



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:35 PM GMT

PDB ID : 1QU3  
Title : INSIGHTS INTO EDITING FROM AN ILE-TRNA SYNTHETASE STRUCTURE WITH TRNA(ILE) AND MUPIROCIN  
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Deposited on : 1999-07-06  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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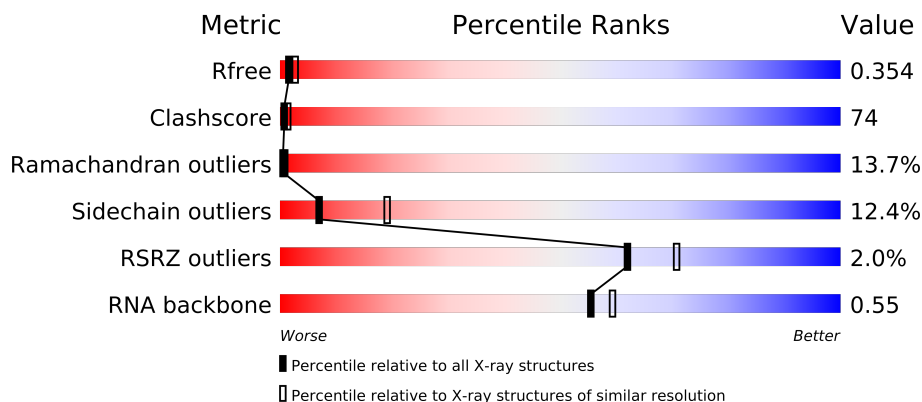
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

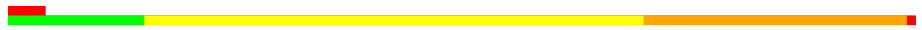
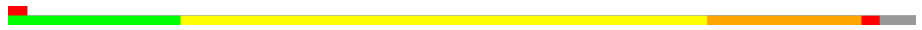
The reported resolution of this entry is 2.90 Å.

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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1053 (2.90-2.90)                                      |
| Clashscore            | 79885                       | 1326 (2.90-2.90)                                      |
| Ramachandran outliers | 78287                       | 1290 (2.90-2.90)                                      |
| Sidechain outliers    | 78261                       | 1292 (2.90-2.90)                                      |
| RSRZ outliers         | 66119                       | 1054 (2.90-2.90)                                      |
| RNA backbone          | 1838                        | 1055 (3.40-2.40)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | T     | 75     |  |
| 2   | A     | 917    |  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 4   | MRC  | A     | 993 | -        | X                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8870 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called ISOLEUCYL-TRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | T     | 75       | Total | C   | N   | O   | P  | 24      | 0       | 0     |
|     |       |          | 1603  | 715 | 289 | 525 | 74 |         |         |       |

- Molecule 2 is a protein called ISOLEUCYL-TRNA SYNTHETASE.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | A     | 880      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7113  | 4537 | 1198 | 1358 | 20 |         |         |       |

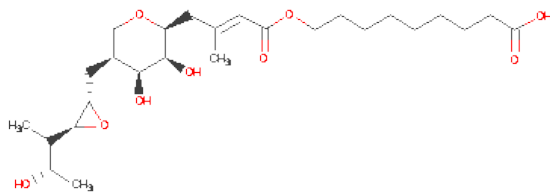
There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 4       | GLU      | LYS    | CONFLICT | UNP P41972 |
| A     | 5       | LYS      | GLU    | CONFLICT | UNP P41972 |
| A     | 295     | TRP      | TYR    | CONFLICT | UNP P41972 |
| A     | 340     | GLN      | LYS    | CONFLICT | UNP P41972 |
| A     | 644     | ASP      | VAL    | CONFLICT | UNP P41972 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is MUPIROCIN (three-letter code: MRC) (formula: C<sub>26</sub>H<sub>44</sub>O<sub>9</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 35    | 26 | 9 |         |         |

- Molecule 5 is water.

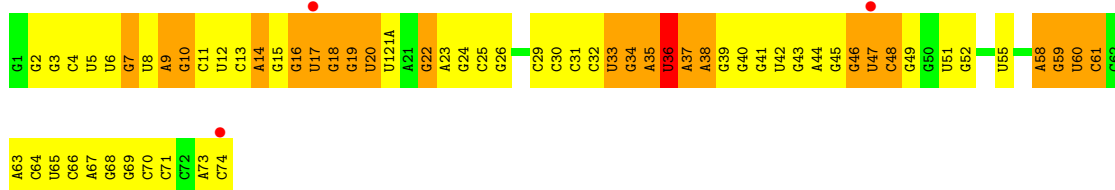
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 82       | Total | O  | 0       | 0       |
|     |       |          | 82    | 82 |         |         |
| 5   | T     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |

### 3 Residue-property plots

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

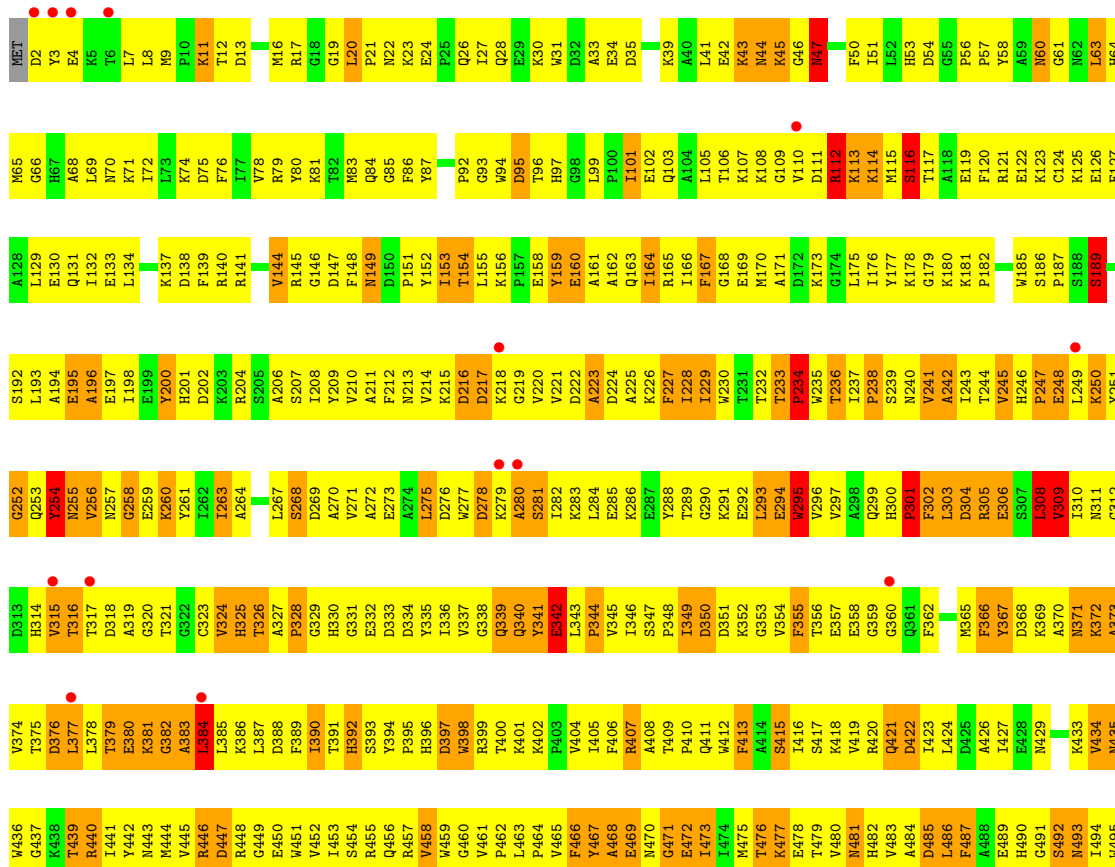
#### • Molecule 1: ISOLEUCYL-TRNA

Chain T: 



#### • Molecule 2: ISOLEUCYL-TRNA SYNTHETASE

Chain A: 



|      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|
| ARG  | K823 | A757 | R686 | M621 | R560 | F496 |
| CYS  | S824 | P758 | S691 | V622 | G561 | E497 |
| TRP  | L825 | I759 |      | S623 | W562 | R498 |
| ASN  | E826 | L760 | N695 | S624 | F563 | E499 |
| TYR  | A827 | H761 |      | T625 | N564 | A500 |
| SER  | K828 | H762 |      | D626 | K501 | K501 |
| GLU  | V829 |      |      | Y627 | I567 | D502 |
| ASP  | T830 |      |      | L628 | T568 | L503 |
| LEU  | I831 | E765 | N698 | A629 | T569 | L504 |
| GLY  | A832 | E766 | P699 | D630 | T569 | P505 |
| ALA  | S833 | V767 | D700 | V631 | S570 | E506 |
| VAL  | N834 | V768 | L702 | R632 | V571 | G507 |
| ASP  | D835 | S769 | N703 | R633 | A572 | F508 |
| GLU  | K836 | H770 | I704 | S634 | T573 | F509 |
| LEU  | F837 | I771 | Y705 | D635 | R574 | H510 |
| THR  | N838 | P772 | Q706 | E636 | G576 | P511 |
| HIS  | A839 | H773 | E707 | I637 | S577 | G512 |
| LEU  | S840 | V774 | V708 | L638 | P578 | S513 |
| CYS  | F841 | K775 | Q709 |      | Y579 | P514 |
| PRO  | F842 | E776 | N710 | S642 | K580 | N515 |
| ARG  | L843 | E777 | F711 | D643 | F581 | F518 |
| GLN  | T844 | S778 | I712 | D644 | L582 | T519 |
| GLN  | A848 | V779 | N713 | Y645 | L583 | K520 |
| VAL  | L849 | H780 | V714 | R646 | S584 | E521 |
| VAL  | H850 | L781 | E715 | K647 | H585 |      |
| LYS  | Q851 | N784 | L716 | I648 | G586 |      |
| LEU  | F853 | D791 | S717 | R649 | F587 | L624 |
| LEU  | V854 | Q792 | N718 | N650 | V588 | M525 |
|      | V855 | A793 | F719 | T651 | M589 | D526 |
| S856 | S856 | L794 | Y720 | L652 | D590 | V527 |
| Q857 | Q857 | L795 | D722 | R653 | G591 | K528 |
| V858 | V858 | L796 | Y723 | F654 | E592 | F529 |
| K859 | K859 | K797 | G724 | M655 | G593 | D530 |
| V860 | V860 | W798 | I727 | G657 | K594 |      |
| V861 | V861 | R799 | L728 | L658 | K595 | S533 |
| D862 | D862 | T800 | I729 | N660 | M596 | S534 |
|      | D865 | F801 | Y730 | D661 | S597 | H535 |
| D866 | D866 | M802 | E731 | P664 | K598 | R536 |
| Q867 | Q867 | N803 | Q732 | D665 | S599 | G537 |
| A868 | A868 | L804 | R733 | T666 | L600 | V538 |
| T869 | T869 | R805 |      | D667 | G601 | L539 |
| A870 | A870 | D806 | H736 | S668 | N602 | R542 |
| Y871 | Y871 | D807 | I737 | I669 | V603 | P543 |
| E872 | E872 | N808 | R738 | P670 | I604 | P544 |
| H873 | H873 | N809 | R739 | S670 | V605 | E544 |
| G874 | G874 | R810 | P670 | E571 | P606 | L545 |
| D875 | D875 | A811 | S740 | G572 | D607 | S546 |
| I876 | I876 | L812 | M741 | E673 | Q608 | F547 |
| V877 | V877 | E813 | Q742 |      | V609 | P548 |
|      | A881 | T814 | T743 | E576 | V610 | A549 |
|      | ASP  | A815 | V744 |      | K611 | D550 |
| GLY  | GLY  | R816 | L745 |      | Q612 | M551 |
| GLU  | GLU  | N817 | Y746 | R679 | K613 | Y552 |
| LYS  | LYS  | E818 | Q747 | Y680 | G614 | L553 |
| CYS  | CYS  | K819 | I748 | L681 | A615 | E554 |
| GLU  | GLU  | V820 | L749 | L682 | D616 | G555 |
|      |      | I821 | V750 | N683 | I617 | S556 |
|      |      | G822 | D751 | R684 | A618 | D557 |
|      |      |      | M752 | L685 | R619 | Q558 |
|      |      |      |      |      | L620 | Y559 |

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 71.00Å 100.00Å 180.00Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 10.00 – 2.90<br>19.93 – 2.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 85.9 (10.00-2.90)<br>55.5 (19.93-2.75)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.10  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.76 (at 2.75Å)   | Xtriage          |
| Refinement program  | unknown   | Depositor        |
| R, $R_{free}$   | 0.234 , 0.345<br>0.239 , 0.354                              | Depositor<br>DCC |
| $R_{free}$ test set   | 902 reflections (5.01%)                                     | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 43.7  | Xtriage          |
| Anisotropy  | 0.418   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 11.6   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Outliers  | 0 of 19777 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 8870  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 34.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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   | T     | 0.53         | 0/1792      | 0.80        | 1/2794 (0.0%)  |
| 2   | A     | 0.44         | 0/7287      | 0.72        | 3/9879 (0.0%)  |
| All | All   | 0.46         | 0/9079      | 0.74        | 4/12673 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | A     | 471 | GLY  | N-CA-C     | -6.82 | 96.06       | 113.10   |
| 2   | A     | 681 | LEU  | CA-CB-CG   | -5.37 | 102.94      | 115.30   |
| 1   | T     | 36  | U    | N1-C1'-C2' | 5.28  | 120.86      | 114.00   |
| 2   | A     | 255 | ASN  | N-CA-C     | 5.25  | 125.18      | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | T     | 1603  | 0        | 811      | 99      | 1            |
| 2   | A     | 7113  | 0        | 6935     | 1135    | 1            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | A     | 35    | 0        | 40       | 5       | 0            |
| 5   | A     | 82    | 0        | 0        | 15      | 0            |
| 5   | T     | 36    | 0        | 0        | 2       | 0            |
| All | All   | 8870  | 0        | 7786     | 1212    | 1            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 74.

All (1212) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:T:13:C:H2'     | 1:T:14:A:H5''    | 1.32        | 1.10     |
| 2:A:366:PHE:H    | 2:A:370:ALA:HB3  | 1.18        | 1.07     |
| 2:A:53:HIS:NE2   | 2:A:534:SER:HB3  | 1.73        | 1.02     |
| 2:A:250:LYS:HG2  | 2:A:290:GLY:N    | 1.77        | 1.00     |
| 2:A:302:PHE:HA   | 2:A:378:LEU:HD13 | 1.43        | 0.99     |
| 2:A:821:ILE:HD13 | 2:A:822:GLY:N    | 1.77        | 0.98     |
| 2:A:481:ASN:HD22 | 2:A:481:ASN:H    | 1.10        | 0.98     |
| 1:T:37:A:H2'     | 2:A:17:ARG:HD2   | 1.45        | 0.98     |
| 2:A:250:LYS:NZ   | 2:A:289:THR:HG23 | 1.78        | 0.97     |
| 2:A:469:GLU:HA   | 2:A:513:SER:N    | 1.79        | 0.97     |
| 2:A:70:ASN:HD22  | 2:A:585:HIS:HE1  | 1.10        | 0.97     |
| 2:A:250:LYS:HD3  | 2:A:289:THR:HA   | 1.45        | 0.97     |
| 2:A:589:MET:HE3  | 2:A:595:LYS:HA   | 1.46        | 0.96     |
| 2:A:596:MET:HB3  | 2:A:603:VAL:HG12 | 1.46        | 0.96     |
| 2:A:821:ILE:HD13 | 2:A:822:GLY:H    | 1.30        | 0.96     |
| 2:A:539:LEU:HD23 | 2:A:545:LEU:HD13 | 1.49        | 0.95     |
| 2:A:481:ASN:N    | 2:A:481:ASN:HD22 | 1.61        | 0.94     |
| 1:T:23:A:H2'     | 1:T:24:G:C8      | 2.03        | 0.94     |
| 2:A:23:LYS:HE3   | 2:A:27:ILE:HD11  | 1.47        | 0.94     |
| 2:A:467:TYR:HB3  | 2:A:472:GLU:CB   | 1.98        | 0.93     |
| 2:A:116:SER:HB3  | 2:A:119:GLU:HG3  | 1.50        | 0.93     |
| 2:A:487:PHE:CE1  | 2:A:492:SER:HA   | 2.02        | 0.93     |
| 2:A:704:ILE:O    | 2:A:708:VAL:HG12 | 1.68        | 0.93     |
| 2:A:411:GLN:HE22 | 2:A:456:GLN:NE2  | 1.65        | 0.93     |
| 2:A:481:ASN:H    | 2:A:481:ASN:ND2  | 1.66        | 0.93     |
| 2:A:857:GLN:NE2  | 2:A:858:VAL:H    | 1.67        | 0.93     |
| 2:A:237:ILE:HA   | 2:A:325:HIS:NE2  | 1.85        | 0.92     |
| 2:A:102:GLU:HA   | 2:A:105:LEU:HD12 | 1.50        | 0.92     |
| 2:A:390:ILE:HG12 | 2:A:391:THR:H    | 1.33        | 0.92     |
| 2:A:336:ILE:HG13 | 2:A:337:VAL:N    | 1.85        | 0.92     |
| 2:A:857:GLN:HE21 | 2:A:858:VAL:H    | 1.11        | 0.92     |
| 2:A:253:GLN:O    | 2:A:254:TYR:HB2  | 1.67        | 0.92     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:749:LEU:HD22 | 2:A:750:VAL:N    | 1.85        | 0.91     |
| 2:A:200:TYR:CE2  | 2:A:395:PRO:HG3  | 2.05        | 0.91     |
| 2:A:296:VAL:HG12 | 2:A:297:VAL:H    | 1.35        | 0.91     |
| 2:A:597:SER:H    | 2:A:602:ASN:HD21 | 1.18        | 0.91     |
| 2:A:105:LEU:HB3  | 2:A:110:VAL:HG21 | 1.53        | 0.90     |
| 2:A:602:ASN:HD22 | 2:A:602:ASN:H    | 1.20        | 0.90     |
| 2:A:250:LYS:HZ2  | 2:A:289:THR:HG23 | 1.37        | 0.89     |
| 2:A:4:GLU:HG3    | 2:A:7:LEU:HD23   | 1.54        | 0.89     |
| 2:A:649:ARG:HH11 | 2:A:649:ARG:HG3  | 1.34        | 0.89     |
| 2:A:355:PHE:HE1  | 2:A:365:MET:HB2  | 1.38        | 0.89     |
| 2:A:121:ARG:HD2  | 2:A:496:PHE:HD1  | 1.37        | 0.89     |
| 2:A:60:ASN:HD22  | 2:A:61:GLY:N     | 1.71        | 0.88     |
| 2:A:551:MET:HB3  | 2:A:581:PHE:HB3  | 1.55        | 0.88     |
| 2:A:467:TYR:HB3  | 2:A:472:GLU:HB3  | 1.57        | 0.87     |
| 2:A:324:VAL:O    | 2:A:325:HIS:HB3  | 1.75        | 0.87     |
| 2:A:829:VAL:HB   | 2:A:858:VAL:HG12 | 1.56        | 0.87     |
| 2:A:218:LYS:HD2  | 2:A:218:LYS:H    | 1.40        | 0.87     |
| 2:A:723:TYR:HA   | 2:A:854:ILE:HD11 | 1.55        | 0.87     |
| 2:A:349:ILE:HG12 | 2:A:355:PHE:HB3  | 1.55        | 0.86     |
| 2:A:749:LEU:HD13 | 2:A:750:VAL:H    | 1.38        | 0.86     |
| 2:A:71:LYS:HG3   | 2:A:139:PHE:CE2  | 2.10        | 0.86     |
| 2:A:578:PRO:HD2  | 5:A:1048:HOH:O   | 1.74        | 0.86     |
| 2:A:237:ILE:HB   | 2:A:238:PRO:HD3  | 1.58        | 0.86     |
| 1:T:33:U:H4'     | 1:T:34:G:O5'     | 1.73        | 0.86     |
| 2:A:105:LEU:HD13 | 2:A:124:CYS:SG   | 2.16        | 0.85     |
| 2:A:290:GLY:HA2  | 2:A:293:LEU:HB3  | 1.59        | 0.85     |
| 2:A:469:GLU:HA   | 2:A:513:SER:H    | 1.38        | 0.84     |
| 2:A:745:LEU:HA   | 2:A:748:ILE:HG22 | 1.57        | 0.84     |
| 2:A:434:VAL:HG13 | 2:A:435:ASN:H    | 1.43        | 0.84     |
| 2:A:240:ASN:ND2  | 2:A:308:LEU:HD21 | 1.93        | 0.84     |
| 2:A:289:THR:HG22 | 2:A:292:GLU:H    | 1.42        | 0.84     |
| 2:A:355:PHE:HD1  | 2:A:355:PHE:H    | 1.24        | 0.83     |
| 2:A:244:THR:HG22 | 2:A:311:ASN:HB2  | 1.58        | 0.83     |
| 2:A:741:MET:HE2  | 2:A:745:LEU:HD11 | 1.58        | 0.83     |
| 2:A:275:LEU:HG   | 2:A:386:LYS:HE3  | 1.61        | 0.83     |
| 2:A:482:HIS:O    | 2:A:486:LEU:HB2  | 1.78        | 0.83     |
| 1:T:13:C:C2'     | 1:T:14:A:H5''    | 2.09        | 0.83     |
| 2:A:384:LEU:O    | 2:A:385:LEU:HD23 | 1.79        | 0.82     |
| 2:A:379:THR:HG23 | 2:A:385:LEU:HB2  | 1.60        | 0.82     |
| 2:A:30:LYS:O     | 2:A:34:GLU:HG2   | 1.80        | 0.81     |
| 2:A:749:LEU:HD13 | 2:A:750:VAL:HG23 | 1.59        | 0.81     |
| 2:A:23:LYS:O     | 2:A:26:GLN:HG2   | 1.81        | 0.81     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:301:PRO:O    | 2:A:303:LEU:N    | 2.14        | 0.81     |
| 2:A:250:LYS:HG2  | 2:A:290:GLY:H    | 1.39        | 0.80     |
| 2:A:167:PHE:CE1  | 2:A:464:PRO:HD2  | 2.16        | 0.80     |
| 1:T:63:A:H2'     | 1:T:64:C:C6      | 2.16        | 0.80     |
| 2:A:212:PHE:CD2  | 2:A:301:PRO:HD2  | 2.17        | 0.80     |
| 2:A:834:ASN:HB2  | 2:A:874:GLY:HA2  | 1.64        | 0.80     |
| 2:A:536:ARG:HH12 | 2:A:574:ARG:CZ   | 1.95        | 0.79     |
| 1:T:33:U:H1'     | 1:T:36:U:H3      | 1.45        | 0.79     |
| 2:A:803:ASN:HB3  | 2:A:873:HIS:CE1  | 2.16        | 0.79     |
| 2:A:708:VAL:HG13 | 2:A:709:GLN:N    | 1.97        | 0.79     |
| 1:T:46:G:H2'     | 1:T:47:U:H5'     | 1.65        | 0.79     |
| 2:A:570:SER:CB   | 2:A:578:PRO:HG3  | 2.13        | 0.79     |
| 2:A:247:PRO:HB3  | 2:A:291:LYS:HA   | 1.65        | 0.78     |
| 2:A:390:ILE:HG12 | 2:A:391:THR:N    | 1.98        | 0.78     |
| 2:A:210:VAL:O    | 2:A:229:ILE:HG22 | 1.83        | 0.78     |
| 2:A:341:TYR:O    | 2:A:343:LEU:HG   | 1.82        | 0.78     |
| 2:A:535:HIS:HD1  | 2:A:536:ARG:N    | 1.81        | 0.78     |
| 2:A:272:ALA:HA   | 2:A:277:TRP:HB2  | 1.65        | 0.78     |
| 2:A:486:LEU:HD11 | 5:A:1020:HOH:O   | 1.83        | 0.78     |
| 2:A:323:CYS:O    | 2:A:324:VAL:HB   | 1.82        | 0.78     |
| 2:A:411:GLN:HE22 | 2:A:456:GLN:HE22 | 1.30        | 0.78     |
| 2:A:831:ILE:HA   | 2:A:875:ASP:O    | 1.83        | 0.78     |
| 2:A:857:GLN:HE21 | 2:A:858:VAL:N    | 1.81        | 0.77     |
| 2:A:154:THR:HA   | 2:A:159:TYR:CD1  | 2.19        | 0.77     |
| 2:A:164:ILE:HD11 | 2:A:484:ALA:HB2  | 1.65        | 0.77     |
| 2:A:501:LYS:CD   | 2:A:501:LYS:H    | 1.98        | 0.77     |
| 2:A:468:ALA:H    | 2:A:472:GLU:HB3  | 1.50        | 0.77     |
| 2:A:234:PRO:HG2  | 2:A:235:TRP:H    | 1.50        | 0.77     |
| 2:A:466:PHE:HA   | 2:A:520:LYS:HA   | 1.67        | 0.77     |
| 2:A:469:GLU:N    | 2:A:472:GLU:HG2  | 1.99        | 0.76     |
| 2:A:198:ILE:HG23 | 2:A:396:HIS:O    | 1.84        | 0.76     |
| 2:A:164:ILE:CD1  | 2:A:484:ALA:HB2  | 2.15        | 0.76     |
| 2:A:181:LYS:HG2  | 2:A:182:PRO:HD2  | 1.68        | 0.76     |
| 2:A:349:ILE:O    | 2:A:350:ASP:O    | 2.03        | 0.76     |
| 2:A:228:ILE:HD12 | 2:A:263:ILE:CG2  | 2.16        | 0.76     |
| 2:A:570:SER:HB2  | 2:A:578:PRO:HG3  | 1.68        | 0.76     |
| 1:T:43:G:O2'     | 1:T:44:A:H5'     | 1.86        | 0.76     |
| 2:A:164:ILE:HG13 | 2:A:165:ARG:N    | 2.01        | 0.75     |
| 2:A:161:ALA:HB1  | 2:A:165:ARG:HH12 | 1.51        | 0.75     |
| 1:T:19:G:O2'     | 1:T:20:U:OP1     | 2.04        | 0.75     |
| 2:A:823:LYS:O    | 2:A:825:LEU:N    | 2.19        | 0.75     |
| 2:A:229:ILE:HD12 | 2:A:323:CYS:HB2  | 1.69        | 0.75     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:178:LYS:HZ2  | 2:A:412:TRP:HE1  | 1.32        | 0.75     |
| 2:A:433:LYS:HB2  | 2:A:583:LEU:HG   | 1.69        | 0.75     |
| 2:A:240:ASN:HB2  | 2:A:308:LEU:HD11 | 1.69        | 0.75     |
| 1:T:37:A:H4'     | 1:T:38:A:OP2     | 1.87        | 0.74     |
| 2:A:462:PRO:HA   | 2:A:524:ILE:HA   | 1.67        | 0.74     |
| 1:T:47:U:O2'     | 1:T:48:C:OP2     | 2.05        | 0.74     |
| 2:A:309:VAL:C    | 2:A:310:ILE:HD12 | 2.08        | 0.74     |
| 2:A:336:ILE:HG13 | 2:A:337:VAL:H    | 1.50        | 0.74     |
| 1:T:63:A:H2'     | 1:T:64:C:H6      | 1.53        | 0.74     |
| 2:A:420:ARG:NH2  | 2:A:449:GLY:H    | 1.86        | 0.74     |
| 2:A:255:ASN:O    | 2:A:260:LYS:HA   | 1.86        | 0.74     |
| 2:A:602:ASN:HD22 | 2:A:602:ASN:N    | 1.84        | 0.74     |
| 2:A:650:ASN:O    | 2:A:653:ARG:HB3  | 1.87        | 0.74     |
| 2:A:54:ASP:OD1   | 2:A:92:PRO:HA    | 1.88        | 0.74     |
| 2:A:64:HIS:CD2   | 2:A:66:GLY:H     | 2.05        | 0.74     |
| 2:A:539:LEU:HD11 | 2:A:549:ALA:HB2  | 1.70        | 0.74     |
| 1:T:41:G:N2      | 5:T:156:HOH:O    | 2.20        | 0.74     |
| 2:A:807:ASP:OD2  | 2:A:871:TYR:HB3  | 1.88        | 0.73     |
| 2:A:653:ARG:HH11 | 2:A:653:ARG:HG2  | 1.52        | 0.73     |
| 2:A:604:ILE:HD12 | 2:A:633:ILE:HG23 | 1.70        | 0.73     |
| 2:A:459:TRP:H    | 2:A:524:ILE:HD13 | 1.51        | 0.73     |
| 2:A:469:GLU:C    | 2:A:471:GLY:H    | 1.89        | 0.73     |
| 2:A:300:HIS:O    | 2:A:304:ASP:HB3  | 1.87        | 0.73     |
| 2:A:293:LEU:O    | 2:A:295:TRP:N    | 2.20        | 0.73     |
| 2:A:468:ALA:N    | 2:A:472:GLU:HB3  | 2.04        | 0.73     |
| 2:A:70:ASN:HD22  | 2:A:585:HIS:CE1  | 2.02        | 0.73     |
| 2:A:58:TYR:CE2   | 2:A:101:ILE:HG13 | 2.23        | 0.73     |
| 2:A:220:VAL:HG22 | 2:A:224:ASP:OD1  | 1.89        | 0.72     |
| 2:A:681:LEU:HD13 | 2:A:720:TYR:CD1  | 2.23        | 0.72     |
| 2:A:745:LEU:HA   | 2:A:748:ILE:CG2  | 2.19        | 0.72     |
| 2:A:362:PHE:HA   | 2:A:365:MET:CG   | 2.20        | 0.72     |
| 1:T:13:C:H4'     | 2:A:702:LEU:HD11 | 1.70        | 0.72     |
| 2:A:289:THR:CG2  | 2:A:291:LYS:HB3  | 2.19        | 0.72     |
| 2:A:865:ASP:HB3  | 2:A:867:GLN:HE21 | 1.54        | 0.72     |
| 2:A:355:PHE:N    | 2:A:355:PHE:CD1  | 2.58        | 0.72     |
| 2:A:437:GLY:O    | 2:A:441:ILE:HG22 | 1.90        | 0.72     |
| 2:A:120:PHE:CD1  | 2:A:124:CYS:SG   | 2.83        | 0.72     |
| 2:A:293:LEU:O    | 2:A:296:VAL:HG23 | 1.90        | 0.72     |
| 2:A:632:ARG:HH11 | 2:A:632:ARG:HG3  | 1.54        | 0.71     |
| 2:A:289:THR:HG23 | 2:A:291:LYS:HB3  | 1.72        | 0.71     |
| 2:A:256:VAL:HG21 | 2:A:282:ILE:HD12 | 1.72        | 0.71     |
| 2:A:501:LYS:HD2  | 2:A:501:LYS:H    | 1.55        | 0.71     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:250:LYS:CG   | 2:A:290:GLY:H    | 2.03        | 0.71     |
| 2:A:163:GLN:HG2  | 2:A:461:VAL:HG11 | 1.71        | 0.71     |
| 2:A:597:SER:H    | 2:A:602:ASN:ND2  | 1.89        | 0.71     |
| 1:T:9:A:H5'      | 1:T:10:G:OP2     | 1.90        | 0.71     |
| 2:A:233:THR:HG23 | 2:A:236:THR:HG21 | 1.71        | 0.71     |
| 1:T:40:G:OP1     | 2:A:717:SER:HB3  | 1.90        | 0.71     |
| 2:A:247:PRO:CB   | 2:A:291:LYS:HA   | 2.20        | 0.71     |
| 2:A:229:ILE:CD1  | 2:A:323:CYS:HB2  | 2.20        | 0.71     |
| 2:A:757:ALA:HB3  | 2:A:758:PRO:HD3  | 1.73        | 0.71     |
| 2:A:255:ASN:ND2  | 2:A:256:VAL:HG23 | 2.06        | 0.70     |
| 2:A:185:TRP:O    | 2:A:404:VAL:HG13 | 1.92        | 0.70     |
| 2:A:499:GLU:HA   | 2:A:520:LYS:NZ   | 2.06        | 0.70     |
| 2:A:250:LYS:HZ1  | 2:A:289:THR:HG23 | 1.57        | 0.70     |
| 2:A:163:GLN:HG2  | 2:A:461:VAL:HG21 | 1.71        | 0.70     |
| 2:A:20:LEU:HD12  | 2:A:20:LEU:H     | 1.56        | 0.70     |
| 2:A:20:LEU:CD1   | 2:A:20:LEU:H     | 2.04        | 0.70     |
| 2:A:239:SER:O    | 2:A:346:ILE:HG12 | 1.90        | 0.70     |
| 2:A:250:LYS:CD   | 2:A:289:THR:HA   | 2.21        | 0.70     |
| 2:A:296:VAL:HG12 | 2:A:297:VAL:N    | 2.04        | 0.69     |
| 2:A:44:ASN:C     | 2:A:47:ASN:HD21  | 1.94        | 0.69     |
| 2:A:181:LYS:HG2  | 2:A:182:PRO:CD   | 2.23        | 0.69     |
| 2:A:493:ASN:O    | 2:A:497:GLU:HG2  | 1.93        | 0.69     |
| 2:A:494:ILE:HA   | 2:A:497:GLU:HG3  | 1.74        | 0.69     |
| 2:A:65:MET:HE3   | 2:A:606:PRO:HG3  | 1.72        | 0.69     |
| 2:A:706:GLN:HA   | 2:A:706:GLN:HE21 | 1.56        | 0.69     |
| 2:A:247:PRO:HA   | 2:A:291:LYS:HA   | 1.73        | 0.69     |
| 2:A:247:PRO:O    | 2:A:248:GLU:HB2  | 1.90        | 0.69     |
| 2:A:421:GLN:HA   | 2:A:424:LEU:HD12 | 1.75        | 0.69     |
| 2:A:473:ILE:HG22 | 2:A:473:ILE:O    | 1.90        | 0.69     |
| 2:A:121:ARG:HD2  | 2:A:496:PHE:CD1  | 2.24        | 0.69     |
| 2:A:749:LEU:CD1  | 2:A:750:VAL:H    | 2.06        | 0.69     |
| 2:A:434:VAL:HG13 | 2:A:435:ASN:N    | 2.08        | 0.69     |
| 2:A:821:ILE:CD1  | 2:A:822:GLY:H    | 2.01        | 0.69     |
| 1:T:69:G:H5''    | 2:A:589:MET:CE   | 2.23        | 0.69     |
| 2:A:246:HIS:CD2  | 2:A:315:VAL:H    | 2.11        | 0.69     |
| 2:A:362:PHE:HA   | 2:A:365:MET:HG3  | 1.72        | 0.69     |
| 2:A:469:GLU:N    | 2:A:513:SER:HB2  | 2.08        | 0.69     |
| 2:A:649:ARG:HG3  | 2:A:649:ARG:NH1  | 2.08        | 0.69     |
| 2:A:23:LYS:HA    | 2:A:26:GLN:HE21  | 1.57        | 0.68     |
| 1:T:43:G:H2'     | 1:T:44:A:C8      | 2.28        | 0.68     |
| 2:A:129:LEU:HA   | 2:A:132:ILE:HG12 | 1.75        | 0.68     |
| 2:A:129:LEU:O    | 2:A:132:ILE:HG12 | 1.93        | 0.68     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:247:PRO:CA   | 2:A:291:LYS:HA   | 2.23        | 0.68     |
| 1:T:32:C:H5'     | 2:A:823:LYS:HB3  | 1.75        | 0.68     |
| 2:A:278:ASP:C    | 2:A:280:ALA:H    | 1.97        | 0.68     |
| 2:A:354:VAL:HG22 | 2:A:365:MET:O    | 1.94        | 0.68     |
| 2:A:634:SER:OG   | 2:A:637:ILE:HG13 | 1.93        | 0.68     |
| 2:A:120:PHE:CE1  | 2:A:124:CYS:SG   | 2.87        | 0.68     |
| 2:A:469:GLU:CB   | 2:A:512:GLY:HA3  | 2.23        | 0.68     |
| 2:A:500:ALA:O    | 2:A:504:LEU:HD23 | 1.94        | 0.68     |
| 2:A:848:ALA:HB1  | 2:A:851:GLN:HB2  | 1.76        | 0.68     |
| 2:A:23:LYS:HG3   | 2:A:27:ILE:HD11  | 1.75        | 0.68     |
| 1:T:23:A:H2'     | 1:T:24:G:H8      | 1.58        | 0.68     |
| 2:A:840:SER:HA   | 2:A:860:VAL:CG1  | 2.23        | 0.68     |
| 2:A:237:ILE:C    | 2:A:239:SER:H    | 1.98        | 0.68     |
| 1:T:58:A:O2'     | 1:T:60:U:H5      | 1.77        | 0.68     |
| 2:A:214:VAL:HG22 | 2:A:227:PHE:CD1  | 2.29        | 0.67     |
| 2:A:829:VAL:O    | 2:A:858:VAL:HA   | 1.94        | 0.67     |
| 2:A:831:ILE:HG22 | 2:A:876:ILE:HG12 | 1.77        | 0.67     |
| 2:A:70:ASN:ND2   | 2:A:585:HIS:HE1  | 1.89        | 0.67     |
| 2:A:228:ILE:HD12 | 2:A:263:ILE:HG21 | 1.74        | 0.67     |
| 2:A:802:MET:HE2  | 2:A:802:MET:HA   | 1.76        | 0.67     |
| 1:T:74:C:H6      | 1:T:74:C:O5'     | 1.77        | 0.67     |
| 2:A:132:ILE:HG13 | 2:A:133:GLU:N    | 2.08        | 0.67     |
| 2:A:71:LYS:HG3   | 2:A:139:PHE:HE2  | 1.57        | 0.67     |
| 2:A:349:ILE:HA   | 2:A:355:PHE:HA   | 1.76        | 0.67     |
| 2:A:105:LEU:HD13 | 2:A:120:PHE:CZ   | 2.30        | 0.67     |
| 2:A:622:VAL:O    | 2:A:625:THR:HG22 | 1.94        | 0.67     |
| 2:A:220:VAL:HG13 | 2:A:224:ASP:OD2  | 1.93        | 0.67     |
| 2:A:351:ASP:HA   | 2:A:407:ARG:NH2  | 2.08        | 0.67     |
| 2:A:366:PHE:H    | 2:A:370:ALA:CB   | 2.03        | 0.67     |
| 2:A:57:PRO:HD2   | 2:A:93:GLY:O     | 1.95        | 0.67     |
| 2:A:808:VAL:O    | 2:A:812:LEU:HG   | 1.95        | 0.67     |
| 1:T:4:C:HO2'     | 2:A:436:TRP:HE3  | 1.40        | 0.67     |
| 1:T:4:C:O2'      | 2:A:436:TRP:HE3  | 1.77        | 0.67     |
| 2:A:484:ALA:C    | 2:A:486:LEU:H    | 1.98        | 0.66     |
| 2:A:467:TYR:HB3  | 2:A:472:GLU:HB2  | 1.77        | 0.66     |
| 2:A:766:GLU:O    | 2:A:770:HIS:HD2  | 1.79        | 0.66     |
| 2:A:175:LEU:HD23 | 2:A:418:LYS:HD2  | 1.77        | 0.66     |
| 2:A:681:LEU:HD13 | 2:A:720:TYR:CG   | 2.30        | 0.66     |
| 2:A:708:VAL:HG13 | 2:A:709:GLN:H    | 1.59        | 0.66     |
| 2:A:237:ILE:O    | 2:A:239:SER:N    | 2.28        | 0.66     |
| 2:A:69:LEU:HD12  | 2:A:622:VAL:HG13 | 1.78        | 0.66     |
| 2:A:453:ILE:HD12 | 2:A:463:LEU:HD21 | 1.77        | 0.66     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:148:PHE:O    | 2:A:151:PRO:HD3  | 1.96        | 0.66     |
| 2:A:294:GLU:HA   | 2:A:310:ILE:HG22 | 1.77        | 0.66     |
| 2:A:275:LEU:HD21 | 2:A:386:LYS:HG3  | 1.76        | 0.66     |
| 2:A:371:ASN:HD22 | 2:A:371:ASN:N    | 1.93        | 0.66     |
| 2:A:544:GLU:H    | 2:A:544:GLU:CD   | 1.96        | 0.66     |
| 2:A:745:LEU:CA   | 2:A:748:ILE:HG22 | 2.26        | 0.65     |
| 2:A:275:LEU:HG   | 2:A:386:LYS:CE   | 2.26        | 0.65     |
| 2:A:499:GLU:HB2  | 2:A:501:LYS:HD2  | 1.79        | 0.65     |
| 2:A:653:ARG:HG2  | 2:A:653:ARG:NH1  | 2.11        | 0.65     |
| 2:A:606:PRO:O    | 2:A:609:VAL:HG12 | 1.95        | 0.65     |
| 2:A:736:HIS:HA   | 5:A:1007:HOH:O   | 1.95        | 0.65     |
| 2:A:254:TYR:CD2  | 2:A:286:LYS:HE3  | 2.32        | 0.65     |
| 2:A:861:VAL:O    | 2:A:862:ASP:HB2  | 1.96        | 0.65     |
| 2:A:96:THR:H     | 2:A:154:THR:CG2  | 2.09        | 0.65     |
| 2:A:256:VAL:HG12 | 2:A:257:ASN:N    | 2.11        | 0.65     |
| 2:A:491:GLY:C    | 2:A:493:ASN:H    | 1.98        | 0.65     |
| 2:A:368:ASP:OD1  | 2:A:372:LYS:HE3  | 1.97        | 0.65     |
| 1:T:69:G:H5'     | 2:A:589:MET:HE1  | 1.79        | 0.65     |
| 2:A:834:ASN:CB   | 2:A:874:GLY:HA2  | 2.27        | 0.65     |
| 2:A:667:ASP:O    | 2:A:668:SER:O    | 2.14        | 0.65     |
| 2:A:706:GLN:HA   | 2:A:706:GLN:NE2  | 2.12        | 0.65     |
| 2:A:300:HIS:CD2  | 2:A:308:LEU:HD12 | 2.31        | 0.65     |
| 2:A:210:VAL:HG13 | 2:A:385:LEU:HD22 | 1.79        | 0.65     |
| 2:A:469:GLU:H    | 2:A:472:GLU:HG2  | 1.61        | 0.65     |
| 2:A:390:ILE:CG1  | 2:A:391:THR:H    | 2.09        | 0.64     |
| 2:A:825:LEU:O    | 2:A:856:SER:HB2  | 1.96        | 0.64     |
| 2:A:451:TRP:O    | 2:A:453:ILE:HG23 | 1.97        | 0.64     |
| 2:A:644:ASP:HA   | 5:A:1040:HOH:O   | 1.97        | 0.64     |
| 2:A:64:HIS:HB2   | 5:A:1071:HOH:O   | 1.97        | 0.64     |
| 2:A:747:GLN:C    | 2:A:749:LEU:N    | 2.48        | 0.64     |
| 2:A:201:HIS:HB2  | 2:A:396:HIS:CD2  | 2.32        | 0.64     |
| 1:T:18:G:O2'     | 1:T:19:G:OP1     | 2.12        | 0.64     |
| 2:A:64:HIS:NE2   | 2:A:66:GLY:HA3   | 2.13        | 0.64     |
| 1:T:5:U:H2'      | 1:T:6:U:C6       | 2.32        | 0.64     |
| 2:A:413:PHE:CD1  | 2:A:413:PHE:N    | 2.65        | 0.64     |
| 2:A:316:THR:HG22 | 2:A:316:THR:O    | 1.97        | 0.64     |
| 2:A:538:VAL:HG23 | 2:A:542:ARG:HD3  | 1.81        | 0.63     |
| 2:A:167:PHE:HD2  | 2:A:167:PHE:C    | 2.01        | 0.63     |
| 2:A:548:PRO:HB2  | 2:A:580:LYS:HE3  | 1.79        | 0.63     |
| 2:A:813:GLU:OE2  | 2:A:813:GLU:HA   | 1.98        | 0.63     |
| 2:A:400:THR:HG22 | 2:A:402:LYS:HG2  | 1.80        | 0.63     |
| 2:A:831:ILE:CG2  | 2:A:876:ILE:HG12 | 2.28        | 0.63     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:876:ILE:HG22 | 2:A:877:VAL:N    | 2.14        | 0.63     |
| 2:A:84:GLN:OE1   | 2:A:84:GLN:HA    | 1.97        | 0.63     |
| 2:A:132:ILE:HG13 | 2:A:133:GLU:H    | 1.63        | 0.63     |
| 2:A:745:LEU:O    | 2:A:748:ILE:HG22 | 1.98        | 0.63     |
| 2:A:81:LYS:HE3   | 2:A:86:PHE:CE2   | 2.33        | 0.63     |
| 2:A:481:ASN:O    | 2:A:484:ALA:N    | 2.32        | 0.63     |
| 2:A:8:LEU:HD13   | 2:A:738:ARG:NE   | 2.14        | 0.63     |
| 2:A:244:THR:CG2  | 2:A:311:ASN:HB2  | 2.29        | 0.62     |
| 2:A:424:LEU:HD22 | 2:A:442:TYR:CE1  | 2.34        | 0.62     |
| 2:A:158:GLU:O    | 2:A:161:ALA:HB3  | 1.99        | 0.62     |
| 1:T:37:A:H8      | 1:T:37:A:OP2     | 1.82        | 0.62     |
| 2:A:535:HIS:CD2  | 2:A:570:SER:HB2  | 2.34        | 0.62     |
| 2:A:141:ARG:HG3  | 2:A:141:ARG:HH11 | 1.64        | 0.62     |
| 2:A:11:LYS:O     | 2:A:12:THR:HG23  | 1.99        | 0.62     |
| 2:A:16:MET:O     | 2:A:649:ARG:HD2  | 1.99        | 0.62     |
| 2:A:854:ILE:O    | 2:A:854:ILE:HG22 | 1.99        | 0.62     |
| 2:A:41:LEU:HB3   | 2:A:87:TYR:CE1   | 2.33        | 0.62     |
| 2:A:701:TYR:O    | 2:A:704:ILE:N    | 2.29        | 0.62     |
| 2:A:171:ALA:HA   | 2:A:176:ILE:HG22 | 1.82        | 0.62     |
| 2:A:500:ALA:HB3  | 2:A:501:LYS:HE3  | 1.81        | 0.62     |
| 2:A:17:ARG:HG2   | 2:A:646:ARG:HH22 | 1.65        | 0.62     |
| 2:A:749:LEU:C    | 2:A:749:LEU:HD22 | 2.20        | 0.62     |
| 1:T:47:U:O2'     | 1:T:48:C:P       | 2.58        | 0.62     |
| 1:T:19:G:OP1     | 1:T:60:U:N3      | 2.33        | 0.62     |
| 2:A:810:ARG:O    | 2:A:814:THR:HG23 | 2.00        | 0.62     |
| 2:A:235:TRP:HB3  | 2:A:371:ASN:HB3  | 1.81        | 0.62     |
| 2:A:166:ILE:HD12 | 2:A:533:SER:OG   | 2.00        | 0.62     |
| 2:A:212:PHE:CE2  | 2:A:300:HIS:HB3  | 2.35        | 0.62     |
| 2:A:379:THR:HA   | 2:A:385:LEU:CD1  | 2.30        | 0.62     |
| 2:A:397:ASP:OD2  | 2:A:400:THR:HB   | 1.99        | 0.62     |
| 1:T:41:G:O2'     | 2:A:813:GLU:HG2  | 2.00        | 0.61     |
| 2:A:676:GLU:HG2  | 2:A:798:TRP:HZ2  | 1.64        | 0.61     |
| 2:A:718:ASN:HB3  | 5:A:1060:HOH:O   | 1.98        | 0.61     |
| 2:A:267:LEU:HG   | 2:A:320:GLY:O    | 1.99        | 0.61     |
| 2:A:228:ILE:HG22 | 2:A:229:ILE:H    | 1.64        | 0.61     |
| 2:A:120:PHE:HA   | 2:A:123:LYS:HB2  | 1.82        | 0.61     |
| 1:T:58:A:O2'     | 1:T:59:G:O5'     | 2.17        | 0.61     |
| 2:A:821:ILE:HG12 | 2:A:826:GLU:HB2  | 1.81        | 0.61     |
| 2:A:80:TYR:O     | 2:A:83:MET:HB2   | 2.00        | 0.61     |
| 2:A:467:TYR:CB   | 2:A:472:GLU:HB3  | 2.29        | 0.61     |
| 2:A:367:TYR:O    | 2:A:371:ASN:OD1  | 2.18        | 0.61     |
| 2:A:124:CYS:O    | 2:A:459:TRP:CZ2  | 2.54        | 0.61     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:332:GLU:O    | 2:A:335:TYR:HB3  | 2.00        | 0.61     |
| 2:A:256:VAL:CG1  | 2:A:257:ASN:N    | 2.63        | 0.61     |
| 2:A:60:ASN:HD22  | 2:A:60:ASN:C     | 1.99        | 0.61     |
| 2:A:424:LEU:HB3  | 2:A:442:TYR:HE1  | 1.65        | 0.61     |
| 2:A:167:PHE:C    | 2:A:167:PHE:CD2  | 2.74        | 0.61     |
| 2:A:708:VAL:CG1  | 2:A:709:GLN:N    | 2.64        | 0.61     |
| 2:A:420:ARG:O    | 2:A:421:GLN:CB   | 2.48        | 0.61     |
| 2:A:105:LEU:CD1  | 2:A:124:CYS:SG   | 2.87        | 0.61     |
| 2:A:125:LYS:HG2  | 2:A:125:LYS:O    | 1.99        | 0.61     |
| 2:A:318:ASP:CG   | 2:A:319:ALA:H    | 2.03        | 0.61     |
| 2:A:64:HIS:CD2   | 2:A:66:GLY:N     | 2.69        | 0.61     |
| 2:A:263:ILE:HD12 | 2:A:271:VAL:HG21 | 1.83        | 0.60     |
| 2:A:536:ARG:HH12 | 2:A:574:ARG:NE   | 1.98        | 0.60     |
| 2:A:434:VAL:HG22 | 2:A:435:ASN:N    | 2.16        | 0.60     |
| 2:A:702:LEU:O    | 2:A:706:GLN:HG2  | 2.00        | 0.60     |
| 2:A:218:LYS:C    | 2:A:220:VAL:H    | 2.04        | 0.60     |
| 2:A:476:THR:O    | 2:A:479:THR:OG1  | 2.17        | 0.60     |
| 2:A:733:ARG:HG3  | 2:A:733:ARG:HH11 | 1.65        | 0.60     |
| 2:A:366:PHE:N    | 2:A:366:PHE:CD2  | 2.67        | 0.60     |
| 2:A:366:PHE:N    | 2:A:370:ALA:HB3  | 2.03        | 0.60     |
| 2:A:398:TRP:CD1  | 2:A:399:ARG:HG3  | 2.35        | 0.60     |
| 2:A:251:TYR:O    | 2:A:253:GLN:N    | 2.34        | 0.60     |
| 2:A:250:LYS:O    | 2:A:264:ALA:HA   | 2.01        | 0.60     |
| 2:A:373:ALA:HA   | 2:A:376:ASP:OD1  | 2.01        | 0.60     |
| 2:A:382:GLY:O    | 2:A:383:ALA:HB2  | 2.01        | 0.60     |
| 2:A:50:PHE:HZ    | 2:A:551:MET:HG2  | 1.67        | 0.60     |
| 2:A:832:ALA:HB2  | 2:A:861:VAL:CG1  | 2.31        | 0.60     |
| 2:A:397:ASP:OD1  | 2:A:400:THR:HB   | 2.02        | 0.60     |
| 2:A:239:SER:HB3  | 2:A:346:ILE:HD13 | 1.83        | 0.60     |
| 2:A:251:TYR:C    | 2:A:253:GLN:H    | 2.04        | 0.60     |
| 2:A:336:ILE:CG1  | 2:A:337:VAL:N    | 2.62        | 0.60     |
| 2:A:4:GLU:HG3    | 2:A:7:LEU:CD2    | 2.30        | 0.60     |
| 2:A:605:VAL:HG13 | 2:A:606:PRO:HD2  | 1.84        | 0.60     |
| 2:A:244:THR:HG21 | 2:A:337:VAL:CG2  | 2.31        | 0.60     |
| 2:A:367:TYR:CE1  | 2:A:405:ILE:HG21 | 2.37        | 0.60     |
| 2:A:164:ILE:CG1  | 2:A:484:ALA:HB2  | 2.31        | 0.60     |
| 2:A:536:ARG:HH12 | 2:A:574:ARG:NH2  | 2.00        | 0.60     |
| 2:A:232:THR:HG21 | 2:A:392:HIS:HE1  | 1.67        | 0.60     |
| 2:A:494:ILE:HA   | 2:A:497:GLU:CG   | 2.31        | 0.59     |
| 2:A:545:LEU:O    | 2:A:546:SER:HB3  | 2.01        | 0.59     |
| 2:A:548:PRO:O    | 2:A:580:LYS:HE3  | 2.02        | 0.59     |
| 2:A:659:ILE:C    | 2:A:659:ILE:HD12 | 2.23        | 0.59     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:749:LEU:CD2  | 2:A:750:VAL:N    | 2.63        | 0.59     |
| 2:A:625:THR:OG1  | 2:A:631:VAL:HG12 | 2.03        | 0.59     |
| 2:A:218:LYS:CD   | 2:A:218:LYS:H    | 2.14        | 0.59     |
| 2:A:223:ALA:HB3  | 2:A:254:TYR:OH   | 2.02        | 0.59     |
| 2:A:470:ASN:N    | 2:A:472:GLU:HG2  | 2.17        | 0.59     |
| 2:A:126:GLU:O    | 2:A:130:GLU:HG3  | 2.02        | 0.59     |
| 2:A:510:HIS:CE1  | 2:A:511:PRO:HG2  | 2.37        | 0.59     |
| 2:A:539:LEU:CD1  | 2:A:549:ALA:HB2  | 2.33        | 0.59     |
| 2:A:215:LYS:HG2  | 2:A:216:ASP:H    | 1.66        | 0.59     |
| 2:A:228:ILE:CG2  | 2:A:321:THR:HG21 | 2.32        | 0.59     |
| 2:A:235:TRP:O    | 2:A:238:PRO:HD2  | 2.02        | 0.59     |
| 2:A:823:LYS:HG2  | 2:A:826:GLU:OE2  | 2.02        | 0.59     |
| 2:A:830:THR:HB   | 2:A:877:VAL:HG22 | 1.83        | 0.59     |
| 2:A:745:LEU:HD23 | 2:A:748:ILE:HG21 | 1.83        | 0.59     |
| 2:A:41:LEU:HB3   | 2:A:87:TYR:HE1   | 1.66        | 0.59     |
| 2:A:220:VAL:HG12 | 2:A:220:VAL:O    | 2.02        | 0.59     |
| 2:A:234:PRO:HG2  | 2:A:235:TRP:N    | 2.17        | 0.59     |
| 2:A:289:THR:O    | 2:A:289:THR:HG22 | 2.02        | 0.59     |
| 2:A:484:ALA:C    | 2:A:486:LEU:N    | 2.56        | 0.59     |
| 2:A:600:LEU:HD23 | 2:A:600:LEU:O    | 2.03        | 0.59     |
| 1:T:38:A:H2'     | 1:T:39:G:H5'     | 1.85        | 0.59     |
| 2:A:499:GLU:HA   | 2:A:520:LYS:HZ2  | 1.68        | 0.59     |
| 2:A:257:ASN:O    | 2:A:258:GLY:C    | 2.41        | 0.59     |
| 2:A:338:GLY:O    | 2:A:343:LEU:HD12 | 2.01        | 0.59     |
| 2:A:535:HIS:HB2  | 2:A:547:PHE:CE1  | 2.38        | 0.59     |
| 2:A:411:GLN:NE2  | 2:A:456:GLN:HE22 | 1.97        | 0.59     |
| 2:A:558:GLN:O    | 2:A:563:PHE:HB2  | 2.03        | 0.59     |
| 2:A:46:GLY:O     | 2:A:47:ASN:O     | 2.20        | 0.58     |
| 2:A:613:LYS:HD3  | 2:A:642:SER:OG   | 2.03        | 0.58     |
| 2:A:178:LYS:NZ   | 2:A:412:TRP:HE1  | 2.01        | 0.58     |
| 2:A:453:ILE:O    | 2:A:453:ILE:HD12 | 2.02        | 0.58     |
| 2:A:589:MET:HB3  | 2:A:594:LYS:O    | 2.04        | 0.58     |
| 2:A:239:SER:HB3  | 2:A:346:ILE:HB   | 1.86        | 0.58     |
| 2:A:834:ASN:HD22 | 2:A:874:GLY:C    | 2.05        | 0.58     |
| 2:A:792:GLN:O    | 2:A:795:LEU:N    | 2.37        | 0.58     |
| 2:A:739:ARG:HD3  | 2:A:742:GLN:NE2  | 2.19        | 0.58     |
| 2:A:419:VAL:HA   | 2:A:422:ASP:OD1  | 2.03        | 0.58     |
| 2:A:469:GLU:HB2  | 2:A:512:GLY:HA3  | 1.83        | 0.58     |
| 2:A:314:HIS:O    | 2:A:315:VAL:HB   | 2.03        | 0.58     |
| 2:A:247:PRO:CD   | 2:A:312:GLY:HA2  | 2.34        | 0.58     |
| 2:A:379:THR:HG23 | 2:A:385:LEU:CB   | 2.31        | 0.58     |
| 2:A:234:PRO:CG   | 2:A:235:TRP:H    | 2.17        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:821:ILE:CD1  | 2:A:822:GLY:N    | 2.61        | 0.58     |
| 2:A:792:GLN:HE22 | 2:A:799:ARG:NH1  | 2.00        | 0.58     |
| 2:A:315:VAL:O    | 2:A:316:THR:OG1  | 2.22        | 0.58     |
| 2:A:616:ASP:OD1  | 2:A:762:HIS:HB2  | 2.04        | 0.58     |
| 2:A:490:HIS:HB2  | 2:A:494:ILE:HB   | 1.84        | 0.58     |
| 2:A:247:PRO:O    | 2:A:248:GLU:CB   | 2.51        | 0.58     |
| 2:A:328:PRO:HA   | 2:A:335:TYR:HA   | 1.86        | 0.58     |
| 2:A:299:GLN:HB3  | 2:A:304:ASP:HB2  | 1.86        | 0.57     |
| 2:A:724:GLY:HA3  | 2:A:741:MET:HE1  | 1.85        | 0.57     |
| 2:A:225:ALA:HB2  | 2:A:254:TYR:CE2  | 2.39        | 0.57     |
| 2:A:387:LEU:C    | 2:A:387:LEU:HD23 | 2.24        | 0.57     |
| 2:A:552:TYR:CD1  | 2:A:579:TYR:HB3  | 2.39        | 0.57     |
| 2:A:192:SER:O    | 2:A:193:LEU:HD23 | 2.04        | 0.57     |
| 2:A:243:ILE:HG23 | 2:A:323:CYS:O    | 2.03        | 0.57     |
| 2:A:250:LYS:HD2  | 2:A:251:TYR:H    | 1.69        | 0.57     |
| 2:A:588:VAL:HG12 | 2:A:596:MET:SD   | 2.44        | 0.57     |
| 2:A:185:TRP:C    | 2:A:404:VAL:HG13 | 2.24        | 0.57     |
| 2:A:69:LEU:CD1   | 2:A:622:VAL:HG13 | 2.34        | 0.57     |
| 1:T:71:C:O2'     | 2:A:560:ARG:NH1  | 2.38        | 0.57     |
| 2:A:209:TYR:O    | 2:A:386:LYS:HB2  | 2.04        | 0.57     |
| 2:A:821:ILE:HD11 | 2:A:824:SER:N    | 2.20        | 0.57     |
| 2:A:469:GLU:C    | 2:A:471:GLY:N    | 2.58        | 0.57     |
| 2:A:625:THR:OG1  | 2:A:631:VAL:CG1  | 2.53        | 0.57     |
| 2:A:809:ASN:O    | 2:A:812:LEU:N    | 2.37        | 0.57     |
| 2:A:163:GLN:NE2  | 2:A:529:PHE:CD2  | 2.73        | 0.57     |
| 2:A:228:ILE:O    | 2:A:229:ILE:HB   | 2.05        | 0.57     |
| 1:T:42:U:O2'     | 1:T:43:G:H5'     | 2.05        | 0.57     |
| 2:A:218:LYS:O    | 2:A:221:VAL:HG23 | 2.05        | 0.57     |
| 2:A:35:ASP:O     | 2:A:39:LYS:HG2   | 2.04        | 0.57     |
| 2:A:708:VAL:CG1  | 2:A:709:GLN:H    | 2.18        | 0.57     |
| 2:A:164:ILE:HG12 | 2:A:484:ALA:HB2  | 1.86        | 0.57     |
| 2:A:23:LYS:HA    | 2:A:26:GLN:NE2   | 2.20        | 0.57     |
| 2:A:741:MET:CE   | 2:A:745:LEU:HD11 | 2.34        | 0.57     |
| 2:A:469:GLU:CG   | 2:A:512:GLY:HA3  | 2.35        | 0.57     |
| 2:A:747:GLN:C    | 2:A:749:LEU:H    | 2.06        | 0.57     |
| 2:A:397:ASP:CG   | 2:A:400:THR:HB   | 2.24        | 0.57     |
| 2:A:336:ILE:CG1  | 2:A:337:VAL:H    | 2.17        | 0.57     |
| 2:A:416:ILE:HD11 | 2:A:451:TRP:HB2  | 1.85        | 0.57     |
| 2:A:842:PHE:C    | 2:A:844:THR:H    | 2.09        | 0.57     |
| 2:A:217:ASP:O    | 2:A:220:VAL:HB   | 2.05        | 0.56     |
| 2:A:296:VAL:O    | 2:A:310:ILE:HD13 | 2.05        | 0.56     |
| 2:A:382:GLY:O    | 2:A:383:ALA:CB   | 2.53        | 0.56     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:A:385:LEU:O   | 2:A:386:LYS:HG2  | 2.05        | 0.56     |
| 2:A:472:GLU:O   | 2:A:473:ILE:HB   | 2.05        | 0.56     |
| 2:A:201:HIS:HB2 | 2:A:396:HIS:NE2  | 2.20        | 0.56     |
| 2:A:160:GLU:O   | 2:A:163:GLN:HB3  | 2.05        | 0.56     |
| 1:T:47:U:HO2'   | 1:T:48:C:P       | 2.28        | 0.56     |
| 2:A:832:ALA:HB2 | 2:A:861:VAL:HG13 | 1.86        | 0.56     |
| 2:A:302:PHE:CD1 | 2:A:303:LEU:N    | 2.74        | 0.56     |
| 2:A:461:VAL:O   | 2:A:525:MET:HG3  | 2.05        | 0.56     |
| 2:A:424:LEU:HB3 | 2:A:442:TYR:CE1  | 2.41        | 0.56     |
| 2:A:553:LEU:O   | 2:A:554:GLU:CD   | 2.44        | 0.56     |
| 2:A:212:PHE:HD2 | 2:A:301:PRO:HD2  | 1.67        | 0.56     |
| 2:A:487:PHE:CD1 | 2:A:492:SER:HA   | 2.40        | 0.56     |
| 1:T:66:C:O2'    | 1:T:67:A:H5'     | 2.05        | 0.56     |
| 2:A:865:ASP:HB3 | 2:A:867:GLN:NE2  | 2.21        | 0.56     |
| 2:A:713:ASN:O   | 2:A:718:ASN:HB2  | 2.05        | 0.56     |
| 2:A:263:ILE:CD1 | 2:A:271:VAL:HG21 | 2.36        | 0.56     |
| 2:A:8:LEU:HD21  | 2:A:733:ARG:NH1  | 2.21        | 0.56     |
| 1:T:43:G:O2'    | 1:T:44:A:C5'     | 2.54        | 0.56     |
| 2:A:79:ARG:HH12 | 2:A:780:HIS:CG   | 2.23        | 0.56     |
| 2:A:218:LYS:HD2 | 2:A:218:LYS:N    | 2.15        | 0.56     |
| 2:A:219:GLY:HA2 | 2:A:297:VAL:H    | 1.70        | 0.56     |
| 2:A:327:ALA:C   | 2:A:329:GLY:H    | 2.08        | 0.56     |
| 2:A:816:ARG:HD2 | 2:A:822:GLY:O    | 2.06        | 0.56     |
| 2:A:468:ALA:HA  | 2:A:472:GLU:OE2  | 2.06        | 0.56     |
| 2:A:749:LEU:O   | 2:A:752:MET:N    | 2.30        | 0.56     |
| 2:A:194:ALA:O   | 2:A:195:GLU:C    | 2.44        | 0.56     |
| 2:A:664:PRO:O   | 2:A:665:ASP:C    | 2.45        | 0.56     |
| 2:A:212:PHE:CE1 | 2:A:229:ILE:HG21 | 2.40        | 0.56     |
| 2:A:254:TYR:HD2 | 2:A:286:LYS:HE3  | 1.69        | 0.56     |
| 2:A:57:PRO:HG3  | 5:A:1013:HOH:O   | 2.06        | 0.56     |
| 2:A:419:VAL:O   | 2:A:420:ARG:C    | 2.45        | 0.56     |
| 2:A:487:PHE:O   | 2:A:491:GLY:N    | 2.37        | 0.56     |
| 2:A:120:PHE:CG  | 2:A:124:CYS:SG   | 2.99        | 0.56     |
| 1:T:51:U:C2     | 1:T:52:G:C8      | 2.94        | 0.56     |
| 2:A:618:ALA:O   | 2:A:621:TRP:HB3  | 2.06        | 0.56     |
| 2:A:64:HIS:HD2  | 2:A:66:GLY:H     | 1.54        | 0.56     |
| 2:A:237:ILE:C   | 2:A:239:SER:N    | 2.58        | 0.55     |
| 2:A:747:GLN:O   | 2:A:749:LEU:N    | 2.39        | 0.55     |
| 2:A:24:GLU:HG2  | 2:A:762:HIS:CD2  | 2.41        | 0.55     |
| 2:A:219:GLY:HA3 | 2:A:297:VAL:O    | 2.06        | 0.55     |
| 2:A:484:ALA:O   | 2:A:486:LEU:N    | 2.39        | 0.55     |
| 2:A:842:PHE:O   | 2:A:844:THR:N    | 2.39        | 0.55     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:212:PHE:CE2  | 2:A:301:PRO:HD2  | 2.40        | 0.55     |
| 2:A:212:PHE:N    | 2:A:227:PHE:O    | 2.37        | 0.55     |
| 2:A:470:ASN:H    | 2:A:472:GLU:HG2  | 1.71        | 0.55     |
| 1:T:63:A:O2'     | 1:T:64:C:H5'     | 2.05        | 0.55     |
| 2:A:293:LEU:HD23 | 2:A:296:VAL:HG23 | 1.89        | 0.55     |
| 2:A:371:ASN:N    | 2:A:371:ASN:ND2  | 2.54        | 0.55     |
| 1:T:31:C:H2'     | 1:T:32:C:H6      | 1.72        | 0.55     |
| 2:A:477:LYS:O    | 2:A:478:GLU:HB3  | 2.06        | 0.55     |
| 2:A:536:ARG:HH22 | 2:A:574:ARG:NH2  | 2.04        | 0.55     |
| 1:T:19:G:HO2'    | 1:T:20:U:P       | 2.28        | 0.55     |
| 2:A:324:VAL:O    | 2:A:325:HIS:CB   | 2.52        | 0.55     |
| 2:A:469:GLU:HB3  | 2:A:472:GLU:H    | 1.72        | 0.55     |
| 2:A:765:GLU:OE1  | 2:A:778:SER:HA   | 2.05        | 0.55     |
| 2:A:535:HIS:HB2  | 2:A:547:PHE:HE1  | 1.70        | 0.55     |
| 1:T:4:C:O2'      | 1:T:5:U:H5'      | 2.07        | 0.55     |
| 2:A:81:LYS:HE3   | 2:A:86:PHE:HE2   | 1.72        | 0.55     |
| 2:A:272:ALA:CA   | 2:A:277:TRP:HB2  | 2.36        | 0.55     |
| 2:A:350:ASP:OD2  | 2:A:351:ASP:N    | 2.38        | 0.55     |
| 2:A:23:LYS:HE3   | 2:A:27:ILE:CD1   | 2.31        | 0.55     |
| 2:A:212:PHE:CD1  | 2:A:229:ILE:HG21 | 2.41        | 0.55     |
| 2:A:74:LYS:O     | 2:A:78:VAL:HG23  | 2.07        | 0.55     |
| 2:A:590:ASP:C    | 2:A:590:ASP:OD1  | 2.44        | 0.55     |
| 2:A:446:ARG:CG   | 2:A:446:ARG:O    | 2.55        | 0.55     |
| 2:A:741:MET:HB2  | 5:A:1063:HOH:O   | 2.07        | 0.55     |
| 2:A:294:GLU:O    | 2:A:295:TRP:HB2  | 2.05        | 0.54     |
| 2:A:290:GLY:HA2  | 2:A:293:LEU:CB   | 2.34        | 0.54     |
| 2:A:164:ILE:HD11 | 2:A:484:ALA:CB   | 2.35        | 0.54     |
| 2:A:494:ILE:HG13 | 2:A:494:ILE:O    | 2.06        | 0.54     |
| 2:A:505:PRO:HB2  | 2:A:508:PHE:HB2  | 1.88        | 0.54     |
| 1:T:2:G:H2'      | 1:T:3:G:C8       | 2.42        | 0.54     |
| 2:A:362:PHE:HE2  | 2:A:374:VAL:CG2  | 2.20        | 0.54     |
| 2:A:453:ILE:CD1  | 2:A:463:LEU:HD21 | 2.36        | 0.54     |
| 2:A:491:GLY:C    | 2:A:493:ASN:N    | 2.60        | 0.54     |
| 2:A:463:LEU:CD1  | 2:A:525:MET:HG2  | 2.36        | 0.54     |
| 2:A:466:PHE:CE1  | 2:A:504:LEU:HD11 | 2.41        | 0.54     |
| 2:A:602:ASN:ND2  | 2:A:602:ASN:N    | 2.54        | 0.54     |
| 2:A:380:GLU:HA   | 2:A:384:LEU:HA   | 1.88        | 0.54     |
| 2:A:23:LYS:CE    | 2:A:27:ILE:HD11  | 2.30        | 0.54     |
| 2:A:415:SER:O    | 2:A:419:VAL:HG22 | 2.08        | 0.54     |
| 2:A:491:GLY:O    | 2:A:494:ILE:HG22 | 2.08        | 0.54     |
| 2:A:595:LYS:NZ   | 4:A:993:MRC:H8'1 | 2.21        | 0.54     |
| 2:A:121:ARG:NH1  | 2:A:496:PHE:CE1  | 2.76        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:81:LYS:HG3   | 2:A:86:PHE:CD2   | 2.42        | 0.54     |
| 2:A:707:GLU:O    | 2:A:708:VAL:C    | 2.46        | 0.54     |
| 2:A:163:GLN:OE1  | 2:A:530:ASP:HA   | 2.08        | 0.54     |
| 1:T:22:G:N7      | 1:T:46:G:N2      | 2.50        | 0.54     |
| 2:A:250:LYS:CD   | 2:A:251:TYR:H    | 2.20        | 0.54     |
| 2:A:372:LYS:C    | 2:A:374:VAL:N    | 2.60        | 0.54     |
| 2:A:374:VAL:HG12 | 2:A:375:THR:N    | 2.23        | 0.54     |
| 2:A:486:LEU:CD2  | 2:A:494:ILE:HG12 | 2.38        | 0.54     |
| 2:A:598:LYS:O    | 2:A:600:LEU:N    | 2.41        | 0.54     |
| 1:T:33:U:H1'     | 1:T:36:U:N3      | 2.19        | 0.54     |
| 2:A:551:MET:HE3  | 2:A:699:PHE:CZ   | 2.43        | 0.54     |
| 2:A:278:ASP:C    | 2:A:280:ALA:N    | 2.60        | 0.54     |
| 2:A:621:TRP:O    | 2:A:624:SER:N    | 2.40        | 0.54     |
| 2:A:706:GLN:CA   | 2:A:706:GLN:HE21 | 2.21        | 0.53     |
| 2:A:321:THR:C    | 2:A:323:CYS:H    | 2.10        | 0.53     |
| 2:A:433:LYS:HG2  | 2:A:583:LEU:HD21 | 1.90        | 0.53     |
| 2:A:768:TRP:HB2  | 2:A:779:VAL:HG22 | 1.89        | 0.53     |
| 2:A:327:ALA:N    | 2:A:334:ASP:OD1  | 2.41        | 0.53     |
| 2:A:420:ARG:HH21 | 2:A:448:ARG:HB3  | 1.71        | 0.53     |
| 2:A:632:ARG:CG   | 2:A:632:ARG:HH11 | 2.21        | 0.53     |
| 2:A:175:LEU:CD2  | 2:A:418:LYS:HD2  | 2.37        | 0.53     |
| 2:A:739:ARG:HA   | 2:A:742:GLN:HE21 | 1.73        | 0.53     |
| 2:A:24:GLU:HG2   | 2:A:762:HIS:CG   | 2.43        | 0.53     |
| 2:A:773:HIS:O    | 2:A:774:VAL:C    | 2.45        | 0.53     |
| 2:A:294:GLU:HA   | 2:A:310:ILE:CG2  | 2.39        | 0.53     |
| 2:A:348:PRO:O    | 2:A:407:ARG:HD3  | 2.09        | 0.53     |
| 2:A:44:ASN:O     | 2:A:45:LYS:O     | 2.25        | 0.53     |
| 2:A:818:GLU:O    | 2:A:819:LYS:HB2  | 2.09        | 0.53     |
| 2:A:243:ILE:O    | 2:A:310:ILE:HA   | 2.08        | 0.53     |
| 2:A:357:GLU:O    | 2:A:359:GLY:N    | 2.39        | 0.53     |
| 2:A:685:LEU:HD13 | 2:A:748:ILE:HA   | 1.89        | 0.53     |
| 2:A:555:GLY:O    | 2:A:557:ASP:N    | 2.42        | 0.53     |
| 2:A:116:SER:N    | 2:A:119:GLU:HB2  | 2.24        | 0.53     |
| 2:A:551:MET:HA   | 2:A:581:PHE:O    | 2.09        | 0.53     |
| 2:A:96:THR:HB    | 2:A:155:LEU:HD23 | 1.91        | 0.53     |
| 2:A:207:SER:HB3  | 2:A:388:ASP:HB2  | 1.90        | 0.53     |
| 2:A:204:ARG:HG3  | 2:A:204:ARG:O    | 2.07        | 0.53     |
| 2:A:331:GLY:HA3  | 2:A:334:ASP:HB3  | 1.90        | 0.53     |
| 1:T:69:G:H5''    | 2:A:589:MET:HE2  | 1.90        | 0.53     |
| 2:A:676:GLU:HG2  | 2:A:798:TRP:CZ2  | 2.44        | 0.53     |
| 2:A:733:ARG:NH1  | 2:A:733:ARG:HG3  | 2.24        | 0.53     |
| 2:A:818:GLU:HB2  | 2:A:820:VAL:HG23 | 1.90        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:661:ASP:C    | 2:A:661:ASP:OD2  | 2.45        | 0.53     |
| 2:A:482:HIS:CD2  | 2:A:486:LEU:HD12 | 2.44        | 0.53     |
| 2:A:547:PHE:HB3  | 2:A:548:PRO:HD3  | 1.91        | 0.53     |
| 2:A:501:LYS:H    | 2:A:501:LYS:CE   | 2.21        | 0.53     |
| 2:A:711:PHE:CE2  | 2:A:752:MET:HE1  | 2.44        | 0.53     |
| 2:A:649:ARG:CG   | 2:A:649:ARG:NH1  | 2.72        | 0.53     |
| 2:A:225:ALA:HB2  | 2:A:254:TYR:CZ   | 2.44        | 0.53     |
| 2:A:350:ASP:HB3  | 2:A:352:LYS:O    | 2.08        | 0.53     |
| 2:A:350:ASP:O    | 2:A:407:ARG:CZ   | 2.57        | 0.53     |
| 2:A:423:ILE:O    | 2:A:426:ALA:N    | 2.42        | 0.53     |
| 2:A:469:GLU:OE1  | 2:A:510:HIS:HE1  | 1.92        | 0.53     |
| 2:A:372:LYS:C    | 2:A:374:VAL:H    | 2.12        | 0.52     |
| 2:A:597:SER:HB2  | 5:A:1021:HOH:O   | 2.09        | 0.52     |
| 2:A:58:TYR:CZ    | 2:A:101:ILE:HG13 | 2.44        | 0.52     |
| 2:A:439:THR:O    | 2:A:440:ARG:C    | 2.48        | 0.52     |
| 2:A:166:ILE:O    | 2:A:170:MET:HG3  | 2.10        | 0.52     |
| 2:A:749:LEU:CG   | 2:A:750:VAL:H    | 2.20        | 0.52     |
| 2:A:182:PRO:HA   | 2:A:407:ARG:O    | 2.09        | 0.52     |
| 2:A:380:GLU:O    | 2:A:382:GLY:N    | 2.41        | 0.52     |
| 2:A:120:PHE:CZ   | 2:A:124:CYS:SG   | 3.03        | 0.52     |
| 2:A:12:THR:HG23  | 2:A:657:GLY:HA2  | 1.91        | 0.52     |
| 2:A:229:ILE:O    | 2:A:229:ILE:HG23 | 2.09        | 0.52     |
| 2:A:823:LYS:HG2  | 2:A:826:GLU:HG3  | 1.91        | 0.52     |
| 2:A:2:ASP:OD2    | 2:A:4:GLU:HB3    | 2.09        | 0.52     |
| 2:A:267:LEU:O    | 2:A:268:SER:C    | 2.47        | 0.52     |
| 2:A:638:LEU:O    | 2:A:642:SER:N    | 2.42        | 0.52     |
| 2:A:309:VAL:HG12 | 2:A:310:ILE:H    | 1.75        | 0.52     |
| 2:A:348:PRO:O    | 2:A:349:ILE:HB   | 2.09        | 0.52     |
| 2:A:691:SER:O    | 2:A:695:ASN:ND2  | 2.43        | 0.52     |
| 2:A:229:ILE:HD11 | 2:A:324:VAL:C    | 2.30        | 0.52     |
| 2:A:372:LYS:O    | 2:A:374:VAL:N    | 2.42        | 0.52     |
| 2:A:176:ILE:O    | 2:A:176:ILE:HG23 | 2.10        | 0.52     |
| 2:A:398:TRP:HA   | 2:A:401:LYS:HD3  | 1.92        | 0.52     |
| 2:A:163:GLN:NE2  | 2:A:529:PHE:HD2  | 2.07        | 0.52     |
| 2:A:278:ASP:OD1  | 2:A:281:SER:HB3  | 2.10        | 0.52     |
| 2:A:802:MET:CE   | 2:A:805:ARG:HD3  | 2.40        | 0.52     |
| 2:A:245:VAL:HG12 | 2:A:246:HIS:H    | 1.74        | 0.52     |
| 2:A:571:VAL:C    | 2:A:573:THR:H    | 2.13        | 0.52     |
| 2:A:226:LYS:HD2  | 2:A:259:GLU:HB2  | 1.91        | 0.51     |
| 2:A:420:ARG:O    | 2:A:421:GLN:HB2  | 2.09        | 0.51     |
| 2:A:107:LYS:O    | 2:A:107:LYS:HG2  | 2.10        | 0.51     |
| 2:A:300:HIS:HD2  | 2:A:308:LEU:HD12 | 1.74        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:802:MET:HA   | 2:A:802:MET:CE   | 2.40        | 0.51     |
| 2:A:560:ARG:HB2  | 2:A:560:ARG:NH1  | 2.25        | 0.51     |
| 2:A:250:LYS:HD2  | 2:A:251:TYR:N    | 2.25        | 0.51     |
| 2:A:280:ALA:O    | 2:A:282:ILE:N    | 2.40        | 0.51     |
| 2:A:377:LEU:O    | 2:A:381:LYS:HB2  | 2.10        | 0.51     |
| 2:A:200:TYR:CD1  | 2:A:200:TYR:N    | 2.79        | 0.51     |
| 2:A:200:TYR:HE2  | 2:A:395:PRO:HG3  | 1.70        | 0.51     |
| 2:A:560:ARG:CB   | 2:A:560:ARG:NH1  | 2.74        | 0.51     |
| 2:A:244:THR:HG21 | 2:A:337:VAL:HG21 | 1.91        | 0.51     |
| 2:A:837:PHE:HD2  | 2:A:873:HIS:O    | 1.94        | 0.51     |
| 2:A:257:ASN:CG   | 2:A:258:GLY:H    | 2.14        | 0.51     |
| 1:T:35:A:C2      | 2:A:654:PHE:HB2  | 2.45        | 0.51     |
| 2:A:876:ILE:CG2  | 2:A:877:VAL:N    | 2.73        | 0.51     |
| 2:A:292:GLU:C    | 2:A:294:GLU:N    | 2.64        | 0.51     |
| 2:A:416:ILE:O    | 2:A:420:ARG:HG2  | 2.10        | 0.51     |
| 2:A:417:SER:HA   | 2:A:420:ARG:HD2  | 1.92        | 0.51     |
| 2:A:470:ASN:N    | 2:A:472:GLU:CG   | 2.73        | 0.51     |
| 2:A:330:HIS:HA   | 2:A:406:PHE:HB3  | 1.92        | 0.51     |
| 2:A:229:ILE:HA   | 2:A:321:THR:OG1  | 2.10        | 0.51     |
| 1:T:4:C:C2'      | 1:T:5:U:H5'      | 2.40        | 0.51     |
| 2:A:129:LEU:CA   | 2:A:132:ILE:HG12 | 2.40        | 0.51     |
| 2:A:328:PRO:HB3  | 2:A:335:TYR:HA   | 1.93        | 0.51     |
| 2:A:194:ALA:O    | 2:A:196:ALA:N    | 2.44        | 0.51     |
| 2:A:777:GLU:O    | 2:A:778:SER:HB3  | 2.11        | 0.51     |
| 2:A:567:ILE:O    | 2:A:571:VAL:HG23 | 2.11        | 0.51     |
| 2:A:417:SER:HA   | 2:A:420:ARG:HG2  | 1.91        | 0.51     |
| 2:A:861:VAL:O    | 2:A:862:ASP:CB   | 2.59        | 0.51     |
| 2:A:679:ARG:HH22 | 2:A:791:ASP:CG   | 2.13        | 0.51     |
| 2:A:195:GLU:O    | 2:A:197:GLU:N    | 2.44        | 0.51     |
| 2:A:768:TRP:CG   | 2:A:779:VAL:HG22 | 2.46        | 0.51     |
| 2:A:250:LYS:HZ2  | 2:A:289:THR:CG2  | 2.18        | 0.51     |
| 2:A:56:PRO:HD3   | 2:A:152:TYR:OH   | 2.10        | 0.51     |
| 2:A:805:ARG:O    | 2:A:808:VAL:N    | 2.44        | 0.51     |
| 2:A:468:ALA:HB2  | 2:A:518:PHE:CD2  | 2.46        | 0.51     |
| 2:A:664:PRO:HG2  | 2:A:746:TYR:CE2  | 2.46        | 0.51     |
| 2:A:279:LYS:O    | 2:A:280:ALA:CB   | 2.58        | 0.51     |
| 2:A:350:ASP:HB2  | 2:A:354:VAL:O    | 2.11        | 0.51     |
| 2:A:809:ASN:C    | 2:A:811:ALA:N    | 2.63        | 0.51     |
| 2:A:512:GLY:O    | 2:A:513:SER:C    | 2.49        | 0.51     |
| 2:A:309:VAL:O    | 2:A:310:ILE:HD12 | 2.11        | 0.50     |
| 2:A:348:PRO:O    | 2:A:407:ARG:HG2  | 2.11        | 0.50     |
| 2:A:181:LYS:HD3  | 2:A:452:VAL:HG21 | 1.92        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:719:PHE:HD1  | 2:A:805:ARG:NH2  | 2.09        | 0.50     |
| 2:A:468:ALA:H    | 2:A:472:GLU:CB   | 2.22        | 0.50     |
| 2:A:110:VAL:O    | 2:A:111:ASP:HB3  | 2.11        | 0.50     |
| 2:A:120:PHE:O    | 2:A:124:CYS:SG   | 2.69        | 0.50     |
| 1:T:58:A:O2'     | 1:T:59:G:P       | 2.68        | 0.50     |
| 1:T:11:C:H5'     | 2:A:636:GLU:OE2  | 2.11        | 0.50     |
| 2:A:218:LYS:HA   | 2:A:221:VAL:HG23 | 1.92        | 0.50     |
| 2:A:213:ASN:ND2  | 2:A:226:LYS:HE3  | 2.26        | 0.50     |
| 2:A:719:PHE:HD1  | 2:A:805:ARG:CZ   | 2.24        | 0.50     |
| 2:A:469:GLU:HG3  | 2:A:512:GLY:HA3  | 1.91        | 0.50     |
| 2:A:727:ILE:HD13 | 2:A:737:ILE:CG1  | 2.41        | 0.50     |
| 1:T:60:U:O2'     | 1:T:61:C:OP1     | 2.26        | 0.50     |
| 1:T:55:U:O5'     | 1:T:55:U:H6      | 1.95        | 0.50     |
| 2:A:366:PHE:HD1  | 2:A:369:LYS:HB3  | 1.75        | 0.50     |
| 2:A:420:ARG:HH22 | 2:A:449:GLY:H    | 1.59        | 0.50     |
| 2:A:652:LEU:HA   | 2:A:655:MET:CE   | 2.42        | 0.50     |
| 2:A:409:THR:HG23 | 2:A:410:PRO:HD2  | 1.92        | 0.50     |
| 2:A:775:LYS:C    | 2:A:776:GLU:HG2  | 2.31        | 0.50     |
| 2:A:223:ALA:CB   | 2:A:254:TYR:OH   | 2.60        | 0.50     |
| 2:A:178:LYS:NZ   | 2:A:412:TRP:NE1  | 2.57        | 0.50     |
| 2:A:443:ASN:ND2  | 2:A:446:ARG:CZ   | 2.74        | 0.50     |
| 2:A:589:MET:HE3  | 2:A:595:LYS:CA   | 2.31        | 0.50     |
| 2:A:603:VAL:HG11 | 4:A:993:MRC:H3'1 | 1.92        | 0.50     |
| 2:A:50:PHE:CZ    | 2:A:551:MET:HG2  | 2.45        | 0.50     |
| 2:A:39:LYS:HA    | 2:A:42:GLU:HB2   | 1.94        | 0.50     |
| 2:A:267:LEU:O    | 2:A:270:ALA:N    | 2.44        | 0.50     |
| 2:A:20:LEU:N     | 2:A:20:LEU:HD12  | 2.24        | 0.50     |
| 1:T:43:G:H2'     | 1:T:44:A:H8      | 1.73        | 0.50     |
| 2:A:186:SER:HB2  | 2:A:404:VAL:HG22 | 1.93        | 0.50     |
| 2:A:230:TRP:CE3  | 2:A:319:ALA:HB1  | 2.47        | 0.50     |
| 2:A:303:LEU:O    | 2:A:305:ARG:N    | 2.45        | 0.50     |
| 2:A:467:TYR:N    | 2:A:519:THR:O    | 2.34        | 0.50     |
| 2:A:112:ARG:NH2  | 2:A:458:VAL:HG21 | 2.27        | 0.50     |
| 1:T:5:U:H2'      | 1:T:6:U:H6       | 1.75        | 0.50     |
| 2:A:292:GLU:O    | 2:A:294:GLU:N    | 2.45        | 0.50     |
| 2:A:510:HIS:CG   | 2:A:511:PRO:HD2  | 2.46        | 0.50     |
| 2:A:359:GLY:HA3  | 2:A:362:PHE:HB2  | 1.92        | 0.50     |
| 2:A:711:PHE:HE2  | 2:A:752:MET:HE1  | 1.76        | 0.50     |
| 2:A:58:TYR:HA    | 2:A:95:ASP:HB2   | 1.94        | 0.50     |
| 2:A:247:PRO:HA   | 2:A:291:LYS:CA   | 2.41        | 0.49     |
| 2:A:277:TRP:C    | 2:A:279:LYS:H    | 2.15        | 0.49     |
| 2:A:116:SER:HB3  | 2:A:119:GLU:CG   | 2.31        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:8:LEU:HB2    | 2:A:729:TYR:O    | 2.11        | 0.49     |
| 2:A:861:VAL:O    | 2:A:861:VAL:CG2  | 2.60        | 0.49     |
| 2:A:853:PHE:O    | 2:A:855:VAL:HG13 | 2.11        | 0.49     |
| 2:A:719:PHE:CD1  | 2:A:805:ARG:CZ   | 2.95        | 0.49     |
| 2:A:805:ARG:O    | 2:A:807:ASP:N    | 2.45        | 0.49     |
| 2:A:476:THR:O    | 2:A:480:VAL:HG23 | 2.12        | 0.49     |
| 2:A:141:ARG:HG3  | 2:A:141:ARG:NH1  | 2.27        | 0.49     |
| 2:A:861:VAL:O    | 2:A:861:VAL:HG22 | 2.11        | 0.49     |
| 2:A:339:GLN:O    | 2:A:341:TYR:N    | 2.46        | 0.49     |
| 2:A:373:ALA:O    | 2:A:376:ASP:HB2  | 2.12        | 0.49     |
| 2:A:451:TRP:CD1  | 2:A:453:ILE:HG22 | 2.46        | 0.49     |
| 2:A:112:ARG:HD2  | 2:A:113:LYS:HD2  | 1.95        | 0.49     |
| 2:A:65:MET:HA    | 2:A:606:PRO:HG3  | 1.93        | 0.49     |
| 2:A:204:ARG:CG   | 2:A:204:ARG:O    | 2.59        | 0.49     |
| 2:A:338:GLY:HA2  | 2:A:343:LEU:HD12 | 1.94        | 0.49     |
| 2:A:341:TYR:CD1  | 2:A:341:TYR:N    | 2.80        | 0.49     |
| 2:A:113:LYS:O    | 2:A:114:LYS:HB2  | 2.11        | 0.49     |
| 2:A:279:LYS:O    | 2:A:280:ALA:HB3  | 2.13        | 0.49     |
| 2:A:443:ASN:ND2  | 2:A:446:ARG:NH1  | 2.60        | 0.49     |
| 2:A:176:ILE:CG2  | 2:A:475:MET:HE3  | 2.43        | 0.49     |
| 2:A:81:LYS:HG3   | 2:A:86:PHE:HD2   | 1.75        | 0.49     |
| 2:A:206:ALA:O    | 2:A:208:ILE:HG23 | 2.11        | 0.49     |
| 1:T:12:U:H5"     | 5:A:1033:HOH:O   | 2.12        | 0.49     |
| 2:A:472:GLU:O    | 2:A:473:ILE:CB   | 2.61        | 0.49     |
| 2:A:255:ASN:CG   | 2:A:256:VAL:N    | 2.66        | 0.49     |
| 2:A:327:ALA:O    | 2:A:329:GLY:N    | 2.45        | 0.49     |
| 2:A:656:LEU:HD21 | 2:A:771:THR:HG23 | 1.95        | 0.49     |
| 2:A:222:ASP:HB3  | 2:A:288:TYR:CE2  | 2.48        | 0.49     |
| 2:A:289:THR:HG21 | 2:A:292:GLU:HG3  | 1.95        | 0.49     |
| 2:A:368:ASP:O    | 2:A:372:LYS:HG3  | 2.13        | 0.49     |
| 2:A:500:ALA:HB3  | 2:A:501:LYS:CE   | 2.41        | 0.49     |
| 2:A:658:ASN:HB3  | 2:A:728:LEU:HD13 | 1.94        | 0.49     |
| 1:T:13:C:O3'     | 2:A:702:LEU:HD21 | 2.13        | 0.49     |
| 2:A:333:ASP:O    | 2:A:337:VAL:HG12 | 2.12        | 0.49     |
| 2:A:833:SER:CB   | 2:A:840:SER:HG   | 2.26        | 0.49     |
| 2:A:44:ASN:C     | 2:A:47:ASN:ND2   | 2.65        | 0.49     |
| 2:A:443:ASN:HD22 | 2:A:446:ARG:NH1  | 2.11        | 0.49     |
| 2:A:411:GLN:HE22 | 2:A:456:GLN:HE21 | 1.56        | 0.49     |
| 2:A:504:LEU:HB3  | 2:A:505:PRO:HD2  | 1.95        | 0.49     |
| 2:A:229:ILE:HA   | 2:A:323:CYS:SG   | 2.53        | 0.48     |
| 2:A:451:TRP:CE2  | 2:A:453:ILE:HG22 | 2.47        | 0.48     |
| 2:A:469:GLU:O    | 2:A:471:GLY:N    | 2.45        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:8:LEU:HD13   | 2:A:738:ARG:HE   | 1.77        | 0.48     |
| 2:A:230:TRP:CZ3  | 2:A:319:ALA:HB1  | 2.46        | 0.48     |
| 2:A:300:HIS:HB2  | 2:A:302:PHE:CE2  | 2.48        | 0.48     |
| 2:A:64:HIS:HD2   | 4:A:993:MRC:H9'2 | 1.78        | 0.48     |
| 2:A:711:PHE:HE2  | 2:A:752:MET:CE   | 2.26        | 0.48     |
| 2:A:65:MET:HE3   | 2:A:65:MET:HA    | 1.94        | 0.48     |
| 2:A:296:VAL:CG1  | 2:A:297:VAL:N    | 2.76        | 0.48     |
| 2:A:719:PHE:O    | 2:A:720:TYR:C    | 2.50        | 0.48     |
| 2:A:807:ASP:O    | 2:A:809:ASN:N    | 2.46        | 0.48     |
| 2:A:416:ILE:HB   | 2:A:449:GLY:O    | 2.13        | 0.48     |
| 2:A:495:TRP:O    | 2:A:520:LYS:HE3  | 2.13        | 0.48     |
| 2:A:466:PHE:HB3  | 2:A:520:LYS:HA   | 1.96        | 0.48     |
| 2:A:739:ARG:HD3  | 2:A:742:GLN:HE22 | 1.78        | 0.48     |
| 2:A:220:VAL:CG1  | 2:A:220:VAL:O    | 2.62        | 0.48     |
| 2:A:23:LYS:HG3   | 2:A:27:ILE:CD1   | 2.40        | 0.48     |
| 2:A:500:ALA:H    | 2:A:501:LYS:HZ2  | 1.62        | 0.48     |
| 2:A:465:VAL:O    | 2:A:521:GLU:CB   | 2.62        | 0.48     |
| 2:A:282:ILE:HG13 | 2:A:282:ILE:O    | 2.14        | 0.48     |
| 2:A:589:MET:CE   | 2:A:595:LYS:HA   | 2.31        | 0.48     |
| 2:A:469:GLU:O    | 2:A:469:GLU:HG2  | 2.13        | 0.48     |
| 2:A:470:ASN:H    | 2:A:472:GLU:CG   | 2.26        | 0.48     |
| 2:A:627:TYR:C    | 2:A:629:ALA:H    | 2.17        | 0.48     |
| 2:A:152:TYR:CD2  | 2:A:538:VAL:HG21 | 2.48        | 0.48     |
| 2:A:840:SER:HA   | 2:A:860:VAL:HG11 | 1.95        | 0.48     |
| 2:A:668:SER:HA   | 2:A:743:THR:OG1  | 2.14        | 0.48     |
| 2:A:547:PHE:O    | 2:A:549:ALA:N    | 2.46        | 0.48     |
| 2:A:711:PHE:CE2  | 2:A:752:MET:CE   | 2.96        | 0.48     |
| 2:A:632:ARG:CZ   | 2:A:632:ARG:HB2  | 2.42        | 0.48     |
| 2:A:254:TYR:CE2  | 2:A:260:LYS:HE2  | 2.49        | 0.48     |
| 2:A:327:ALA:H    | 2:A:334:ASP:CG   | 2.17        | 0.48     |
| 2:A:165:ARG:O    | 2:A:169:GLU:HG3  | 2.14        | 0.48     |
| 2:A:99:LEU:O     | 2:A:103:GLN:HG3  | 2.13        | 0.48     |
| 2:A:749:LEU:O    | 2:A:751:ASP:N    | 2.46        | 0.48     |
| 2:A:138:ASP:O    | 2:A:141:ARG:N    | 2.47        | 0.48     |
| 1:T:16:G:H5'     | 1:T:17:U:OP2     | 2.14        | 0.48     |
| 2:A:332:GLU:O    | 2:A:335:TYR:N    | 2.45        | 0.48     |
| 1:T:65:U:O2'     | 1:T:66:C:H5'     | 2.14        | 0.48     |
| 2:A:180:LYS:HD3  | 2:A:408:ALA:HB1  | 1.96        | 0.48     |
| 2:A:350:ASP:CB   | 2:A:354:VAL:O    | 2.62        | 0.48     |
| 2:A:357:GLU:C    | 2:A:359:GLY:H    | 2.18        | 0.48     |
| 2:A:800:THR:O    | 2:A:803:ASN:HB2  | 2.14        | 0.48     |
| 1:T:69:G:O2'     | 2:A:630:ASP:OD2  | 2.25        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:849:LEU:HB2  | 2:A:858:VAL:HG21 | 1.96        | 0.48     |
| 2:A:243:ILE:HD11 | 2:A:300:HIS:NE2  | 2.28        | 0.47     |
| 2:A:504:LEU:O    | 2:A:506:GLU:N    | 2.47        | 0.47     |
| 2:A:840:SER:OG   | 2:A:862:ASP:HA   | 2.14        | 0.47     |
| 2:A:106:THR:HG21 | 2:A:399:ARG:HH12 | 1.79        | 0.47     |
| 2:A:194:ALA:O    | 2:A:197:GLU:N    | 2.42        | 0.47     |
| 2:A:369:LYS:HA   | 2:A:372:LYS:HD2  | 1.96        | 0.47     |
| 2:A:481:ASN:O    | 2:A:483:VAL:N    | 2.47        | 0.47     |
| 2:A:569:THR:CG2  | 2:A:570:SER:N    | 2.76        | 0.47     |
| 2:A:153:ILE:HG13 | 2:A:156:LYS:HG2  | 1.94        | 0.47     |
| 1:T:2:G:H2'      | 1:T:3:G:H8       | 1.78        | 0.47     |
| 2:A:241:VAL:O    | 2:A:242:ALA:HB2  | 2.14        | 0.47     |
| 2:A:248:GLU:C    | 2:A:249:LEU:HG   | 2.34        | 0.47     |
| 2:A:293:LEU:HD23 | 2:A:293:LEU:O    | 2.14        | 0.47     |
| 2:A:366:PHE:O    | 2:A:371:ASN:ND2  | 2.44        | 0.47     |
| 2:A:724:GLY:HA3  | 2:A:741:MET:CE   | 2.44        | 0.47     |
| 2:A:722:ASP:O    | 2:A:723:TYR:C    | 2.53        | 0.47     |
| 2:A:398:TRP:C    | 2:A:400:THR:H    | 2.17        | 0.47     |
| 2:A:321:THR:O    | 2:A:323:CYS:N    | 2.42        | 0.47     |
| 2:A:324:VAL:CG1  | 2:A:326:THR:HG23 | 2.45        | 0.47     |
| 2:A:535:HIS:ND1  | 2:A:536:ARG:N    | 2.55        | 0.47     |
| 2:A:535:HIS:NE2  | 2:A:569:THR:CG2  | 2.77        | 0.47     |
| 2:A:848:ALA:HA   | 2:A:850:HIS:CE1  | 2.49        | 0.47     |
| 2:A:220:VAL:HG13 | 2:A:224:ASP:CG   | 2.34        | 0.47     |
| 2:A:717:SER:O    | 2:A:719:PHE:N    | 2.47        | 0.47     |
| 2:A:811:ALA:HA   | 2:A:871:TYR:OH   | 2.14        | 0.47     |
| 2:A:552:TYR:CD2  | 2:A:562:TRP:CZ3  | 3.03        | 0.47     |
| 2:A:567:ILE:HG23 | 2:A:568:THR:N    | 2.30        | 0.47     |
| 1:T:24:G:H2'     | 1:T:25:C:O4'     | 2.14        | 0.47     |
| 1:T:51:U:O2'     | 1:T:52:G:H5'     | 2.14        | 0.47     |
| 2:A:591:GLY:O    | 2:A:592:GLU:C    | 2.52        | 0.47     |
| 2:A:379:THR:HA   | 2:A:385:LEU:HD12 | 1.97        | 0.47     |
| 2:A:296:VAL:CG1  | 2:A:297:VAL:H    | 2.16        | 0.47     |
| 2:A:446:ARG:O    | 2:A:446:ARG:HG2  | 2.15        | 0.47     |
| 2:A:466:PHE:CD2  | 2:A:504:LEU:HD21 | 2.49        | 0.47     |
| 2:A:4:GLU:HA     | 2:A:7:LEU:HB2    | 1.96        | 0.47     |
| 2:A:551:MET:HE3  | 2:A:699:PHE:CE2  | 2.50        | 0.47     |
| 2:A:434:VAL:HG11 | 2:A:436:TRP:NE1  | 2.30        | 0.47     |
| 2:A:652:LEU:HD22 | 2:A:767:VAL:HG21 | 1.97        | 0.47     |
| 2:A:680:TYR:CE1  | 2:A:798:TRP:HB2  | 2.48        | 0.47     |
| 2:A:701:TYR:O    | 2:A:702:LEU:C    | 2.53        | 0.47     |
| 2:A:242:ALA:N    | 2:A:308:LEU:HD13 | 2.30        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:275:LEU:HD11 | 2:A:386:LYS:HD2  | 1.97        | 0.47     |
| 2:A:285:GLU:OE2  | 2:A:285:GLU:HA   | 2.15        | 0.47     |
| 1:T:46:G:C2'     | 1:T:47:U:H5'     | 2.39        | 0.47     |
| 2:A:433:LYS:O    | 2:A:433:LYS:HD2  | 2.14        | 0.47     |
| 2:A:366:PHE:CG   | 2:A:370:ALA:HB2  | 2.50        | 0.47     |
| 2:A:467:TYR:CA   | 2:A:472:GLU:HB3  | 2.44        | 0.47     |
| 2:A:23:LYS:HE2   | 2:A:766:GLU:OE2  | 2.14        | 0.47     |
| 2:A:849:LEU:CB   | 2:A:858:VAL:HG21 | 2.44        | 0.47     |
| 2:A:571:VAL:HG13 | 2:A:575:GLY:HA2  | 1.97        | 0.47     |
| 1:T:55:U:H3'     | 1:T:55:U:C6      | 2.50        | 0.47     |
| 2:A:587:PHE:HA   | 4:A:993:MRC:H152 | 1.96        | 0.47     |
| 2:A:596:MET:HB3  | 2:A:603:VAL:CG1  | 2.30        | 0.47     |
| 2:A:42:GLU:O     | 2:A:43:LYS:C     | 2.53        | 0.47     |
| 2:A:571:VAL:O    | 2:A:573:THR:N    | 2.42        | 0.47     |
| 2:A:239:SER:HB3  | 2:A:346:ILE:CG1  | 2.45        | 0.46     |
| 2:A:802:MET:O    | 2:A:805:ARG:HB3  | 2.15        | 0.46     |
| 2:A:831:ILE:CD1  | 2:A:839:ALA:HB1  | 2.44        | 0.46     |
| 2:A:96:THR:OG1   | 2:A:154:THR:HG23 | 2.15        | 0.46     |
| 2:A:632:ARG:NH1  | 2:A:632:ARG:HG3  | 2.28        | 0.46     |
| 2:A:127:PHE:O    | 2:A:130:GLU:HB2  | 2.15        | 0.46     |
| 2:A:598:LYS:C    | 2:A:600:LEU:H    | 2.19        | 0.46     |
| 2:A:229:ILE:HA   | 2:A:321:THR:HG1  | 1.79        | 0.46     |
| 2:A:163:GLN:HG2  | 2:A:461:VAL:CG1  | 2.44        | 0.46     |
| 2:A:549:ALA:O    | 2:A:580:LYS:HG3  | 2.15        | 0.46     |
| 2:A:749:LEU:O    | 2:A:750:VAL:C    | 2.53        | 0.46     |
| 2:A:63:LEU:HD12  | 2:A:138:ASP:HB2  | 1.96        | 0.46     |
| 1:T:9:A:H2'      | 1:T:11:C:H41     | 1.80        | 0.46     |
| 1:T:25:C:H2'     | 1:T:26:G:O4'     | 2.15        | 0.46     |
| 2:A:210:VAL:HG11 | 2:A:212:PHE:CE2  | 2.50        | 0.46     |
| 2:A:219:GLY:HA2  | 2:A:296:VAL:HG12 | 1.97        | 0.46     |
| 2:A:327:ALA:C    | 2:A:334:ASP:OD1  | 2.54        | 0.46     |
| 2:A:211:ALA:HB3  | 2:A:385:LEU:HD23 | 1.98        | 0.46     |
| 2:A:493:ASN:HA   | 2:A:493:ASN:HD22 | 1.59        | 0.46     |
| 2:A:500:ALA:N    | 2:A:501:LYS:HZ2  | 2.14        | 0.46     |
| 2:A:436:TRP:N    | 2:A:436:TRP:CD1  | 2.82        | 0.46     |
| 2:A:433:LYS:CB   | 2:A:583:LEU:HG   | 2.43        | 0.46     |
| 2:A:560:ARG:HB3  | 2:A:560:ARG:HH11 | 1.81        | 0.46     |
| 2:A:97:HIS:CG    | 2:A:460:GLY:HA2  | 2.50        | 0.46     |
| 2:A:216:ASP:O    | 2:A:220:VAL:HG23 | 2.15        | 0.46     |
| 2:A:228:ILE:O    | 2:A:229:ILE:CB   | 2.62        | 0.46     |
| 2:A:238:PRO:HB3  | 2:A:362:PHE:CE1  | 2.51        | 0.46     |
| 2:A:812:LEU:O    | 2:A:816:ARG:N    | 2.47        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:424:LEU:O    | 2:A:427:ILE:HB   | 2.15        | 0.46     |
| 2:A:504:LEU:HB3  | 2:A:505:PRO:CD   | 2.45        | 0.46     |
| 2:A:609:VAL:CG1  | 2:A:610:VAL:N    | 2.79        | 0.46     |
| 2:A:252:GLY:HA2  | 2:A:263:ILE:O    | 2.15        | 0.46     |
| 2:A:289:THR:CG2  | 2:A:292:GLU:HG3  | 2.46        | 0.46     |
| 2:A:53:HIS:HE1   | 2:A:152:TYR:CE2  | 2.32        | 0.46     |
| 2:A:200:TYR:HB3  | 2:A:393:SER:O    | 2.16        | 0.46     |
| 2:A:632:ARG:CG   | 2:A:632:ARG:NH1  | 2.77        | 0.46     |
| 2:A:397:ASP:O    | 2:A:397:ASP:CG   | 2.52        | 0.46     |
| 2:A:383:ALA:O    | 2:A:384:LEU:O    | 2.33        | 0.46     |
| 2:A:237:ILE:HB   | 2:A:238:PRO:CD   | 2.37        | 0.46     |
| 2:A:802:MET:HE2  | 2:A:805:ARG:HD3  | 1.97        | 0.46     |
| 2:A:805:ARG:O    | 2:A:806:ASP:C    | 2.54        | 0.46     |
| 2:A:160:GLU:O    | 2:A:161:ALA:C    | 2.54        | 0.46     |
| 2:A:170:MET:O    | 2:A:173:LYS:HB2  | 2.16        | 0.46     |
| 2:A:536:ARG:NH1  | 2:A:574:ARG:NH2  | 2.63        | 0.46     |
| 2:A:857:GLN:NE2  | 2:A:858:VAL:N    | 2.47        | 0.46     |
| 1:T:58:A:HO2'    | 1:T:59:G:P       | 2.38        | 0.46     |
| 2:A:240:ASN:ND2  | 2:A:302:PHE:HZ   | 2.14        | 0.46     |
| 2:A:293:LEU:HD23 | 2:A:296:VAL:CG2  | 2.45        | 0.46     |
| 2:A:329:GLY:HA3  | 2:A:346:ILE:HD12 | 1.98        | 0.46     |
| 2:A:542:ARG:O    | 2:A:544:GLU:N    | 2.49        | 0.46     |
| 2:A:102:GLU:O    | 2:A:105:LEU:HB2  | 2.16        | 0.46     |
| 2:A:323:CYS:O    | 2:A:324:VAL:CB   | 2.55        | 0.46     |
| 2:A:211:ALA:H    | 2:A:385:LEU:HD22 | 1.81        | 0.46     |
| 2:A:500:ALA:HB3  | 2:A:501:LYS:NZ   | 2.31        | 0.46     |
| 2:A:75:ASP:OD2   | 2:A:619:ARG:NH2  | 2.49        | 0.46     |
| 2:A:285:GLU:C    | 2:A:286:LYS:HG2  | 2.37        | 0.46     |
| 2:A:310:ILE:CG2  | 2:A:311:ASN:N    | 2.78        | 0.46     |
| 2:A:162:ALA:HB1  | 2:A:536:ARG:CG   | 2.47        | 0.46     |
| 1:T:18:G:O2'     | 1:T:19:G:P       | 2.74        | 0.46     |
| 2:A:397:ASP:O    | 2:A:401:LYS:N    | 2.42        | 0.46     |
| 2:A:255:ASN:HD21 | 2:A:256:VAL:HG23 | 1.81        | 0.45     |
| 2:A:362:PHE:O    | 2:A:365:MET:HG2  | 2.16        | 0.45     |
| 1:T:74:C:OP1     | 2:A:333:ASP:CG   | 2.55        | 0.45     |
| 2:A:160:GLU:O    | 2:A:163:GLN:N    | 2.50        | 0.45     |
| 2:A:481:ASN:O    | 2:A:482:HIS:C    | 2.53        | 0.45     |
| 2:A:176:ILE:HG23 | 2:A:475:MET:HE3  | 1.98        | 0.45     |
| 2:A:20:LEU:HA    | 2:A:23:LYS:HB3   | 1.97        | 0.45     |
| 2:A:120:PHE:O    | 2:A:124:CYS:N    | 2.50        | 0.45     |
| 1:T:34:G:H1'     | 2:A:9:MET:HE1    | 1.99        | 0.45     |
| 2:A:394:TYR:HA   | 2:A:395:PRO:HD3  | 1.85        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:840:SER:HA   | 2:A:860:VAL:HG13 | 1.96        | 0.45     |
| 1:T:67:A:H2'     | 1:T:68:G:O5'     | 2.15        | 0.45     |
| 2:A:240:ASN:ND2  | 2:A:302:PHE:CZ   | 2.84        | 0.45     |
| 2:A:121:ARG:NH1  | 2:A:496:PHE:HE1  | 2.14        | 0.45     |
| 2:A:198:ILE:HG21 | 2:A:395:PRO:HB3  | 1.98        | 0.45     |
| 2:A:609:VAL:HG13 | 2:A:610:VAL:N    | 2.30        | 0.45     |
| 2:A:792:GLN:O    | 2:A:794:LEU:N    | 2.50        | 0.45     |
| 2:A:679:ARG:NH2  | 2:A:794:LEU:HD22 | 2.32        | 0.45     |
| 2:A:684:ARG:NH1  | 2:A:684:ARG:HB3  | 2.31        | 0.45     |
| 1:T:14:A:H2'     | 1:T:15:G:O4'     | 2.16        | 0.45     |
| 1:T:24:G:H2'     | 1:T:25:C:C6      | 2.51        | 0.45     |
| 2:A:445:VAL:C    | 2:A:447:ASP:H    | 2.20        | 0.45     |
| 2:A:560:ARG:HB2  | 2:A:560:ARG:CZ   | 2.46        | 0.45     |
| 2:A:765:GLU:HA   | 2:A:765:GLU:OE1  | 2.17        | 0.45     |
| 1:T:24:G:H2'     | 1:T:25:C:H6      | 1.82        | 0.45     |
| 2:A:372:LYS:O    | 2:A:375:THR:N    | 2.50        | 0.45     |
| 2:A:451:TRP:NE1  | 2:A:453:ILE:HG22 | 2.32        | 0.45     |
| 2:A:494:ILE:O    | 2:A:503:LEU:HD21 | 2.16        | 0.45     |
| 2:A:60:ASN:C     | 2:A:60:ASN:ND2   | 2.67        | 0.45     |
| 2:A:865:ASP:CB   | 2:A:867:GLN:HE21 | 2.26        | 0.45     |
| 2:A:367:TYR:C    | 2:A:371:ASN:ND2  | 2.70        | 0.45     |
| 2:A:421:GLN:CA   | 2:A:424:LEU:HD12 | 2.45        | 0.45     |
| 2:A:831:ILE:HD11 | 2:A:843:LEU:HD11 | 1.99        | 0.45     |
| 2:A:46:GLY:O     | 2:A:47:ASN:C     | 2.55        | 0.45     |
| 2:A:64:HIS:CD2   | 4:A:993:MRC:H9'2 | 2.51        | 0.45     |
| 2:A:749:LEU:HD11 | 2:A:771:THR:CG2  | 2.45        | 0.45     |
| 1:T:17:U:C5'     | 1:T:18:G:H5'     | 2.47        | 0.45     |
| 2:A:240:ASN:HD21 | 2:A:306:GLU:CB   | 2.29        | 0.45     |
| 2:A:479:THR:O    | 2:A:483:VAL:HG23 | 2.17        | 0.45     |
| 2:A:683:ASN:O    | 2:A:686:ARG:HB2  | 2.17        | 0.45     |
| 2:A:257:ASN:ND2  | 2:A:258:GLY:H    | 2.15        | 0.45     |
| 2:A:749:LEU:HD11 | 2:A:771:THR:HG21 | 1.98        | 0.45     |
| 1:T:24:G:O2'     | 1:T:25:C:H5'     | 2.16        | 0.45     |
| 2:A:235:TRP:C    | 2:A:238:PRO:HD2  | 2.37        | 0.45     |
| 2:A:225:ALA:HB1  | 2:A:260:LYS:HB2  | 1.99        | 0.45     |
| 2:A:480:VAL:O    | 2:A:483:VAL:HB   | 2.17        | 0.45     |
| 2:A:467:TYR:N    | 2:A:467:TYR:CD1  | 2.85        | 0.45     |
| 2:A:71:LYS:NZ    | 5:A:1073:HOH:O   | 2.44        | 0.45     |
| 2:A:559:TYR:HA   | 2:A:563:PHE:HD1  | 1.82        | 0.45     |
| 2:A:616:ASP:OD1  | 2:A:762:HIS:ND1  | 2.48        | 0.45     |
| 2:A:560:ARG:CB   | 2:A:560:ARG:HH11 | 2.30        | 0.45     |
| 2:A:285:GLU:C    | 2:A:286:LYS:CG   | 2.86        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:500:ALA:N    | 2:A:520:LYS:HZ3  | 2.15        | 0.45     |
| 2:A:579:TYR:CD2  | 2:A:579:TYR:N    | 2.85        | 0.45     |
| 1:T:7:G:H1       | 1:T:66:C:H42     | 1.64        | 0.45     |
| 2:A:99:LEU:HD22  | 2:A:457:ARG:HD2  | 1.97        | 0.45     |
| 2:A:365:MET:HB3  | 2:A:370:ALA:CB   | 2.47        | 0.44     |
| 1:T:17:U:H5'     | 1:T:18:G:C5'     | 2.47        | 0.44     |
| 2:A:343:LEU:HA   | 2:A:344:PRO:HD3  | 1.88        | 0.44     |
| 2:A:681:LEU:O    | 2:A:682:LEU:C    | 2.54        | 0.44     |
| 2:A:417:SER:HA   | 2:A:420:ARG:CD   | 2.48        | 0.44     |
| 2:A:508:PHE:CD1  | 2:A:509:THR:N    | 2.86        | 0.44     |
| 1:T:34:G:H5''    | 1:T:36:U:C5      | 2.52        | 0.44     |
| 2:A:832:ALA:O    | 2:A:833:SER:C    | 2.54        | 0.44     |
| 2:A:813:GLU:O    | 2:A:817:ASN:N    | 2.46        | 0.44     |
| 2:A:605:VAL:HG13 | 2:A:606:PRO:CD   | 2.47        | 0.44     |
| 2:A:376:ASP:O    | 2:A:378:LEU:N    | 2.51        | 0.44     |
| 2:A:550:ASP:HA   | 2:A:580:LYS:HD2  | 1.99        | 0.44     |
| 2:A:810:ARG:NH1  | 2:A:814:THR:HG23 | 2.32        | 0.44     |
| 2:A:328:PRO:CA   | 2:A:335:TYR:HA   | 2.47        | 0.44     |
| 2:A:3:TYR:N      | 2:A:3:TYR:CD1    | 2.85        | 0.44     |
| 2:A:277:TRP:O    | 2:A:279:LYS:N    | 2.48        | 0.44     |
| 2:A:807:ASP:C    | 2:A:809:ASN:N    | 2.70        | 0.44     |
| 1:T:17:U:H5'     | 1:T:18:G:H5'     | 2.00        | 0.44     |
| 2:A:215:LYS:HG2  | 2:A:216:ASP:N    | 2.32        | 0.44     |
| 2:A:251:TYR:C    | 2:A:253:GLN:N    | 2.70        | 0.44     |
| 2:A:353:GLY:HA3  | 2:A:367:TYR:HB3  | 1.98        | 0.44     |
| 2:A:804:LEU:HD12 | 2:A:837:PHE:HE2  | 1.82        | 0.44     |
| 2:A:439:THR:O    | 2:A:442:TYR:N    | 2.50        | 0.44     |
| 2:A:749:LEU:CG   | 2:A:750:VAL:N    | 2.81        | 0.44     |
| 2:A:153:ILE:O    | 2:A:155:LEU:N    | 2.50        | 0.44     |
| 2:A:627:TYR:C    | 2:A:629:ALA:N    | 2.71        | 0.44     |
| 2:A:178:LYS:HG3  | 2:A:179:GLY:H    | 1.82        | 0.44     |
| 2:A:555:GLY:HA2  | 2:A:585:HIS:O    | 2.17        | 0.44     |
| 2:A:120:PHE:O    | 2:A:121:ARG:C    | 2.56        | 0.44     |
| 2:A:211:ALA:N    | 2:A:385:LEU:HD22 | 2.33        | 0.44     |
| 2:A:807:ASP:C    | 2:A:809:ASN:H    | 2.21        | 0.44     |
| 2:A:417:SER:CA   | 2:A:420:ARG:HG2  | 2.48        | 0.44     |
| 2:A:446:ARG:O    | 2:A:446:ARG:CD   | 2.65        | 0.44     |
| 2:A:481:ASN:C    | 2:A:483:VAL:N    | 2.72        | 0.44     |
| 2:A:13:ASP:OD1   | 2:A:770:HIS:CE1  | 2.71        | 0.44     |
| 2:A:598:LYS:C    | 2:A:600:LEU:N    | 2.71        | 0.44     |
| 2:A:362:PHE:HE2  | 2:A:374:VAL:HG22 | 1.83        | 0.44     |
| 2:A:423:ILE:O    | 2:A:424:LEU:C    | 2.55        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:13:ASP:OD2   | 2:A:770:HIS:HE1  | 2.01        | 0.44     |
| 2:A:737:ILE:HG23 | 2:A:738:ARG:N    | 2.32        | 0.44     |
| 2:A:768:TRP:HB2  | 2:A:779:VAL:CG2  | 2.48        | 0.44     |
| 2:A:694:ASN:O    | 2:A:698:ASN:ND2  | 2.50        | 0.44     |
| 2:A:229:ILE:HA   | 2:A:323:CYS:HB2  | 1.99        | 0.43     |
| 2:A:234:PRO:CG   | 2:A:235:TRP:N    | 2.75        | 0.43     |
| 2:A:355:PHE:CE1  | 2:A:365:MET:HB2  | 2.30        | 0.43     |
| 1:T:70:C:OP1     | 2:A:595:LYS:HD3  | 2.18        | 0.43     |
| 2:A:749:LEU:C    | 2:A:749:LEU:CD2  | 2.85        | 0.43     |
| 2:A:648:ILE:O    | 2:A:652:LEU:HD12 | 2.18        | 0.43     |
| 2:A:83:MET:HB3   | 2:A:784:MET:HG2  | 1.99        | 0.43     |
| 2:A:446:ARG:O    | 2:A:447:ASP:CG   | 2.57        | 0.43     |
| 1:T:70:C:O2      | 2:A:440:ARG:NH2  | 2.47        | 0.43     |
| 2:A:212:PHE:O    | 2:A:227:PHE:N    | 2.42        | 0.43     |
| 2:A:250:LYS:O    | 2:A:251:TYR:HB2  | 2.19        | 0.43     |
| 2:A:723:TYR:CE1  | 2:A:852:LEU:HD23 | 2.53        | 0.43     |
| 2:A:606:PRO:O    | 2:A:607:ASP:C    | 2.56        | 0.43     |
| 2:A:134:LEU:HA   | 2:A:134:LEU:HD23 | 1.84        | 0.43     |
| 2:A:233:THR:HG23 | 2:A:236:THR:CG2  | 2.44        | 0.43     |
| 2:A:241:VAL:HG11 | 2:A:343:LEU:HB3  | 2.00        | 0.43     |
| 2:A:804:LEU:HD23 | 2:A:808:VAL:HG23 | 2.00        | 0.43     |
| 2:A:4:GLU:O      | 2:A:4:GLU:HG2    | 2.18        | 0.43     |
| 2:A:275:LEU:O    | 2:A:276:ASP:C    | 2.56        | 0.43     |
| 2:A:162:ALA:HB1  | 2:A:536:ARG:HG3  | 2.01        | 0.43     |
| 1:T:13:C:H4'     | 2:A:702:LEU:HD21 | 1.99        | 0.43     |
| 2:A:240:ASN:O    | 2:A:241:VAL:HG23 | 2.18        | 0.43     |
| 2:A:275:LEU:HA   | 2:A:275:LEU:HD12 | 1.81        | 0.43     |
| 2:A:318:ASP:OD2  | 2:A:319:ALA:N    | 2.49        | 0.43     |
| 2:A:670:PRO:HG2  | 2:A:673:GLU:OE2  | 2.18        | 0.43     |
| 1:T:22:G:OP2     | 5:T:152:HOH:O    | 2.22        | 0.43     |
| 2:A:832:ALA:CB   | 2:A:861:VAL:HG13 | 2.47        | 0.43     |
| 2:A:795:LEU:HA   | 2:A:795:LEU:HD23 | 1.81        | 0.43     |
| 2:A:259:GLU:O    | 2:A:260:LYS:HB2  | 2.19        | 0.43     |
| 2:A:240:ASN:HD21 | 2:A:306:GLU:HB2  | 1.84        | 0.43     |
| 2:A:324:VAL:HG12 | 2:A:325:HIS:N    | 2.32        | 0.43     |
| 2:A:161:ALA:HB1  | 2:A:165:ARG:NH1  | 2.27        | 0.43     |
| 2:A:79:ARG:NH1   | 2:A:780:HIS:ND1  | 2.66        | 0.43     |
| 2:A:842:PHE:C    | 2:A:844:THR:N    | 2.71        | 0.43     |
| 2:A:777:GLU:O    | 2:A:778:SER:CB   | 2.66        | 0.43     |
| 2:A:240:ASN:HD22 | 2:A:308:LEU:HD21 | 1.77        | 0.43     |
| 2:A:422:ASP:OD2  | 2:A:422:ASP:N    | 2.41        | 0.43     |
| 2:A:129:LEU:C    | 2:A:132:ILE:HG12 | 2.39        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:68:ALA:O     | 2:A:72:ILE:HG13  | 2.18        | 0.43     |
| 2:A:338:GLY:C    | 2:A:343:LEU:HD12 | 2.39        | 0.43     |
| 2:A:166:ILE:O    | 2:A:167:PHE:C    | 2.58        | 0.43     |
| 2:A:466:PHE:CA   | 2:A:520:LYS:HA   | 2.44        | 0.43     |
| 2:A:830:THR:HB   | 2:A:877:VAL:CG2  | 2.48        | 0.43     |
| 2:A:187:PRO:C    | 2:A:189:SER:H    | 2.22        | 0.43     |
| 2:A:654:PHE:HE1  | 2:A:729:TYR:HH   | 1.65        | 0.42     |
| 2:A:727:ILE:HD13 | 2:A:737:ILE:HG12 | 2.01        | 0.42     |
| 2:A:727:ILE:CG2  | 2:A:738:ARG:HA   | 2.48        | 0.42     |
| 2:A:434:VAL:HG22 | 2:A:435:ASN:H    | 1.83        | 0.42     |
| 2:A:324:VAL:HG11 | 2:A:326:THR:HG23 | 2.01        | 0.42     |
| 2:A:821:ILE:HG13 | 2:A:827:ALA:HB2  | 2.01        | 0.42     |
| 2:A:632:ARG:HD3  | 5:A:1074:HOH:O   | 2.19        | 0.42     |
| 2:A:81:LYS:HE3   | 2:A:86:PHE:CD2   | 2.54        | 0.42     |
| 2:A:76:PHE:CE2   | 2:A:759:ILE:HA   | 2.54        | 0.42     |
| 2:A:379:THR:HG23 | 2:A:385:LEU:CG   | 2.50        | 0.42     |
| 2:A:809:ASN:C    | 2:A:811:ALA:H    | 2.22        | 0.42     |
| 2:A:525:MET:SD   | 2:A:529:PHE:CD2  | 3.13        | 0.42     |
| 2:A:577:SER:HA   | 2:A:578:PRO:HD3  | 1.89        | 0.42     |
| 2:A:129:LEU:O    | 2:A:132:ILE:CG1  | 2.65        | 0.42     |
| 2:A:144:VAL:CG1  | 2:A:145:ARG:N    | 2.81        | 0.42     |
| 2:A:454:SER:O    | 2:A:455:ARG:HD3  | 2.19        | 0.42     |
| 2:A:816:ARG:CD   | 2:A:822:GLY:O    | 2.67        | 0.42     |
| 2:A:417:SER:HA   | 2:A:420:ARG:CG   | 2.49        | 0.42     |
| 2:A:491:GLY:O    | 2:A:493:ASN:N    | 2.53        | 0.42     |
| 2:A:111:ASP:O    | 2:A:112:ARG:O    | 2.36        | 0.42     |
| 2:A:731:GLU:HG3  | 2:A:737:ILE:HG21 | 2.02        | 0.42     |
| 2:A:71:LYS:HE2   | 2:A:139:PHE:CE2  | 2.54        | 0.42     |
| 2:A:830:THR:O    | 2:A:877:VAL:HG22 | 2.20        | 0.42     |
| 1:T:55:U:C3'     | 1:T:55:U:C6      | 3.02        | 0.42     |
| 2:A:218:LYS:C    | 2:A:220:VAL:N    | 2.71        | 0.42     |
| 2:A:339:GLN:O    | 2:A:340:GLN:C    | 2.57        | 0.42     |
| 2:A:177:TYR:HD1  | 2:A:178:LYS:O    | 2.03        | 0.42     |
| 2:A:413:PHE:HA   | 2:A:451:TRP:O    | 2.20        | 0.42     |
| 2:A:513:SER:O    | 2:A:515:ASN:N    | 2.47        | 0.42     |
| 2:A:115:MET:HB3  | 2:A:119:GLU:HB3  | 2.01        | 0.42     |
| 2:A:122:GLU:C    | 2:A:124:CYS:H    | 2.23        | 0.42     |
| 2:A:434:VAL:HG21 | 2:A:436:TRP:CD1  | 2.55        | 0.42     |
| 2:A:436:TRP:HD1  | 2:A:436:TRP:H    | 1.64        | 0.42     |
| 2:A:30:LYS:O     | 2:A:33:ALA:HB3   | 2.19        | 0.42     |
| 1:T:45:G:H5'     | 1:T:46:G:OP2     | 2.20        | 0.42     |
| 2:A:644:ASP:O    | 2:A:648:ILE:HG13 | 2.20        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:84:GLN:OE1   | 2:A:784:MET:HB2  | 2.19        | 0.42     |
| 2:A:664:PRO:O    | 2:A:666:THR:N    | 2.53        | 0.42     |
| 2:A:821:ILE:CG1  | 2:A:822:GLY:H    | 2.32        | 0.42     |
| 1:T:38:A:C2'     | 1:T:39:G:H5'     | 2.49        | 0.42     |
| 2:A:501:LYS:N    | 2:A:501:LYS:HE3  | 2.35        | 0.42     |
| 2:A:792:GLN:NE2  | 2:A:796:ASP:OD1  | 2.51        | 0.42     |
| 2:A:775:LYS:O    | 2:A:776:GLU:CB   | 2.67        | 0.42     |
| 2:A:289:THR:HG22 | 2:A:292:GLU:N    | 2.21        | 0.42     |
| 2:A:832:ALA:HB2  | 2:A:861:VAL:HG12 | 1.99        | 0.42     |
| 1:T:41:G:O2'     | 1:T:42:U:H5'     | 2.20        | 0.42     |
| 2:A:44:ASN:OD1   | 2:A:85:GLY:HA2   | 2.20        | 0.42     |
| 2:A:56:PRO:HA    | 2:A:57:PRO:HD2   | 1.97        | 0.42     |
| 2:A:178:LYS:HG3  | 2:A:179:GLY:N    | 2.35        | 0.42     |
| 2:A:548:PRO:HB2  | 2:A:580:LYS:CE   | 2.49        | 0.42     |
| 2:A:462:PRO:HG3  | 2:A:496:PHE:CZ   | 2.55        | 0.42     |
| 2:A:623:SER:O    | 2:A:702:LEU:HA   | 2.19        | 0.42     |
| 2:A:228:ILE:HD11 | 2:A:261:TYR:HB3  | 2.02        | 0.42     |
| 2:A:326:THR:HA   | 2:A:334:ASP:OD2  | 2.20        | 0.42     |
| 2:A:365:MET:HB3  | 2:A:370:ALA:HB1  | 2.01        | 0.42     |
| 1:T:29:C:H2'     | 1:T:30:C:C6      | 2.55        | 0.42     |
| 2:A:226:LYS:HD2  | 2:A:259:GLU:CB   | 2.50        | 0.42     |
| 2:A:325:HIS:C    | 2:A:325:HIS:ND1  | 2.73        | 0.42     |
| 2:A:350:ASP:OD1  | 2:A:352:LYS:HD3  | 2.19        | 0.42     |
| 2:A:376:ASP:O    | 2:A:377:LEU:C    | 2.57        | 0.42     |
| 2:A:163:GLN:HG2  | 2:A:461:VAL:CG2  | 2.44        | 0.42     |
| 2:A:110:VAL:HG11 | 2:A:120:PHE:CZ   | 2.55        | 0.42     |
| 2:A:8:LEU:CD2    | 2:A:733:ARG:NH1  | 2.81        | 0.42     |
| 2:A:292:GLU:C    | 2:A:294:GLU:H    | 2.22        | 0.41     |
| 2:A:179:GLY:HA3  | 2:A:413:PHE:CE1  | 2.55        | 0.41     |
| 2:A:116:SER:O    | 2:A:117:THR:C    | 2.59        | 0.41     |
| 2:A:43:LYS:HG2   | 2:A:44:ASN:N     | 2.35        | 0.41     |
| 2:A:269:ASP:O    | 2:A:270:ALA:C    | 2.58        | 0.41     |
| 1:T:51:U:H2'     | 1:T:52:G:H8      | 1.85        | 0.41     |
| 2:A:256:VAL:CG1  | 2:A:257:ASN:H    | 2.32        | 0.41     |
| 2:A:296:VAL:C    | 2:A:310:ILE:HD13 | 2.40        | 0.41     |
| 2:A:152:TYR:HB2  | 5:A:1041:HOH:O   | 2.20        | 0.41     |
| 2:A:163:GLN:CG   | 2:A:461:VAL:HG21 | 2.44        | 0.41     |
| 2:A:477:LYS:O    | 2:A:479:THR:N    | 2.45        | 0.41     |
| 2:A:469:GLU:O    | 2:A:470:ASN:HB2  | 2.20        | 0.41     |
| 2:A:141:ARG:HH21 | 2:A:611:LYS:NZ   | 2.18        | 0.41     |
| 2:A:831:ILE:HG13 | 2:A:832:ALA:N    | 2.33        | 0.41     |
| 2:A:131:GLN:O    | 2:A:132:ILE:C    | 2.57        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:146:GLY:O    | 2:A:148:PHE:N    | 2.50        | 0.41     |
| 2:A:106:THR:C    | 2:A:108:LYS:H    | 2.23        | 0.41     |
| 2:A:216:ASP:O    | 2:A:219:GLY:N    | 2.53        | 0.41     |
| 2:A:538:VAL:HG23 | 2:A:542:ARG:CD   | 2.50        | 0.41     |
| 2:A:469:GLU:O    | 2:A:469:GLU:CG   | 2.68        | 0.41     |
| 2:A:536:ARG:NH2  | 2:A:574:ARG:NH2  | 2.66        | 0.41     |
| 2:A:539:LEU:HD23 | 2:A:539:LEU:HA   | 1.85        | 0.41     |
| 2:A:505:PRO:O    | 2:A:506:GLU:C    | 2.58        | 0.41     |
| 2:A:51:ILE:HD12  | 2:A:51:ILE:N     | 2.36        | 0.41     |
| 2:A:325:HIS:C    | 2:A:325:HIS:HD1  | 2.23        | 0.41     |
| 2:A:170:MET:O    | 2:A:171:ALA:C    | 2.59        | 0.41     |
| 2:A:79:ARG:O     | 2:A:80:TYR:C     | 2.58        | 0.41     |
| 2:A:318:ASP:CG   | 2:A:319:ALA:N    | 2.72        | 0.41     |
| 2:A:300:HIS:C    | 2:A:304:ASP:HB3  | 2.40        | 0.41     |
| 2:A:341:TYR:O    | 2:A:342:GLU:C    | 2.58        | 0.41     |
| 2:A:745:LEU:C    | 2:A:748:ILE:HG22 | 2.39        | 0.41     |
| 2:A:138:ASP:O    | 2:A:139:PHE:C    | 2.58        | 0.41     |
| 2:A:798:TRP:HA   | 2:A:801:PHE:HB3  | 2.02        | 0.41     |
| 2:A:214:VAL:HG12 | 2:A:219:GLY:O    | 2.21        | 0.41     |
| 2:A:236:THR:HG23 | 2:A:237:ILE:H    | 1.86        | 0.41     |
| 2:A:327:ALA:C    | 2:A:329:GLY:N    | 2.73        | 0.41     |
| 2:A:367:TYR:CD1  | 2:A:405:ILE:HD13 | 2.54        | 0.41     |
| 2:A:466:PHE:N    | 2:A:466:PHE:CD1  | 2.87        | 0.41     |
| 2:A:749:LEU:HD13 | 2:A:750:VAL:CG2  | 2.41        | 0.41     |
| 2:A:443:ASN:HD21 | 2:A:446:ARG:NH2  | 2.18        | 0.41     |
| 2:A:463:LEU:HG   | 2:A:525:MET:HE3  | 2.02        | 0.41     |
| 2:A:162:ALA:O    | 2:A:166:ILE:HG13 | 2.20        | 0.41     |
| 2:A:170:MET:O    | 2:A:173:LYS:N    | 2.53        | 0.41     |
| 2:A:828:LYS:HG3  | 2:A:857:GLN:HB2  | 2.02        | 0.41     |
| 2:A:137:LYS:O    | 2:A:141:ARG:HB2  | 2.21        | 0.41     |
| 2:A:664:PRO:CG   | 2:A:746:TYR:CE2  | 3.03        | 0.41     |
| 2:A:564:ASN:HA   | 2:A:567:ILE:HG22 | 2.03        | 0.41     |
| 2:A:75:ASP:O     | 2:A:76:PHE:C     | 2.58        | 0.41     |
| 1:T:12:U:H2'     | 1:T:13:C:O4'     | 2.21        | 0.41     |
| 2:A:239:SER:HB3  | 2:A:346:ILE:CD1  | 2.48        | 0.41     |
| 2:A:539:LEU:HA   | 2:A:545:LEU:CD1  | 2.51        | 0.41     |
| 2:A:583:LEU:HD23 | 2:A:584:SER:H    | 1.85        | 0.41     |
| 2:A:328:PRO:CB   | 2:A:335:TYR:HA   | 2.50        | 0.41     |
| 2:A:765:GLU:HA   | 2:A:779:VAL:HG23 | 2.02        | 0.41     |
| 2:A:28:GLN:O     | 2:A:31:TRP:N     | 2.54        | 0.41     |
| 2:A:301:PRO:O    | 2:A:302:PHE:C    | 2.58        | 0.41     |
| 2:A:348:PRO:O    | 2:A:407:ARG:CD   | 2.68        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:210:VAL:HG22 | 2:A:385:LEU:HD13 | 2.03        | 0.41     |
| 2:A:367:TYR:CD1  | 2:A:367:TYR:O    | 2.74        | 0.41     |
| 1:T:73:A:H2'     | 1:T:74:C:H5'     | 2.03        | 0.41     |
| 2:A:823:LYS:HG2  | 2:A:826:GLU:CD   | 2.40        | 0.41     |
| 2:A:445:VAL:HA   | 2:A:448:ARG:HB2  | 2.02        | 0.41     |
| 2:A:171:ALA:C    | 2:A:173:LYS:H    | 2.25        | 0.41     |
| 2:A:539:LEU:HA   | 2:A:545:LEU:HD12 | 2.02        | 0.41     |
| 2:A:747:GLN:O    | 2:A:748:ILE:C    | 2.59        | 0.41     |
| 2:A:185:TRP:H    | 2:A:404:VAL:CG1  | 2.34        | 0.41     |
| 2:A:740:SER:O    | 2:A:743:THR:HB   | 2.20        | 0.41     |
| 2:A:80:TYR:O     | 2:A:83:MET:N     | 2.51        | 0.41     |
| 1:T:67:A:C2'     | 1:T:68:G:O5'     | 2.69        | 0.41     |
| 2:A:684:ARG:HB3  | 2:A:684:ARG:CZ   | 2.51        | 0.41     |
| 2:A:140:ARG:NH2  | 2:A:149:ASN:HD22 | 2.19        | 0.41     |
| 2:A:338:GLY:CA   | 2:A:343:LEU:HD12 | 2.50        | 0.41     |
| 2:A:477:LYS:HB2  | 2:A:477:LYS:HE3  | 1.87        | 0.41     |
| 2:A:116:SER:O    | 2:A:119:GLU:N    | 2.54        | 0.41     |
| 2:A:79:ARG:HH11  | 2:A:79:ARG:HG2   | 1.86        | 0.41     |
| 2:A:482:HIS:HE1  | 5:A:1014:HOH:O   | 2.05        | 0.40     |
| 2:A:495:TRP:HD1  | 2:A:496:PHE:CD2  | 2.39        | 0.40     |
| 2:A:727:ILE:HD12 | 5:A:1063:HOH:O   | 2.20        | 0.40     |
| 2:A:24:GLU:CD    | 2:A:615:ALA:H    | 2.24        | 0.40     |
| 1:T:71:C:O3'     | 2:A:560:ARG:HD2  | 2.21        | 0.40     |
| 2:A:229:ILE:HD13 | 2:A:323:CYS:CB   | 2.51        | 0.40     |
| 2:A:251:TYR:N    | 2:A:251:TYR:CD1  | 2.88        | 0.40     |
| 2:A:304:ASP:C    | 2:A:306:GLU:H    | 2.24        | 0.40     |
| 2:A:327:ALA:HB1  | 2:A:346:ILE:HD11 | 2.03        | 0.40     |
| 2:A:168:GLY:O    | 2:A:169:GLU:C    | 2.59        | 0.40     |
| 2:A:476:THR:C    | 2:A:477:LYS:O    | 2.59        | 0.40     |
| 2:A:120:PHE:HD1  | 2:A:123:LYS:CB   | 2.34        | 0.40     |
| 1:T:35:A:C2'     | 1:T:36:U:OP1     | 2.70        | 0.40     |
| 1:T:5:U:H5'      | 2:A:436:TRP:CE3  | 2.56        | 0.40     |
| 2:A:426:ALA:O    | 2:A:429:ASN:N    | 2.54        | 0.40     |
| 2:A:120:PHE:CD2  | 2:A:124:CYS:SG   | 3.15        | 0.40     |
| 2:A:44:ASN:CA    | 2:A:47:ASN:HD21  | 2.35        | 0.40     |
| 2:A:74:LYS:HE2   | 2:A:553:LEU:O    | 2.21        | 0.40     |
| 2:A:367:TYR:C    | 2:A:371:ASN:HD21 | 2.25        | 0.40     |
| 2:A:367:TYR:CD1  | 2:A:405:ILE:HG21 | 2.56        | 0.40     |
| 1:T:51:U:H2'     | 1:T:52:G:C8      | 2.57        | 0.40     |
| 2:A:180:LYS:HG2  | 2:A:409:THR:C    | 2.41        | 0.40     |
| 2:A:781:LEU:HD23 | 2:A:781:LEU:HA   | 1.91        | 0.40     |
| 2:A:19:GLY:C     | 2:A:21:PRO:HD2   | 2.42        | 0.40     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 2:A:171:ALA:HB1 | 2:A:475:MET:HE3 | 2.03        | 0.40     |
| 2:A:112:ARG:HB3 | 2:A:113:LYS:H   | 1.47        | 0.40     |
| 2:A:867:GLN:HG3 | 2:A:868:ALA:N   | 2.36        | 0.40     |
| 2:A:610:VAL:O   | 2:A:614:GLY:HA2 | 2.22        | 0.40     |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1       | Atom-2               | Distance(Å) | Clash(Å) |
|--------------|----------------------|-------------|----------|
| 1:T:19:G:O2' | 2:A:672:SER:O[4_576] | 2.19        | 0.01     |

## 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       |
|-----|-------|---------------|-----------|-----------|-----------|-------------------|
| 2   | A     | 878/917 (96%) | 572 (65%) | 186 (21%) | 120 (14%) | <b>0</b> <b>1</b> |

All (120) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 45  | LYS  |
| 2   | A     | 47  | ASN  |
| 2   | A     | 112 | ARG  |
| 2   | A     | 114 | LYS  |
| 2   | A     | 195 | GLU  |
| 2   | A     | 229 | ILE  |
| 2   | A     | 248 | GLU  |
| 2   | A     | 254 | TYR  |
| 2   | A     | 256 | VAL  |
| 2   | A     | 263 | ILE  |
| 2   | A     | 268 | SER  |
| 2   | A     | 283 | LYS  |
| 2   | A     | 294 | GLU  |
| 2   | A     | 295 | TRP  |
| 2   | A     | 301 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 302 | PHE  |
| 2   | A     | 304 | ASP  |
| 2   | A     | 316 | THR  |
| 2   | A     | 344 | PRO  |
| 2   | A     | 347 | SER  |
| 2   | A     | 350 | ASP  |
| 2   | A     | 376 | ASP  |
| 2   | A     | 377 | LEU  |
| 2   | A     | 383 | ALA  |
| 2   | A     | 421 | GLN  |
| 2   | A     | 439 | THR  |
| 2   | A     | 469 | GLU  |
| 2   | A     | 473 | ILE  |
| 2   | A     | 506 | GLU  |
| 2   | A     | 556 | SER  |
| 2   | A     | 668 | SER  |
| 2   | A     | 750 | VAL  |
| 2   | A     | 776 | GLU  |
| 2   | A     | 824 | SER  |
| 2   | A     | 843 | LEU  |
| 2   | A     | 43  | LYS  |
| 2   | A     | 44  | ASN  |
| 2   | A     | 116 | SER  |
| 2   | A     | 147 | ASP  |
| 2   | A     | 154 | THR  |
| 2   | A     | 196 | ALA  |
| 2   | A     | 223 | ALA  |
| 2   | A     | 234 | PRO  |
| 2   | A     | 258 | GLY  |
| 2   | A     | 280 | ALA  |
| 2   | A     | 281 | SER  |
| 2   | A     | 293 | LEU  |
| 2   | A     | 303 | LEU  |
| 2   | A     | 315 | VAL  |
| 2   | A     | 340 | GLN  |
| 2   | A     | 360 | GLY  |
| 2   | A     | 372 | LYS  |
| 2   | A     | 379 | THR  |
| 2   | A     | 381 | LYS  |
| 2   | A     | 384 | LEU  |
| 2   | A     | 390 | ILE  |
| 2   | A     | 472 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 546 | SER  |
| 2   | A     | 561 | GLY  |
| 2   | A     | 572 | ALA  |
| 2   | A     | 599 | SER  |
| 2   | A     | 606 | PRO  |
| 2   | A     | 731 | GLU  |
| 2   | A     | 793 | ALA  |
| 2   | A     | 840 | SER  |
| 2   | A     | 113 | LYS  |
| 2   | A     | 189 | SER  |
| 2   | A     | 216 | ASP  |
| 2   | A     | 238 | PRO  |
| 2   | A     | 308 | LEU  |
| 2   | A     | 324 | VAL  |
| 2   | A     | 342 | GLU  |
| 2   | A     | 349 | ILE  |
| 2   | A     | 358 | GLU  |
| 2   | A     | 382 | GLY  |
| 2   | A     | 415 | SER  |
| 2   | A     | 440 | ARG  |
| 2   | A     | 447 | ASP  |
| 2   | A     | 468 | ALA  |
| 2   | A     | 485 | ASP  |
| 2   | A     | 505 | PRO  |
| 2   | A     | 527 | VAL  |
| 2   | A     | 543 | PRO  |
| 2   | A     | 665 | ASP  |
| 2   | A     | 718 | ASN  |
| 2   | A     | 778 | SER  |
| 2   | A     | 806 | ASP  |
| 2   | A     | 822 | GLY  |
| 2   | A     | 833 | SER  |
| 2   | A     | 63  | LEU  |
| 2   | A     | 260 | LYS  |
| 2   | A     | 278 | ASP  |
| 2   | A     | 328 | PRO  |
| 2   | A     | 356 | THR  |
| 2   | A     | 373 | ALA  |
| 2   | A     | 434 | VAL  |
| 2   | A     | 435 | ASN  |
| 2   | A     | 446 | ARG  |
| 2   | A     | 477 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 489 | GLU  |
| 2   | A     | 497 | GLU  |
| 2   | A     | 664 | PRO  |
| 2   | A     | 773 | HIS  |
| 2   | A     | 808 | VAL  |
| 2   | A     | 862 | ASP  |
| 2   | A     | 109 | GLY  |
| 2   | A     | 217 | ASP  |
| 2   | A     | 242 | ALA  |
| 2   | A     | 252 | GLY  |
| 2   | A     | 380 | GLU  |
| 2   | A     | 492 | SER  |
| 2   | A     | 228 | ILE  |
| 2   | A     | 241 | VAL  |
| 2   | A     | 339 | GLN  |
| 2   | A     | 501 | LYS  |
| 2   | A     | 309 | VAL  |
| 2   | A     | 101 | ILE  |
| 2   | A     | 761 | VAL  |
| 2   | A     | 247 | PRO  |
| 2   | A     | 245 | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|-------------|
| 2   | A     | 772/806 (96%) | 676 (88%) | 96 (12%) | 7 19        |

All (96) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 11  | LYS  |
| 2   | A     | 20  | LEU  |
| 2   | A     | 22  | ASN  |
| 2   | A     | 47  | ASN  |
| 2   | A     | 60  | ASN  |
| 2   | A     | 94  | TRP  |
| 2   | A     | 95  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 112 | ARG  |
| 2   | A     | 116 | SER  |
| 2   | A     | 144 | VAL  |
| 2   | A     | 149 | ASN  |
| 2   | A     | 153 | ILE  |
| 2   | A     | 159 | TYR  |
| 2   | A     | 160 | GLU  |
| 2   | A     | 164 | ILE  |
| 2   | A     | 167 | PHE  |
| 2   | A     | 189 | SER  |
| 2   | A     | 200 | TYR  |
| 2   | A     | 202 | ASP  |
| 2   | A     | 227 | PHE  |
| 2   | A     | 233 | THR  |
| 2   | A     | 234 | PRO  |
| 2   | A     | 236 | THR  |
| 2   | A     | 250 | LYS  |
| 2   | A     | 254 | TYR  |
| 2   | A     | 273 | GLU  |
| 2   | A     | 275 | LEU  |
| 2   | A     | 284 | LEU  |
| 2   | A     | 295 | TRP  |
| 2   | A     | 301 | PRO  |
| 2   | A     | 305 | ARG  |
| 2   | A     | 306 | GLU  |
| 2   | A     | 308 | LEU  |
| 2   | A     | 309 | VAL  |
| 2   | A     | 317 | THR  |
| 2   | A     | 325 | HIS  |
| 2   | A     | 326 | THR  |
| 2   | A     | 341 | TYR  |
| 2   | A     | 342 | GLU  |
| 2   | A     | 345 | VAL  |
| 2   | A     | 355 | PHE  |
| 2   | A     | 366 | PHE  |
| 2   | A     | 367 | TYR  |
| 2   | A     | 371 | ASN  |
| 2   | A     | 384 | LEU  |
| 2   | A     | 389 | PHE  |
| 2   | A     | 392 | HIS  |
| 2   | A     | 397 | ASP  |
| 2   | A     | 398 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 407 | ARG  |
| 2   | A     | 413 | PHE  |
| 2   | A     | 422 | ASP  |
| 2   | A     | 444 | MET  |
| 2   | A     | 450 | GLU  |
| 2   | A     | 458 | VAL  |
| 2   | A     | 466 | PHE  |
| 2   | A     | 467 | TYR  |
| 2   | A     | 476 | THR  |
| 2   | A     | 481 | ASN  |
| 2   | A     | 485 | ASP  |
| 2   | A     | 486 | LEU  |
| 2   | A     | 487 | PHE  |
| 2   | A     | 493 | ASN  |
| 2   | A     | 499 | GLU  |
| 2   | A     | 501 | LYS  |
| 2   | A     | 526 | ASP  |
| 2   | A     | 527 | VAL  |
| 2   | A     | 535 | HIS  |
| 2   | A     | 544 | GLU  |
| 2   | A     | 551 | MET  |
| 2   | A     | 560 | ARG  |
| 2   | A     | 569 | THR  |
| 2   | A     | 573 | THR  |
| 2   | A     | 583 | LEU  |
| 2   | A     | 602 | ASN  |
| 2   | A     | 616 | ASP  |
| 2   | A     | 630 | ASP  |
| 2   | A     | 644 | ASP  |
| 2   | A     | 646 | ARG  |
| 2   | A     | 649 | ARG  |
| 2   | A     | 666 | THR  |
| 2   | A     | 681 | LEU  |
| 2   | A     | 715 | GLU  |
| 2   | A     | 723 | TYR  |
| 2   | A     | 732 | GLN  |
| 2   | A     | 749 | LEU  |
| 2   | A     | 773 | HIS  |
| 2   | A     | 807 | ASP  |
| 2   | A     | 813 | GLU  |
| 2   | A     | 821 | ILE  |
| 2   | A     | 830 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 831 | ILE  |
| 2   | A     | 836 | LYS  |
| 2   | A     | 857 | GLN  |
| 2   | A     | 869 | THR  |
| 2   | A     | 875 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 26  | GLN  |
| 2   | A     | 36  | GLN  |
| 2   | A     | 38  | HIS  |
| 2   | A     | 47  | ASN  |
| 2   | A     | 53  | HIS  |
| 2   | A     | 60  | ASN  |
| 2   | A     | 62  | ASN  |
| 2   | A     | 131 | GLN  |
| 2   | A     | 149 | ASN  |
| 2   | A     | 240 | ASN  |
| 2   | A     | 246 | HIS  |
| 2   | A     | 299 | GLN  |
| 2   | A     | 339 | GLN  |
| 2   | A     | 371 | ASN  |
| 2   | A     | 392 | HIS  |
| 2   | A     | 396 | HIS  |
| 2   | A     | 443 | ASN  |
| 2   | A     | 456 | GLN  |
| 2   | A     | 481 | ASN  |
| 2   | A     | 482 | HIS  |
| 2   | A     | 490 | HIS  |
| 2   | A     | 493 | ASN  |
| 2   | A     | 585 | HIS  |
| 2   | A     | 602 | ASN  |
| 2   | A     | 612 | GLN  |
| 2   | A     | 650 | ASN  |
| 2   | A     | 698 | ASN  |
| 2   | A     | 706 | GLN  |
| 2   | A     | 713 | ASN  |
| 2   | A     | 732 | GLN  |
| 2   | A     | 736 | HIS  |
| 2   | A     | 742 | GLN  |
| 2   | A     | 770 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 773 | HIS  |
| 2   | A     | 792 | GLN  |
| 2   | A     | 809 | ASN  |
| 2   | A     | 851 | GLN  |
| 2   | A     | 857 | GLN  |
| 2   | A     | 867 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 1   | T     | 74/75 (98%) | 21 (28%)          | 12 (16%)        |

All (21) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | T     | 8      | U    |
| 1   | T     | 9      | A    |
| 1   | T     | 10     | G    |
| 1   | T     | 14     | A    |
| 1   | T     | 16     | G    |
| 1   | T     | 17     | U    |
| 1   | T     | 18     | G    |
| 1   | T     | 19     | G    |
| 1   | T     | 20     | U    |
| 1   | T     | 121(A) | U    |
| 1   | T     | 22     | G    |
| 1   | T     | 34     | G    |
| 1   | T     | 35     | A    |
| 1   | T     | 36     | U    |
| 1   | T     | 37     | A    |
| 1   | T     | 38     | A    |
| 1   | T     | 46     | G    |
| 1   | T     | 48     | C    |
| 1   | T     | 49     | G    |
| 1   | T     | 59     | G    |
| 1   | T     | 61     | C    |

All (12) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 7   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 9   | A    |
| 1   | T     | 18  | G    |
| 1   | T     | 19  | G    |
| 1   | T     | 33  | U    |
| 1   | T     | 34  | G    |
| 1   | T     | 36  | U    |
| 1   | T     | 37  | A    |
| 1   | T     | 47  | U    |
| 1   | T     | 48  | C    |
| 1   | T     | 58  | A    |
| 1   | T     | 60  | U    |

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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 | $\# Z  > 2$ |
| 4   | MRC  | A     | 993 | -    | 36,36,36     | 2.20 | 10 (27%)    | 48,48,48    | 2.14 | 11 (22%)    |

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

| Mol | Type | Chain | Res | Link | Chirals   | Torsions   | Rings   |
|-----|------|-------|-----|------|-----------|------------|---------|
| 4   | MRC  | A     | 993 | -    | 1/1/11/12 | 0/32/54/54 | 0/1/2/2 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | A     | 993 | MRC  | C11-C10 | -7.40 | 1.36        | 1.46     |
| 4   | A     | 993 | MRC  | C8-C7   | 4.56  | 1.59        | 1.53     |
| 4   | A     | 993 | MRC  | O1A-C1  | 3.82  | 1.43        | 1.34     |
| 4   | A     | 993 | MRC  | C9-C8   | 3.22  | 1.60        | 1.53     |
| 4   | A     | 993 | MRC  | C4-C5   | 2.97  | 1.58        | 1.53     |
| 4   | A     | 993 | MRC  | C2-C3   | 2.75  | 1.39        | 1.33     |
| 4   | A     | 993 | MRC  | C2-C1   | -2.74 | 1.39        | 1.47     |
| 4   | A     | 993 | MRC  | C16-C8  | 2.42  | 1.55        | 1.51     |
| 4   | A     | 993 | MRC  | C4-C3   | 2.30  | 1.54        | 1.51     |
| 4   | A     | 993 | MRC  | C9-C10  | 2.06  | 1.56        | 1.52     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | A     | 993 | MRC  | C16-C8-C7   | -6.48 | 102.91      | 108.72   |
| 4   | A     | 993 | MRC  | C11-O10-C10 | -5.34 | 57.39       | 60.59    |
| 4   | A     | 993 | MRC  | C9-C8-C7    | 4.40  | 119.33      | 113.19   |
| 4   | A     | 993 | MRC  | C11-C12-C13 | 4.30  | 120.59      | 110.71   |
| 4   | A     | 993 | MRC  | O1A-C1-C2   | 3.97  | 118.98      | 110.65   |
| 4   | A     | 993 | MRC  | C17-C12-C11 | 3.59  | 118.34      | 111.46   |
| 4   | A     | 993 | MRC  | C8-C9-C10   | 3.47  | 121.81      | 115.07   |
| 4   | A     | 993 | MRC  | C17-C12-C13 | 3.38  | 120.10      | 112.94   |
| 4   | A     | 993 | MRC  | C9'-O1A-C1  | -3.28 | 110.72      | 116.64   |
| 4   | A     | 993 | MRC  | C5-C4-C3    | 2.77  | 120.99      | 113.62   |
| 4   | A     | 993 | MRC  | C12-C11-C10 | 2.46  | 128.37      | 123.28   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 4   | A     | 993 | MRC  | C12  |

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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   | T     | 75/75 (100%)  | -0.01  | 3 (4%) 36 43  | 5, 30, 78, 100        | 2 (2%) |
| 2   | A     | 880/917 (95%) | -0.30  | 16 (1%) 65 74 | 3, 32, 70, 83         | 0      |
| All | All   | 955/992 (96%) | -0.27  | 19 (1%) 62 71 | 3, 32, 70, 100        | 2 (0%) |

All (19) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | A     | 2   | ASP  | 5.3  |
| 2   | A     | 3   | TYR  | 5.1  |
| 2   | A     | 4   | GLU  | 5.1  |
| 1   | T     | 74  | C    | 4.7  |
| 2   | A     | 280 | ALA  | 4.0  |
| 2   | A     | 377 | LEU  | 3.6  |
| 2   | A     | 249 | LEU  | 3.4  |
| 2   | A     | 384 | LEU  | 3.4  |
| 2   | A     | 279 | LYS  | 3.2  |
| 2   | A     | 315 | VAL  | 3.1  |
| 2   | A     | 866 | ASP  | 3.0  |
| 2   | A     | 317 | THR  | 2.9  |
| 2   | A     | 6   | THR  | 2.9  |
| 2   | A     | 360 | GLY  | 2.8  |
| 1   | T     | 17  | U    | 2.7  |
| 2   | A     | 110 | VAL  | 2.7  |
| 2   | A     | 218 | LYS  | 2.4  |
| 2   | A     | 865 | ASP  | 2.4  |
| 1   | T     | 47  | U    | 2.1  |

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|----------------------------|-------|
| 4   | MRC  | A     | 993 | 35/35 | 0.20 | 2.32  | 22,29,57,58                | 0     |
| 3   | ZN   | A     | 992 | 1/1   | 0.03 | -1.48 | 35,35,35,35                | 0     |

### 6.5 Other polymers

There are no such residues in this entry.