0.50              |
| 1:A:622:PHE:O    | 1:A:625:ASP:CB   | 2.59                     | 0.50              |
| 1:A:631:PHE:CD2  | 1:A:663:MSE:HE2  | 2.47                     | 0.50              |
| 1:A:160:SER:CB   | 1:A:207:GLU:OE1  | 2.60                     | 0.50              |
| 1:A:181:LEU:O    | 1:A:185:LEU:HB2  | 2.11                     | 0.50              |
| 1:A:48:GLN:HG2   | 1:A:48:GLN:O     | 2.12                     | 0.50              |
| 1:A:122:PRO:HD2  | 1:A:165:SER:HA   | 1.94                     | 0.50              |
| 1:A:158:PRO:O    | 1:A:162:LEU:HD12 | 2.11                     | 0.50              |
| 1:A:581:TYR:HE1  | 1:A:630:SER:CA   | 2.24                     | 0.50              |
| 1:A:700:ILE:HD13 | 4:A:836:HOH:O    | 2.12                     | 0.50              |
| 1:A:510:THR:CG2  | 1:A:513:GLY:H    | 2.24                     | 0.50              |
| 1:A:657:ILE:HG23 | 1:A:658:HIS:N    | 2.27                     | 0.50              |
| 1:A:738:ARG:CZ   | 1:A:738:ARG:HA   | 2.41                     | 0.50              |
| 1:A:396:GLU:O    | 1:A:399:GLN:HB2  | 2.12                     | 0.49              |
| 1:A:677:GLU:O    | 1:A:721:VAL:HG21 | 2.12                     | 0.49              |
| 1:A:212:MSE:HE1  | 1:A:615:LEU:CD1  | 2.41                     | 0.49              |
| 1:A:318:GLY:O    | 1:A:320:ASP:N    | 2.44                     | 0.49              |
| 1:A:337:LEU:HB3  | 1:A:356:GLN:CD   | 2.38                     | 0.49              |
| 1:A:347:ILE:O    | 1:A:350:TRP:N    | 2.40                     | 0.49              |
| 1:A:575:PRO:CB   | 1:A:577:HIS:CE1  | 2.89                     | 0.49              |
| 1:A:587:ILE:HG22 | 1:A:634:THR:HG23 | 1.93                     | 0.49              |
| 1:A:687:VAL:O    | 1:A:688:LYS:HB2  | 2.11                     | 0.49              |
| 1:A:223:THR:HG23 | 4:A:907:HOH:O    | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:684:ARG:HA   | 1:A:688:LYS:H    | 1.77                     | 0.49              |
| 1:A:359:VAL:O    | 1:A:362:ASN:N    | 2.45                     | 0.49              |
| 1:A:416:VAL:HG13 | 1:A:417:SER:N    | 2.27                     | 0.49              |
| 1:A:581:TYR:HE1  | 1:A:630:SER:HB2  | 1.69                     | 0.49              |
| 1:A:431:ILE:HG22 | 1:A:432:LEU:CD1  | 2.42                     | 0.49              |
| 1:A:541:PHE:O    | 1:A:545:MSE:HB2  | 2.13                     | 0.49              |
| 1:A:558:LEU:HB2  | 1:A:604:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:611:GLU:CD   | 1:A:611:GLU:N    | 2.68                     | 0.49              |
| 1:A:489:GLY:C    | 1:A:491:PRO:HD3  | 2.37                     | 0.49              |
| 1:A:587:ILE:CG2  | 1:A:634:THR:HG23 | 2.43                     | 0.49              |
| 1:A:657:ILE:CD1  | 1:A:687:VAL:HG21 | 2.43                     | 0.49              |
| 1:A:679:LEU:O    | 1:A:682:VAL:HG13 | 2.12                     | 0.49              |
| 1:A:414:THR:HG22 | 1:A:418:ALA:HB3  | 1.95                     | 0.49              |
| 1:A:463:TYR:HA   | 1:A:466:ALA:CB   | 2.41                     | 0.49              |
| 1:A:464:VAL:HG13 | 1:A:465:LYS:HE2  | 1.94                     | 0.49              |
| 1:A:748:LYS:HB2  | 1:A:748:LYS:NZ   | 2.28                     | 0.49              |
| 1:A:89:ILE:HG23  | 1:A:93:VAL:HB    | 1.95                     | 0.49              |
| 1:A:468:LYS:O    | 1:A:472:LYS:HG3  | 2.13                     | 0.49              |
| 1:A:67:GLN:HG2   | 1:A:68:VAL:H     | 1.77                     | 0.49              |
| 1:A:89:ILE:HG22  | 1:A:90:GLY:N     | 2.28                     | 0.49              |
| 1:A:239:LEU:O    | 1:A:239:LEU:HD13 | 2.13                     | 0.49              |
| 1:A:760:GLN:NE2  | 1:A:760:GLN:N    | 2.60                     | 0.49              |
| 1:A:399:GLN:HE21 | 1:A:400:LYS:N    | 2.10                     | 0.48              |
| 1:A:593:ASP:O    | 1:A:597:GLY:N    | 2.45                     | 0.48              |
| 1:A:695:PRO:HD2  | 1:A:718:MSE:CE   | 2.43                     | 0.48              |
| 1:A:30:THR:O     | 1:A:32:GLU:N     | 2.46                     | 0.48              |
| 1:A:667:VAL:HG21 | 1:A:728:TRP:CE2  | 2.48                     | 0.48              |
| 1:A:725:ASN:C    | 1:A:726:ILE:HG12 | 2.37                     | 0.48              |
| 1:A:755:LYS:O    | 1:A:758:ARG:HB3  | 2.13                     | 0.48              |
| 1:A:101:ASN:C    | 1:A:101:ASN:HD22 | 2.19                     | 0.48              |
| 1:A:107:MSE:SE   | 1:A:123:GLU:OE2  | 2.81                     | 0.48              |
| 1:A:436:THR:HA   | 1:A:731:PRO:CD   | 2.44                     | 0.48              |
| 1:A:639:GLN:NE2  | 1:A:639:GLN:HA   | 2.28                     | 0.48              |
| 1:A:319:LYS:O    | 1:A:320:ASP:CB   | 2.62                     | 0.48              |
| 1:A:331:LEU:HD13 | 1:A:331:LEU:C    | 2.39                     | 0.48              |
| 1:A:442:GLN:HB3  | 1:A:445:GLU:CG   | 2.43                     | 0.48              |
| 1:A:600:GLY:O    | 1:A:642:THR:HG23 | 2.13                     | 0.48              |
| 1:A:757:ILE:HB   | 4:A:826:HOH:O    | 2.13                     | 0.48              |
| 1:A:24:PHE:HB2   | 4:A:848:HOH:O    | 2.13                     | 0.48              |
| 1:A:114:ASP:OD1  | 1:A:296:ARG:NH2  | 2.46                     | 0.48              |
| 1:A:486:LEU:O    | 1:A:555:LYS:HG2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:499:TYR:O    | 1:A:501:GLY:N    | 2.46                     | 0.48              |
| 1:A:516:GLN:N    | 4:A:838:HOH:O    | 2.45                     | 0.48              |
| 1:A:112:TRP:HB2  | 1:A:117:TYR:HD2  | 1.78                     | 0.48              |
| 1:A:700:ILE:HG12 | 1:A:733:CYS:H    | 1.78                     | 0.48              |
| 1:A:157:GLY:O    | 1:A:158:PRO:C    | 2.54                     | 0.48              |
| 1:A:192:ILE:HG21 | 1:A:232:THR:HG22 | 1.96                     | 0.48              |
| 1:A:220:GLN:O    | 1:A:221:ALA:C    | 2.56                     | 0.48              |
| 1:A:437:ILE:HD11 | 1:A:731:PRO:O    | 2.14                     | 0.48              |
| 1:A:471:ILE:HD13 | 1:A:549:MSE:HE2  | 1.94                     | 0.48              |
| 1:A:64:HIS:HB3   | 1:A:95:PHE:CZ    | 2.49                     | 0.48              |
| 1:A:90:GLY:O     | 1:A:92:ASP:N     | 2.46                     | 0.48              |
| 1:A:311:GLN:HA   | 1:A:314:GLU:HG2  | 1.96                     | 0.48              |
| 1:A:484:ASP:O    | 1:A:552:ARG:HB3  | 2.13                     | 0.48              |
| 1:A:526:PRO:HA   | 4:A:814:HOH:O    | 2.14                     | 0.48              |
| 1:A:62:PHE:CG    | 1:A:63:ALA:N     | 2.78                     | 0.48              |
| 1:A:387:ARG:C    | 1:A:389:SER:H    | 2.22                     | 0.48              |
| 1:A:609:LEU:HB3  | 1:A:650:TYR:OH   | 2.14                     | 0.48              |
| 1:A:656:ILE:HG23 | 1:A:656:ILE:O    | 2.14                     | 0.48              |
| 1:A:6:VAL:HG13   | 1:A:326:THR:OG1  | 2.13                     | 0.48              |
| 1:A:588:LYS:HE3  | 1:A:636:CYS:SG   | 2.54                     | 0.48              |
| 1:A:590:GLU:O    | 1:A:594:LEU:HD12 | 2.14                     | 0.48              |
| 1:A:49:MSE:O     | 1:A:54:THR:CB    | 2.62                     | 0.47              |
| 1:A:476:ASP:OD1  | 1:A:476:ASP:C    | 2.57                     | 0.47              |
| 1:A:46:TRP:CE2   | 1:A:144:ALA:HB2  | 2.49                     | 0.47              |
| 1:A:145:LYS:HA   | 1:A:149:VAL:O    | 2.13                     | 0.47              |
| 1:A:273:LYS:HB3  | 1:A:273:LYS:HZ2  | 1.75                     | 0.47              |
| 1:A:647:HIS:C    | 1:A:648:MSE:HG3  | 2.39                     | 0.47              |
| 1:A:705:ILE:HD13 | 1:A:705:ILE:N    | 2.29                     | 0.47              |
| 1:A:77:ALA:O     | 1:A:78:VAL:C     | 2.58                     | 0.47              |
| 1:A:158:PRO:O    | 1:A:161:TYR:HB3  | 2.14                     | 0.47              |
| 1:A:205:LEU:O    | 1:A:240:VAL:HA   | 2.13                     | 0.47              |
| 1:A:333:THR:HG23 | 1:A:334:ALA:O    | 2.14                     | 0.47              |
| 1:A:547:GLN:HB2  | 1:A:554:MSE:CB   | 2.44                     | 0.47              |
| 1:A:170:GLY:O    | 1:A:171:VAL:C    | 2.58                     | 0.47              |
| 1:A:395:ASN:OD1  | 1:A:396:GLU:N    | 2.48                     | 0.47              |
| 1:A:436:THR:HA   | 1:A:731:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:689:TYR:O    | 1:A:690:GLY:C    | 2.57                     | 0.47              |
| 1:A:69:LEU:HD21  | 1:A:97:MSE:HE3   | 1.96                     | 0.47              |
| 1:A:240:VAL:HG22 | 1:A:261:VAL:CG1  | 2.44                     | 0.47              |
| 1:A:558:LEU:HD12 | 1:A:604:ILE:CD1  | 2.44                     | 0.47              |
| 1:A:698:TYR:CD1  | 1:A:698:TYR:C    | 2.92                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:723:GLU:HG3  | 1:A:724:GLN:H    | 1.79                     | 0.47              |
| 1:A:109:MSE:HE1  | 1:A:518:TYR:CE1  | 2.50                     | 0.47              |
| 1:A:217:GLN:H    | 1:A:217:GLN:HE21 | 1.63                     | 0.47              |
| 1:A:311:GLN:O    | 1:A:314:GLU:HG2  | 2.15                     | 0.47              |
| 1:A:335:VAL:HG12 | 1:A:336:ASP:H    | 1.78                     | 0.47              |
| 1:A:583:ILE:O    | 1:A:583:ILE:HG22 | 2.14                     | 0.47              |
| 1:A:37:VAL:O     | 1:A:38:SER:C     | 2.58                     | 0.47              |
| 1:A:59:SER:HB3   | 1:A:151:THR:CB   | 2.44                     | 0.47              |
| 1:A:69:LEU:HD13  | 1:A:94:TYR:CE1   | 2.50                     | 0.47              |
| 1:A:432:LEU:CD1  | 1:A:727:LEU:HB3  | 2.45                     | 0.47              |
| 1:A:510:THR:HG22 | 1:A:524:LYS:HD3  | 1.97                     | 0.47              |
| 1:A:559:THR:HG22 | 1:A:559:THR:O    | 2.15                     | 0.47              |
| 1:A:622:PHE:O    | 1:A:625:ASP:HB3  | 2.14                     | 0.47              |
| 1:A:111:LYS:H    | 1:A:111:LYS:NZ   | 2.08                     | 0.47              |
| 1:A:501:GLY:C    | 1:A:503:GLN:H    | 2.22                     | 0.47              |
| 1:A:667:VAL:HG21 | 1:A:728:TRP:NE1  | 2.30                     | 0.47              |
| 1:A:573:ASP:OD1  | 1:A:573:ASP:N    | 2.48                     | 0.46              |
| 1:A:602:ILE:O    | 1:A:644:ILE:HG23 | 2.15                     | 0.46              |
| 1:A:669:THR:C    | 1:A:670:ILE:HG23 | 2.40                     | 0.46              |
| 1:A:680:LEU:O    | 1:A:683:PHE:HD2  | 1.98                     | 0.46              |
| 1:A:700:ILE:HG13 | 1:A:733:CYS:H    | 1.79                     | 0.46              |
| 1:A:4:HIS:HE1    | 1:A:6:VAL:HG12   | 1.80                     | 0.46              |
| 1:A:204:GLN:HG3  | 1:A:239:LEU:CD1  | 2.45                     | 0.46              |
| 1:A:347:ILE:O    | 1:A:350:TRP:HB2  | 2.15                     | 0.46              |
| 1:A:471:ILE:HD12 | 1:A:474:VAL:HB   | 1.97                     | 0.46              |
| 1:A:547:GLN:NE2  | 1:A:547:GLN:HA   | 2.28                     | 0.46              |
| 1:A:18:LYS:CE    | 1:A:521:ARG:NH2  | 2.78                     | 0.46              |
| 1:A:191:VAL:CG1  | 1:A:195:LEU:HD11 | 2.37                     | 0.46              |
| 1:A:698:TYR:HE2  | 1:A:731:PRO:HG3  | 1.79                     | 0.46              |
| 1:A:751:VAL:O    | 1:A:755:LYS:HG3  | 2.15                     | 0.46              |
| 1:A:12:GLY:HA2   | 4:A:966:HOH:O    | 2.15                     | 0.46              |
| 1:A:341:THR:CG2  | 1:A:342:LYS:NZ   | 2.79                     | 0.46              |
| 1:A:468:LYS:HG2  | 1:A:472:LYS:NZ   | 2.30                     | 0.46              |
| 1:A:507:PHE:N    | 1:A:529:TYR:CE2  | 2.83                     | 0.46              |
| 1:A:717:LYS:O    | 1:A:721:VAL:HG22 | 2.15                     | 0.46              |
| 1:A:723:GLU:HG3  | 1:A:724:GLN:N    | 2.30                     | 0.46              |
| 1:A:421:ASP:O    | 1:A:424:GLN:HB2  | 2.16                     | 0.46              |
| 1:A:699:ASP:OD1  | 1:A:732:ASP:OD1  | 2.33                     | 0.46              |
| 1:A:739:LYS:HB3  | 1:A:742:GLU:HG2  | 1.97                     | 0.46              |
| 1:A:760:GLN:N    | 1:A:760:GLN:CD   | 2.73                     | 0.46              |
| 1:A:145:LYS:C    | 1:A:147:LEU:H    | 2.22                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:LEU:CD2  | 1:A:228:GLU:HG2  | 2.37                     | 0.46              |
| 1:A:193:THR:HA   | 1:A:196:LYS:HB2  | 1.98                     | 0.46              |
| 1:A:313:LEU:C    | 1:A:315:GLY:N    | 2.73                     | 0.46              |
| 1:A:555:LYS:HA   | 1:A:601:VAL:O    | 2.15                     | 0.46              |
| 1:A:558:LEU:HD12 | 1:A:604:ILE:HD11 | 1.98                     | 0.46              |
| 1:A:158:PRO:O    | 1:A:159:VAL:C    | 2.59                     | 0.46              |
| 1:A:411:ARG:NH2  | 1:A:419:ARG:CD   | 2.78                     | 0.46              |
| 1:A:581:TYR:HE1  | 1:A:630:SER:CB   | 2.28                     | 0.46              |
| 1:A:9:PRO:HA     | 1:A:331:LEU:HD23 | 1.98                     | 0.46              |
| 1:A:247:ILE:H    | 1:A:247:ILE:CD1  | 2.20                     | 0.46              |
| 1:A:529:TYR:CD1  | 1:A:530:GLY:N    | 2.83                     | 0.46              |
| 1:A:558:LEU:HD12 | 1:A:604:ILE:CG1  | 2.46                     | 0.46              |
| 1:A:757:ILE:H    | 1:A:757:ILE:CD1  | 2.15                     | 0.46              |
| 1:A:195:LEU:HD12 | 1:A:195:LEU:H    | 1.81                     | 0.46              |
| 1:A:283:PRO:O    | 1:A:284:GLU:O    | 2.33                     | 0.46              |
| 1:A:340:GLU:OE2  | 1:A:512:ASN:N    | 2.37                     | 0.46              |
| 1:A:405:LEU:HD13 | 1:A:405:LEU:N    | 2.31                     | 0.46              |
| 1:A:525:PRO:HB3  | 1:A:568:SER:HA   | 1.98                     | 0.46              |
| 1:A:670:ILE:CD1  | 1:A:670:ILE:N    | 2.76                     | 0.46              |
| 1:A:711:ILE:O    | 1:A:715:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:372:LYS:O    | 1:A:374:GLU:N    | 2.49                     | 0.46              |
| 1:A:495:ASP:HB3  | 1:A:498:GLU:CB   | 2.45                     | 0.46              |
| 1:A:679:LEU:O    | 1:A:682:VAL:HG22 | 2.16                     | 0.46              |
| 1:A:725:ASN:O    | 1:A:725:ASN:CG   | 2.59                     | 0.46              |
| 1:A:9:PRO:HG3    | 1:A:331:LEU:HA   | 1.98                     | 0.45              |
| 1:A:36:LYS:HB2   | 4:A:1010:HOH:O   | 2.15                     | 0.45              |
| 1:A:254:THR:O    | 1:A:258:LEU:HG   | 2.15                     | 0.45              |
| 1:A:341:THR:O    | 1:A:342:LYS:C    | 2.59                     | 0.45              |
| 1:A:653:PHE:CZ   | 1:A:670:ILE:HG21 | 2.49                     | 0.45              |
| 1:A:693:ILE:C    | 1:A:695:PRO:HD3  | 2.41                     | 0.45              |
| 1:A:176:GLU:C    | 1:A:178:LEU:N    | 2.74                     | 0.45              |
| 1:A:240:VAL:HG22 | 1:A:261:VAL:HG11 | 1.98                     | 0.45              |
| 1:A:254:THR:HG23 | 4:A:1055:HOH:O   | 2.15                     | 0.45              |
| 1:A:397:GLY:O    | 1:A:399:GLN:N    | 2.47                     | 0.45              |
| 1:A:431:ILE:O    | 1:A:432:LEU:C    | 2.59                     | 0.45              |
| 1:A:437:ILE:HG12 | 1:A:731:PRO:HB2  | 1.98                     | 0.45              |
| 1:A:534:ARG:NH2  | 1:A:536:LYS:C    | 2.74                     | 0.45              |
| 1:A:136:LYS:O    | 1:A:137:ALA:C    | 2.58                     | 0.45              |
| 1:A:217:GLN:H    | 1:A:217:GLN:NE2  | 2.14                     | 0.45              |
| 1:A:250:GLU:HB2  | 4:A:856:HOH:O    | 2.16                     | 0.45              |
| 1:A:305:ALA:O    | 1:A:306:SER:C    | 2.59                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:310:LEU:CD1  | 1:A:364:LEU:HD13 | 2.47                     | 0.45              |
| 1:A:492:GLU:O    | 1:A:493:ARG:HG3  | 2.16                     | 0.45              |
| 1:A:577:HIS:HA   | 1:A:580:CYS:HB3  | 1.99                     | 0.45              |
| 1:A:661:ILE:HG13 | 1:A:689:TYR:CD1  | 2.50                     | 0.45              |
| 1:A:79:PRO:HB3   | 1:A:80:PRO:HD2   | 1.99                     | 0.45              |
| 1:A:248:PRO:O    | 1:A:249:ALA:C    | 2.60                     | 0.45              |
| 1:A:361:VAL:O    | 1:A:365:ALA:HB2  | 2.17                     | 0.45              |
| 1:A:408:SER:HA   | 1:A:629:HIS:CE1  | 2.51                     | 0.45              |
| 1:A:411:ARG:NH1  | 1:A:644:ILE:HD13 | 2.31                     | 0.45              |
| 1:A:13:PRO:HD3   | 4:A:966:HOH:O    | 2.16                     | 0.45              |
| 1:A:50:SER:HB3   | 1:A:57:ILE:CD1   | 2.47                     | 0.45              |
| 1:A:350:TRP:HH2  | 1:A:390:SER:CB   | 2.29                     | 0.45              |
| 1:A:373:ASP:OD2  | 1:A:375:ALA:HB3  | 2.17                     | 0.45              |
| 1:A:516:GLN:HG2  | 1:A:518:TYR:H    | 1.80                     | 0.45              |
| 1:A:610:ARG:NH2  | 1:A:653:PHE:HA   | 2.27                     | 0.45              |
| 1:A:705:ILE:H    | 1:A:705:ILE:CD1  | 2.29                     | 0.45              |
| 1:A:632:ARG:HH11 | 1:A:632:ARG:CB   | 2.29                     | 0.45              |
| 1:A:656:ILE:O    | 1:A:656:ILE:HG12 | 2.17                     | 0.45              |
| 1:A:186:PRO:O    | 1:A:190:GLU:HG2  | 2.17                     | 0.45              |
| 1:A:220:GLN:O    | 1:A:222:PHE:N    | 2.49                     | 0.45              |
| 1:A:420:LEU:HA   | 1:A:423:GLN:OE1  | 2.17                     | 0.45              |
| 1:A:434:THR:HA   | 1:A:729:VAL:HB   | 1.99                     | 0.45              |
| 1:A:577:HIS:HB3  | 1:A:626:TRP:CG   | 2.52                     | 0.45              |
| 1:A:628:VAL:O    | 1:A:629:HIS:C    | 2.60                     | 0.45              |
| 1:A:639:GLN:C    | 1:A:641:SER:N    | 2.75                     | 0.45              |
| 1:A:684:ARG:HA   | 1:A:688:LYS:N    | 2.32                     | 0.45              |
| 1:A:105:PRO:HA   | 4:A:877:HOH:O    | 2.16                     | 0.45              |
| 1:A:419:ARG:HD3  | 4:A:888:HOH:O    | 2.16                     | 0.45              |
| 1:A:652:HIS:NE2  | 1:A:679:LEU:HD13 | 2.32                     | 0.45              |
| 1:A:59:SER:O     | 1:A:60:ASN:CB    | 2.64                     | 0.44              |
| 1:A:272:THR:HA   | 1:A:275:LEU:CD1  | 2.47                     | 0.44              |
| 1:A:437:ILE:HG13 | 1:A:731:PRO:HB2  | 1.99                     | 0.44              |
| 1:A:468:LYS:HG2  | 1:A:472:LYS:HZ1  | 1.81                     | 0.44              |
| 1:A:380:ASN:C    | 1:A:382:ALA:N    | 2.73                     | 0.44              |
| 1:A:417:SER:HA   | 1:A:420:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:700:ILE:HG23 | 1:A:731:PRO:HB3  | 1.99                     | 0.44              |
| 1:A:739:LYS:CG   | 1:A:740:TYR:N    | 2.80                     | 0.44              |
| 1:A:299:TRP:HA   | 1:A:351:MSE:HA   | 1.98                     | 0.44              |
| 1:A:335:VAL:HG23 | 4:A:884:HOH:O    | 2.16                     | 0.44              |
| 1:A:357:LYS:O    | 1:A:360:GLU:HB2  | 2.17                     | 0.44              |
| 1:A:471:ILE:O    | 1:A:475:VAL:HG23 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:533:SER:C    | 1:A:535:PRO:HD3  | 2.41                     | 0.44              |
| 1:A:622:PHE:C    | 1:A:622:PHE:CD2  | 2.94                     | 0.44              |
| 1:A:638:VAL:CG2  | 1:A:642:THR:HB   | 2.47                     | 0.44              |
| 1:A:653:PHE:CE2  | 1:A:670:ILE:HG21 | 2.52                     | 0.44              |
| 1:A:6:VAL:HG22   | 1:A:329:SER:HA   | 2.00                     | 0.44              |
| 1:A:176:GLU:O    | 1:A:178:LEU:N    | 2.50                     | 0.44              |
| 1:A:416:VAL:C    | 1:A:418:ALA:N    | 2.76                     | 0.44              |
| 1:A:581:TYR:CE1  | 1:A:633:ILE:HD12 | 2.52                     | 0.44              |
| 1:A:313:LEU:O    | 1:A:314:GLU:C    | 2.60                     | 0.44              |
| 1:A:341:THR:HG23 | 1:A:342:LYS:H    | 1.83                     | 0.44              |
| 1:A:576:ARG:HG3  | 3:A:771:SO4:O1   | 2.17                     | 0.44              |
| 1:A:62:PHE:O     | 1:A:63:ALA:CB    | 2.65                     | 0.44              |
| 1:A:159:VAL:HG11 | 1:A:222:PHE:CD2  | 2.53                     | 0.44              |
| 1:A:364:LEU:O    | 1:A:368:LEU:HB2  | 2.17                     | 0.44              |
| 1:A:395:ASN:C    | 1:A:397:GLY:N    | 2.70                     | 0.44              |
| 1:A:571:ARG:HD2  | 1:A:573:ASP:CG   | 2.43                     | 0.44              |
| 1:A:680:LEU:O    | 1:A:683:PHE:CD2  | 2.71                     | 0.44              |
| 1:A:218:LYS:O    | 1:A:219:LEU:C    | 2.59                     | 0.44              |
| 1:A:318:GLY:C    | 1:A:320:ASP:N    | 2.70                     | 0.44              |
| 1:A:495:ASP:HB3  | 1:A:498:GLU:HB2  | 1.99                     | 0.44              |
| 1:A:650:TYR:HB2  | 1:A:653:PHE:HD2  | 1.82                     | 0.44              |
| 1:A:35:GLN:HE21  | 1:A:35:GLN:CA    | 2.17                     | 0.44              |
| 1:A:191:VAL:O    | 1:A:192:ILE:C    | 2.60                     | 0.44              |
| 1:A:350:TRP:CZ2  | 1:A:386:SER:HB2  | 2.48                     | 0.44              |
| 1:A:471:ILE:HD13 | 1:A:549:MSE:CE   | 2.48                     | 0.44              |
| 1:A:307:LEU:HD12 | 1:A:377:PHE:HE2  | 1.83                     | 0.44              |
| 1:A:345:ASP:O    | 1:A:347:ILE:N    | 2.51                     | 0.44              |
| 1:A:653:PHE:HB2  | 1:A:656:ILE:HG23 | 1.98                     | 0.44              |
| 1:A:67:GLN:HG2   | 1:A:68:VAL:HG23  | 2.00                     | 0.43              |
| 1:A:107:MSE:CE   | 1:A:120:ILE:HG21 | 2.35                     | 0.43              |
| 1:A:305:ALA:O    | 1:A:308:SER:HB3  | 2.18                     | 0.43              |
| 1:A:415:ASN:C    | 1:A:415:ASN:HD22 | 2.25                     | 0.43              |
| 1:A:519:GLY:HA3  | 4:A:829:HOH:O    | 2.17                     | 0.43              |
| 1:A:64:HIS:HB3   | 1:A:95:PHE:HZ    | 1.82                     | 0.43              |
| 1:A:307:LEU:HD21 | 1:A:368:LEU:HG   | 1.99                     | 0.43              |
| 1:A:503:GLN:O    | 1:A:504:LEU:HD23 | 2.18                     | 0.43              |
| 1:A:684:ARG:HG2  | 1:A:684:ARG:NH1  | 2.32                     | 0.43              |
| 1:A:687:VAL:O    | 1:A:688:LYS:CB   | 2.66                     | 0.43              |
| 1:A:329:SER:O    | 1:A:331:LEU:N    | 2.45                     | 0.43              |
| 1:A:362:ASN:HA   | 1:A:365:ALA:HB3  | 1.99                     | 0.43              |
| 1:A:390:SER:C    | 1:A:392:ARG:H    | 2.26                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:15:ARG:O     | 1:A:18:LYS:HB3   | 2.18                     | 0.43              |
| 1:A:68:VAL:HG21  | 1:A:119:TYR:CG   | 2.53                     | 0.43              |
| 1:A:126:PRO:HG3  | 1:A:175:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:436:THR:C    | 1:A:731:PRO:HD2  | 2.43                     | 0.43              |
| 1:A:521:ARG:HE   | 1:A:521:ARG:CA   | 2.23                     | 0.43              |
| 1:A:617:LYS:C    | 1:A:619:GLU:H    | 2.26                     | 0.43              |
| 1:A:79:PRO:HB2   | 1:A:82:TYR:CE2   | 2.53                     | 0.43              |
| 1:A:102:ALA:O    | 1:A:103:SER:HB3  | 2.18                     | 0.43              |
| 1:A:195:LEU:O    | 1:A:196:LYS:C    | 2.61                     | 0.43              |
| 1:A:477:LEU:HD13 | 1:A:487:VAL:H    | 1.82                     | 0.43              |
| 1:A:546:ALA:O    | 1:A:548:SER:N    | 2.50                     | 0.43              |
| 1:A:562:VAL:HG23 | 1:A:606:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:581:TYR:O    | 1:A:582:GLN:C    | 2.61                     | 0.43              |
| 1:A:636:CYS:HB2  | 4:A:847:HOH:O    | 2.18                     | 0.43              |
| 1:A:195:LEU:C    | 1:A:198:ALA:H    | 2.26                     | 0.43              |
| 1:A:739:LYS:HG2  | 1:A:740:TYR:H    | 1.83                     | 0.43              |
| 1:A:562:VAL:CG2  | 1:A:606:GLU:OE2  | 2.66                     | 0.43              |
| 1:A:617:LYS:C    | 1:A:619:GLU:N    | 2.74                     | 0.43              |
| 1:A:340:GLU:OE2  | 1:A:511:ALA:HB3  | 2.18                     | 0.43              |
| 1:A:406:LYS:HB3  | 1:A:406:LYS:HE2  | 1.80                     | 0.43              |
| 1:A:255:LEU:C    | 1:A:257:SER:N    | 2.77                     | 0.43              |
| 1:A:407:GLY:O    | 1:A:408:SER:O    | 2.37                     | 0.43              |
| 1:A:475:VAL:O    | 1:A:479:GLU:HG2  | 2.19                     | 0.43              |
| 1:A:610:ARG:O    | 1:A:613:LEU:HG   | 2.18                     | 0.43              |
| 1:A:632:ARG:HB2  | 1:A:632:ARG:NH1  | 2.34                     | 0.43              |
| 1:A:37:VAL:O     | 1:A:40:ASP:N     | 2.52                     | 0.43              |
| 1:A:341:THR:CG2  | 1:A:342:LYS:N    | 2.82                     | 0.43              |
| 1:A:395:ASN:CG   | 1:A:396:GLU:N    | 2.77                     | 0.43              |
| 1:A:430:PRO:HB2  | 1:A:758:ARG:HH22 | 1.84                     | 0.43              |
| 1:A:534:ARG:HH21 | 1:A:537:ALA:N    | 2.16                     | 0.43              |
| 1:A:680:LEU:HD23 | 1:A:683:PHE:HE2  | 1.84                     | 0.43              |
| 1:A:120:ILE:HG22 | 4:A:834:HOH:O    | 2.18                     | 0.42              |
| 1:A:345:ASP:O    | 1:A:346:GLU:C    | 2.61                     | 0.42              |
| 1:A:697:VAL:O    | 1:A:698:TYR:CB   | 2.63                     | 0.42              |
| 1:A:700:ILE:C    | 1:A:702:SER:H    | 2.27                     | 0.42              |
| 1:A:18:LYS:HE2   | 1:A:521:ARG:NH2  | 2.35                     | 0.42              |
| 1:A:481:LEU:O    | 1:A:482:ASP:CB   | 2.66                     | 0.42              |
| 1:A:521:ARG:NE   | 1:A:521:ARG:CA   | 2.68                     | 0.42              |
| 1:A:521:ARG:NH2  | 4:A:997:HOH:O    | 2.52                     | 0.42              |
| 1:A:560:GLY:O    | 1:A:564:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:605:ASP:HA   | 1:A:647:HIS:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:689:TYR:CD2  | 1:A:691:ALA:HB3  | 2.53                     | 0.42              |
| 1:A:119:TYR:CD1  | 1:A:119:TYR:C    | 2.97                     | 0.42              |
| 1:A:162:LEU:O    | 1:A:165:SER:N    | 2.50                     | 0.42              |
| 1:A:181:LEU:HD23 | 1:A:181:LEU:HA   | 1.82                     | 0.42              |
| 1:A:353:PHE:O    | 1:A:354:ALA:C    | 2.60                     | 0.42              |
| 1:A:528:ILE:N    | 1:A:528:ILE:HD12 | 2.34                     | 0.42              |
| 1:A:610:ARG:C    | 1:A:612:GLY:H    | 2.27                     | 0.42              |
| 1:A:631:PHE:O    | 1:A:634:THR:HB   | 2.19                     | 0.42              |
| 1:A:708:SER:HB2  | 1:A:749:ASN:HB3  | 2.01                     | 0.42              |
| 1:A:269:VAL:CG2  | 1:A:327:SER:HB3  | 2.50                     | 0.42              |
| 1:A:311:GLN:O    | 1:A:314:GLU:N    | 2.50                     | 0.42              |
| 1:A:341:THR:O    | 1:A:343:LEU:N    | 2.52                     | 0.42              |
| 1:A:481:LEU:HD13 | 1:A:751:VAL:CG1  | 2.50                     | 0.42              |
| 1:A:541:PHE:O    | 1:A:545:MSE:N    | 2.52                     | 0.42              |
| 1:A:563:THR:O    | 1:A:564:ILE:C    | 2.61                     | 0.42              |
| 1:A:607:ALA:HB1  | 1:A:649:CYS:SG   | 2.59                     | 0.42              |
| 1:A:79:PRO:HB2   | 1:A:82:TYR:HD2   | 1.80                     | 0.42              |
| 1:A:223:THR:C    | 1:A:225:ALA:N    | 2.77                     | 0.42              |
| 1:A:388:ARG:HB2  | 4:A:831:HOH:O    | 2.20                     | 0.42              |
| 1:A:411:ARG:O    | 1:A:412:ARG:C    | 2.62                     | 0.42              |
| 1:A:594:LEU:HB2  | 1:A:602:ILE:CD1  | 2.49                     | 0.42              |
| 1:A:730:ASN:HB2  | 1:A:731:PRO:CD   | 2.49                     | 0.42              |
| 1:A:740:TYR:C    | 1:A:743:VAL:HG22 | 2.44                     | 0.42              |
| 1:A:754:ALA:C    | 1:A:756:LEU:N    | 2.77                     | 0.42              |
| 1:A:273:LYS:NZ   | 1:A:273:LYS:CB   | 2.76                     | 0.42              |
| 1:A:690:GLY:O    | 1:A:691:ALA:HB2  | 2.19                     | 0.42              |
| 1:A:181:LEU:HB2  | 1:A:182:PRO:HD3  | 2.02                     | 0.42              |
| 1:A:78:VAL:HG11  | 1:A:84:TYR:CG    | 2.55                     | 0.42              |
| 1:A:110:THR:C    | 1:A:111:LYS:HZ2  | 2.20                     | 0.42              |
| 1:A:217:GLN:NE2  | 1:A:217:GLN:N    | 2.68                     | 0.42              |
| 1:A:219:LEU:O    | 1:A:220:GLN:C    | 2.63                     | 0.42              |
| 1:A:373:ASP:HB3  | 1:A:376:LEU:HG   | 2.02                     | 0.42              |
| 1:A:423:GLN:HE22 | 1:A:666:ASP:CG   | 2.27                     | 0.42              |
| 1:A:615:LEU:HA   | 4:A:914:HOH:O    | 2.19                     | 0.42              |
| 1:A:119:TYR:OH   | 1:A:164:LEU:O    | 2.36                     | 0.42              |
| 1:A:211:VAL:HG12 | 1:A:247:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:350:TRP:CZ2  | 1:A:387:ARG:HA   | 2.54                     | 0.42              |
| 1:A:423:GLN:HE21 | 1:A:643:GLN:CA   | 2.33                     | 0.42              |
| 1:A:434:THR:HG22 | 1:A:729:VAL:HB   | 2.01                     | 0.42              |
| 1:A:500:PHE:CD1  | 1:A:538:MSE:CE   | 3.03                     | 0.42              |
| 1:A:22:GLU:O     | 1:A:23:SER:C     | 2.62                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:143:GLU:O    | 1:A:144:ALA:C    | 2.63                     | 0.42              |
| 1:A:286:LYS:HA   | 1:A:286:LYS:HD3  | 1.88                     | 0.42              |
| 1:A:297:ASN:HB3  | 1:A:298:ILE:H    | 1.71                     | 0.42              |
| 1:A:384:LEU:O    | 1:A:385:ALA:C    | 2.63                     | 0.42              |
| 1:A:416:VAL:HG23 | 1:A:419:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:513:GLY:O    | 1:A:524:LYS:HG3  | 2.20                     | 0.42              |
| 1:A:557:MSE:SE   | 1:A:603:GLN:NE2  | 3.03                     | 0.42              |
| 1:A:609:LEU:HD23 | 1:A:650:TYR:CE2  | 2.33                     | 0.42              |
| 1:A:709:GLU:HG3  | 1:A:709:GLU:H    | 1.57                     | 0.42              |
| 1:A:18:LYS:HE3   | 1:A:521:ARG:NH2  | 2.34                     | 0.41              |
| 1:A:54:THR:CG2   | 1:A:57:ILE:HG12  | 2.50                     | 0.41              |
| 1:A:65:TYR:CD1   | 1:A:98:ALA:HB1   | 2.55                     | 0.41              |
| 1:A:501:GLY:O    | 1:A:503:GLN:N    | 2.47                     | 0.41              |
| 1:A:581:TYR:O    | 1:A:584:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:303:PHE:CD1  | 1:A:380:ASN:ND2  | 2.88                     | 0.41              |
| 1:A:480:GLU:C    | 1:A:482:ASP:N    | 2.78                     | 0.41              |
| 1:A:675:SER:HB3  | 1:A:676:ASP:H    | 1.69                     | 0.41              |
| 1:A:693:ILE:HD11 | 1:A:695:PRO:HG3  | 2.02                     | 0.41              |
| 1:A:49:MSE:O     | 1:A:54:THR:HB    | 2.20                     | 0.41              |
| 1:A:205:LEU:HD23 | 1:A:205:LEU:HA   | 1.87                     | 0.41              |
| 1:A:11:MSE:HE3   | 4:A:903:HOH:O    | 2.20                     | 0.41              |
| 1:A:12:GLY:C     | 1:A:14:LYS:H     | 2.27                     | 0.41              |
| 1:A:264:PHE:CD2  | 1:A:264:PHE:N    | 2.88                     | 0.41              |
| 1:A:633:ILE:O    | 1:A:633:ILE:CG2  | 2.62                     | 0.41              |
| 1:A:635:ASN:O    | 1:A:638:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:647:HIS:HA   | 1:A:669:THR:HG22 | 2.02                     | 0.41              |
| 1:A:756:LEU:C    | 1:A:758:ARG:N    | 2.78                     | 0.41              |
| 1:A:41:LEU:O     | 1:A:42:ARG:C     | 2.63                     | 0.41              |
| 1:A:239:LEU:HD11 | 1:A:241:GLU:OE2  | 2.20                     | 0.41              |
| 1:A:284:GLU:HB2  | 1:A:285:GLY:H    | 1.52                     | 0.41              |
| 1:A:301:ASN:HB3  | 1:A:360:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:415:ASN:C    | 1:A:415:ASN:ND2  | 2.78                     | 0.41              |
| 1:A:523:VAL:C    | 1:A:525:PRO:HD3  | 2.45                     | 0.41              |
| 1:A:576:ARG:HG3  | 3:A:771:SO4:S    | 2.60                     | 0.41              |
| 1:A:604:ILE:CG2  | 1:A:631:PHE:HE1  | 2.33                     | 0.41              |
| 1:A:622:PHE:HD2  | 1:A:622:PHE:C    | 2.28                     | 0.41              |
| 1:A:658:HIS:O    | 1:A:659:SER:C    | 2.63                     | 0.41              |
| 1:A:187:ILE:O    | 1:A:187:ILE:HG22 | 2.20                     | 0.41              |
| 1:A:426:LYS:C    | 1:A:427:LEU:HG   | 2.45                     | 0.41              |
| 1:A:623:TYR:C    | 1:A:625:ASP:N    | 2.78                     | 0.41              |
| 1:A:625:ASP:HB3  | 1:A:626:TRP:H    | 1.74                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:667:VAL:CG1  | 1:A:668:ILE:N    | 2.83                     | 0.41              |
| 1:A:29:SER:HB2   | 1:A:33:ASP:CG    | 2.45                     | 0.41              |
| 1:A:135:HIS:HB3  | 1:A:138:VAL:CG1  | 2.50                     | 0.41              |
| 1:A:755:LYS:O    | 1:A:756:LEU:O    | 2.39                     | 0.41              |
| 1:A:79:PRO:HG2   | 1:A:107:MSE:SE   | 2.71                     | 0.41              |
| 1:A:270:ARG:NH1  | 1:A:296:ARG:CZ   | 2.83                     | 0.41              |
| 1:A:327:SER:OG   | 1:A:328:CYS:N    | 2.54                     | 0.41              |
| 1:A:339:ASN:HB3  | 1:A:512:ASN:HD22 | 1.85                     | 0.41              |
| 1:A:381:ALA:HA   | 1:A:384:LEU:CD1  | 2.51                     | 0.41              |
| 1:A:470:GLU:HG2  | 1:A:491:PRO:HG3  | 2.01                     | 0.41              |
| 1:A:505:SER:OG   | 1:A:533:SER:HB3  | 2.20                     | 0.41              |
| 1:A:595:GLU:OE1  | 1:A:638:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:81:ARG:O     | 1:A:104:VAL:HG11 | 2.20                     | 0.41              |
| 1:A:111:LYS:HE3  | 1:A:118:HIS:CD2  | 2.56                     | 0.41              |
| 1:A:220:GLN:C    | 1:A:222:PHE:N    | 2.77                     | 0.41              |
| 1:A:286:LYS:O    | 1:A:321:LYS:HB3  | 2.20                     | 0.41              |
| 1:A:424:GLN:O    | 1:A:427:LEU:O    | 2.38                     | 0.41              |
| 1:A:581:TYR:CE1  | 1:A:630:SER:CB   | 2.97                     | 0.41              |
| 1:A:648:MSE:HE3  | 1:A:648:MSE:HB2  | 1.99                     | 0.41              |
| 1:A:723:GLU:HG3  | 1:A:725:ASN:H    | 1.85                     | 0.41              |
| 1:A:19:PHE:C     | 1:A:21:LEU:N     | 2.78                     | 0.41              |
| 1:A:293:VAL:O    | 1:A:294:ASP:C    | 2.63                     | 0.41              |
| 1:A:357:LYS:O    | 1:A:358:VAL:C    | 2.63                     | 0.41              |
| 1:A:380:ASN:C    | 1:A:382:ALA:H    | 2.29                     | 0.41              |
| 1:A:411:ARG:HH21 | 1:A:419:ARG:HD2  | 1.86                     | 0.41              |
| 1:A:623:TYR:C    | 1:A:625:ASP:H    | 2.29                     | 0.41              |
| 1:A:11:MSE:O     | 1:A:16:GLU:N     | 2.54                     | 0.40              |
| 1:A:427:LEU:HD11 | 1:A:641:SER:O    | 2.21                     | 0.40              |
| 1:A:430:PRO:HB2  | 1:A:758:ARG:NH2  | 2.36                     | 0.40              |
| 1:A:718:MSE:HG2  | 1:A:722:LEU:HD11 | 2.02                     | 0.40              |
| 1:A:186:PRO:C    | 1:A:188:TYR:N    | 2.77                     | 0.40              |
| 1:A:504:LEU:HD21 | 1:A:538:MSE:SE   | 2.71                     | 0.40              |
| 1:A:506:GLY:O    | 1:A:528:ILE:HA   | 2.21                     | 0.40              |
| 1:A:610:ARG:N    | 1:A:650:TYR:OH   | 2.39                     | 0.40              |
| 1:A:664:ASP:N    | 4:A:1046:HOH:O   | 2.55                     | 0.40              |
| 1:A:715:VAL:O    | 1:A:718:MSE:HB2  | 2.21                     | 0.40              |
| 1:A:247:ILE:HG22 | 1:A:251:ALA:HB3  | 2.03                     | 0.40              |
| 1:A:272:THR:O    | 1:A:275:LEU:HD13 | 2.21                     | 0.40              |
| 1:A:307:LEU:HD12 | 1:A:377:PHE:CE2  | 2.56                     | 0.40              |
| 1:A:352:ALA:HA   | 1:A:356:GLN:HG2  | 2.03                     | 0.40              |
| 1:A:401:ALA:C    | 1:A:403:ALA:N    | 2.79                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:69:LEU:HD23  | 1:A:72:THR:HB    | 2.03                     | 0.40              |
| 1:A:123:GLU:HA   | 1:A:166:LYS:O    | 2.20                     | 0.40              |
| 1:A:350:TRP:CZ2  | 1:A:386:SER:C    | 3.00                     | 0.40              |
| 1:A:390:SER:C    | 1:A:392:ARG:N    | 2.80                     | 0.40              |
| 1:A:495:ASP:C    | 1:A:497:VAL:N    | 2.79                     | 0.40              |
| 1:A:557:MSE:HE1  | 4:A:987:HOH:O    | 2.21                     | 0.40              |
| 1:A:558:LEU:CD1  | 1:A:591:VAL:HG13 | 2.38                     | 0.40              |
| 1:A:698:TYR:O    | 1:A:698:TYR:CG   | 2.73                     | 0.40              |
| 1:A:700:ILE:HG12 | 1:A:733:CYS:N    | 2.37                     | 0.40              |
| 1:A:78:VAL:HA    | 1:A:97:MSE:SE    | 2.72                     | 0.40              |
| 1:A:84:TYR:CZ    | 1:A:86:GLY:CA    | 3.00                     | 0.40              |
| 1:A:175:PHE:CE2  | 1:A:177:LEU:HA   | 2.57                     | 0.40              |
| 1:A:303:PHE:O    | 1:A:304:ALA:C    | 2.64                     | 0.40              |
| 1:A:609:LEU:N    | 1:A:650:TYR:OH   | 2.54                     | 0.40              |
| 1:A:629:HIS:HA   | 1:A:632:ARG:CZ   | 2.52                     | 0.40              |
| 1:A:711:ILE:HA   | 1:A:714:ARG:HB2  | 2.03                     | 0.40              |
| 1:A:724:GLN:C    | 1:A:726:ILE:H    | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles       |
|-----|-------|---------------|-----------|-----------|----------|-------------------|
| 1   | A     | 742/765 (97%) | 478 (64%) | 172 (23%) | 92 (12%) | <b>0</b> <b>0</b> |

All (92) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | ALA  |
| 1   | A     | 79  | PRO  |
| 1   | A     | 91  | LEU  |
| 1   | A     | 169 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 171 | VAL  |
| 1   | A     | 284 | GLU  |
| 1   | A     | 302 | ASP  |
| 1   | A     | 408 | SER  |
| 1   | A     | 412 | ARG  |
| 1   | A     | 416 | VAL  |
| 1   | A     | 428 | ASN  |
| 1   | A     | 481 | LEU  |
| 1   | A     | 499 | TYR  |
| 1   | A     | 505 | SER  |
| 1   | A     | 518 | TYR  |
| 1   | A     | 599 | ILE  |
| 1   | A     | 611 | GLU  |
| 1   | A     | 621 | ALA  |
| 1   | A     | 633 | ILE  |
| 1   | A     | 698 | TYR  |
| 1   | A     | 726 | ILE  |
| 1   | A     | 756 | LEU  |
| 1   | A     | 757 | ILE  |
| 1   | A     | 25  | TRP  |
| 1   | A     | 31  | ALA  |
| 1   | A     | 103 | SER  |
| 1   | A     | 113 | PHE  |
| 1   | A     | 137 | ALA  |
| 1   | A     | 192 | ILE  |
| 1   | A     | 319 | LYS  |
| 1   | A     | 320 | ASP  |
| 1   | A     | 371 | GLN  |
| 1   | A     | 398 | VAL  |
| 1   | A     | 415 | ASN  |
| 1   | A     | 423 | GLN  |
| 1   | A     | 500 | PHE  |
| 1   | A     | 502 | GLU  |
| 1   | A     | 506 | GLY  |
| 1   | A     | 531 | ASP  |
| 1   | A     | 540 | VAL  |
| 1   | A     | 548 | SER  |
| 1   | A     | 560 | GLY  |
| 1   | A     | 615 | LEU  |
| 1   | A     | 672 | ASN  |
| 1   | A     | 687 | VAL  |
| 1   | A     | 688 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 696 | GLY  |
| 1   | A     | 739 | LYS  |
| 1   | A     | 748 | LYS  |
| 1   | A     | 158 | PRO  |
| 1   | A     | 174 | SER  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 221 | ALA  |
| 1   | A     | 306 | SER  |
| 1   | A     | 317 | VAL  |
| 1   | A     | 338 | ILE  |
| 1   | A     | 346 | GLU  |
| 1   | A     | 352 | ALA  |
| 1   | A     | 373 | ASP  |
| 1   | A     | 385 | ALA  |
| 1   | A     | 414 | THR  |
| 1   | A     | 482 | ASP  |
| 1   | A     | 496 | MSE  |
| 1   | A     | 571 | ARG  |
| 1   | A     | 625 | ASP  |
| 1   | A     | 673 | SER  |
| 1   | A     | 691 | ALA  |
| 1   | A     | 24  | PHE  |
| 1   | A     | 60  | ASN  |
| 1   | A     | 330 | LEU  |
| 1   | A     | 354 | ALA  |
| 1   | A     | 484 | ASP  |
| 1   | A     | 567 | TRP  |
| 1   | A     | 620 | HIS  |
| 1   | A     | 684 | ARG  |
| 1   | A     | 106 | ALA  |
| 1   | A     | 256 | THR  |
| 1   | A     | 388 | ARG  |
| 1   | A     | 483 | ILE  |
| 1   | A     | 490 | GLU  |
| 1   | A     | 658 | HIS  |
| 1   | A     | 393 | VAL  |
| 1   | A     | 430 | PRO  |
| 1   | A     | 468 | LYS  |
| 1   | A     | 532 | VAL  |
| 1   | A     | 335 | VAL  |
| 1   | A     | 438 | GLY  |
| 1   | A     | 564 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | PRO  |
| 1   | A     | 656 | ILE  |
| 1   | A     | 668 | ILE  |
| 1   | A     | 89  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|----------|-------------|
| 1   | A     | 622/619 (100%) | 551 (89%) | 71 (11%) | 5 16        |

All (71) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | VAL  |
| 1   | A     | 11  | MSE  |
| 1   | A     | 15  | ARG  |
| 1   | A     | 33  | ASP  |
| 1   | A     | 35  | GLN  |
| 1   | A     | 48  | GLN  |
| 1   | A     | 55  | LYS  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 101 | ASN  |
| 1   | A     | 111 | LYS  |
| 1   | A     | 121 | VAL  |
| 1   | A     | 160 | SER  |
| 1   | A     | 169 | LYS  |
| 1   | A     | 176 | GLU  |
| 1   | A     | 185 | LEU  |
| 1   | A     | 196 | LYS  |
| 1   | A     | 201 | THR  |
| 1   | A     | 217 | GLN  |
| 1   | A     | 220 | GLN  |
| 1   | A     | 223 | THR  |
| 1   | A     | 228 | GLU  |
| 1   | A     | 229 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 239 | LEU  |
| 1   | A     | 240 | VAL  |
| 1   | A     | 247 | ILE  |
| 1   | A     | 255 | LEU  |
| 1   | A     | 288 | LEU  |
| 1   | A     | 297 | ASN  |
| 1   | A     | 307 | LEU  |
| 1   | A     | 314 | GLU  |
| 1   | A     | 317 | VAL  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 347 | ILE  |
| 1   | A     | 348 | LYS  |
| 1   | A     | 353 | PHE  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 386 | SER  |
| 1   | A     | 399 | GLN  |
| 1   | A     | 405 | LEU  |
| 1   | A     | 434 | THR  |
| 1   | A     | 436 | THR  |
| 1   | A     | 446 | LEU  |
| 1   | A     | 476 | ASP  |
| 1   | A     | 477 | LEU  |
| 1   | A     | 492 | GLU  |
| 1   | A     | 507 | PHE  |
| 1   | A     | 510 | THR  |
| 1   | A     | 518 | TYR  |
| 1   | A     | 521 | ARG  |
| 1   | A     | 542 | TRP  |
| 1   | A     | 591 | VAL  |
| 1   | A     | 599 | ILE  |
| 1   | A     | 605 | ASP  |
| 1   | A     | 611 | GLU  |
| 1   | A     | 616 | ARG  |
| 1   | A     | 652 | HIS  |
| 1   | A     | 653 | PHE  |
| 1   | A     | 670 | ILE  |
| 1   | A     | 684 | ARG  |
| 1   | A     | 697 | VAL  |
| 1   | A     | 698 | TYR  |
| 1   | A     | 705 | ILE  |
| 1   | A     | 709 | GLU  |
| 1   | A     | 719 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 725 | ASN  |
| 1   | A     | 726 | ILE  |
| 1   | A     | 736 | LYS  |
| 1   | A     | 738 | ARG  |
| 1   | A     | 740 | TYR  |
| 1   | A     | 748 | LYS  |
| 1   | A     | 757 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 35  | GLN  |
| 1   | A     | 101 | ASN  |
| 1   | A     | 217 | GLN  |
| 1   | A     | 220 | GLN  |
| 1   | A     | 297 | ASN  |
| 1   | A     | 311 | GLN  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 362 | ASN  |
| 1   | A     | 399 | GLN  |
| 1   | A     | 415 | ASN  |
| 1   | A     | 424 | GLN  |
| 1   | A     | 428 | ASN  |
| 1   | A     | 494 | ASN  |
| 1   | A     | 512 | ASN  |
| 1   | A     | 547 | GLN  |
| 1   | A     | 574 | GLN  |
| 1   | A     | 577 | HIS  |
| 1   | A     | 603 | GLN  |
| 1   | A     | 629 | HIS  |
| 1   | A     | 639 | GLN  |
| 1   | A     | 645 | HIS  |
| 1   | A     | 652 | HIS  |
| 1   | A     | 654 | ASN  |
| 1   | A     | 760 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SO4  | A     | 769 | -    | 4,4,4        | 0.38 | 0           | 6,6,6       | 0.09 | 0           |
| 3   | SO4  | A     | 771 | -    | 4,4,4        | 0.37 | 0           | 6,6,6       | 0.08 | 0           |
| 3   | SO4  | A     | 770 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.07 | 0           |
| 3   | SO4  | A     | 768 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.07 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 771 | SO4  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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     | 728/765 (95%) | -1.39  | 0 100 100 | 12, 52, 86, 100       | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | SO4  | A     | 769 | 5/5   | 0.97 | 0.05 | 124,124,124,125            | 0     |
| 3   | SO4  | A     | 771 | 5/5   | 0.97 | 0.08 | 133,134,134,134            | 0     |
| 3   | SO4  | A     | 770 | 5/5   | 0.99 | 0.08 | 105,105,106,106            | 0     |
| 3   | SO4  | A     | 768 | 5/5   | 0.99 | 0.05 | 94,95,95,96                | 0     |
| 2   | ZN   | A     | 766 | 1/1   | 1.00 | 0.03 | 65,65,65,65                | 0     |
| 2   | ZN   | A     | 767 | 1/1   | 1.00 | 0.02 | 37,37,37,37                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.