



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 PM UTC

PDB ID : 1AM4 / pdb\_00001am4  
Title : COMPLEX BETWEEN CDC42HS.GMPPNP AND P50 RHOGAP (H. SAPI-  
ENS)  
Authors : Rittinger, K.; Walker, P.; Gamblin, S.J.; Smerdon, S.J.  
Deposited on : 1997-06-22  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | <b>NOT EXECUTED</b>                                              |
| EDS                            | : | <b>NOT EXECUTED</b>                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

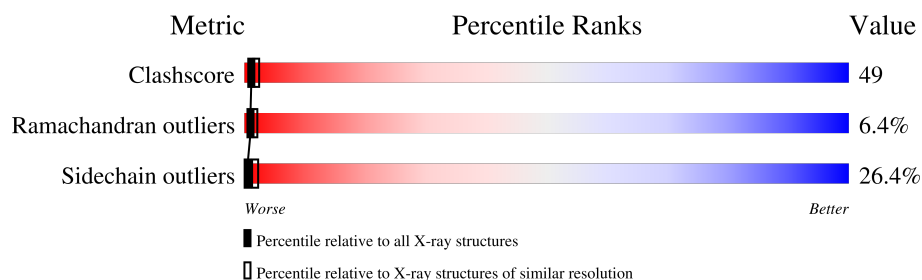
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 199    |                  |
| 1   | B     | 199    |                  |
| 1   | C     | 199    |                  |
| 2   | D     | 177    |                  |
| 2   | E     | 177    |                  |
| 2   | F     | 177    |                  |

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

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | GNP  | D     | 678 | -         | X        | X       | -                |
| 4   | GNP  | E     | 678 | -         | X        | -       | -                |
| 4   | GNP  | F     | 678 | -         | X        | -       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9191 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called P50-RHOGAP.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1593  | 1032 | 273 | 286 | 2 |         |         |       |
| 1   | B     | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1593  | 1032 | 273 | 286 | 2 |         |         |       |
| 1   | C     | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1593  | 1032 | 273 | 286 | 2 |         |         |       |

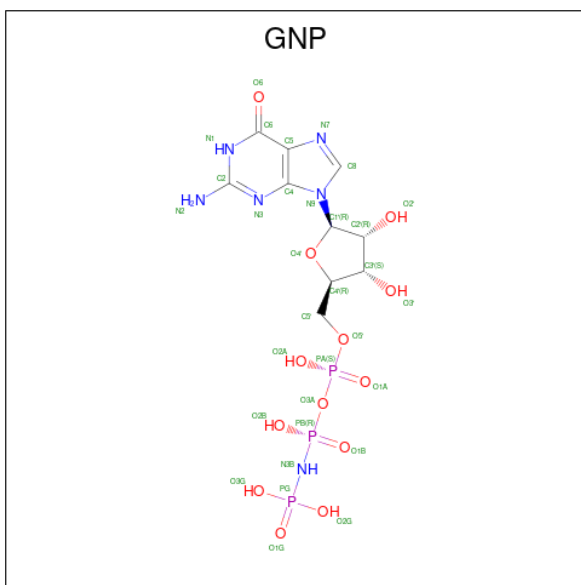
- Molecule 2 is a protein called CDC42HS.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | D     | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1337  | 861 | 218 | 252 | 6 |         |         |       |
| 2   | E     | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1337  | 861 | 218 | 252 | 6 |         |         |       |
| 2   | F     | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1337  | 861 | 218 | 252 | 6 |         |         |       |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | F     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 4   | D     | 1        | Total<br>32 | C<br>10 | N<br>6 | O<br>13 | P<br>3 | 0       | 0       |
| 4   | E     | 1        | Total<br>32 | C<br>10 | N<br>6 | O<br>13 | P<br>3 | 0       | 0       |
| 4   | F     | 1        | Total<br>32 | C<br>10 | N<br>6 | O<br>13 | P<br>3 | 0       | 0       |

- Molecule 5 is water.

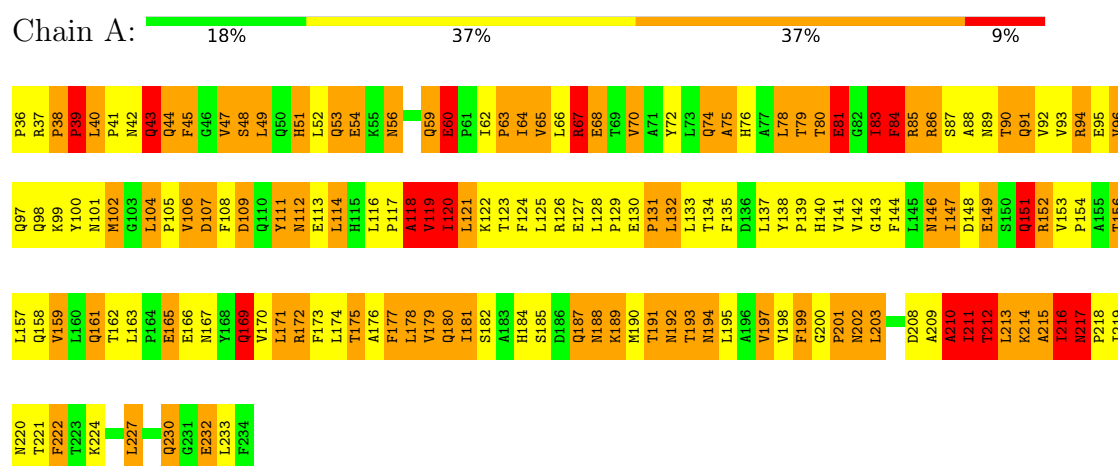
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5   | A     | 63       | Total O<br>63 63 | 0       | 0       |
| 5   | D     | 36       | Total O<br>36 36 | 0       | 0       |
| 5   | B     | 62       | Total O<br>62 62 | 0       | 0       |
| 5   | E     | 39       | Total O<br>39 39 | 0       | 0       |
| 5   | C     | 62       | Total O<br>62 62 | 0       | 0       |
| 5   | F     | 40       | Total O<br>40 40 | 0       | 0       |

### 3 Residue-property plots

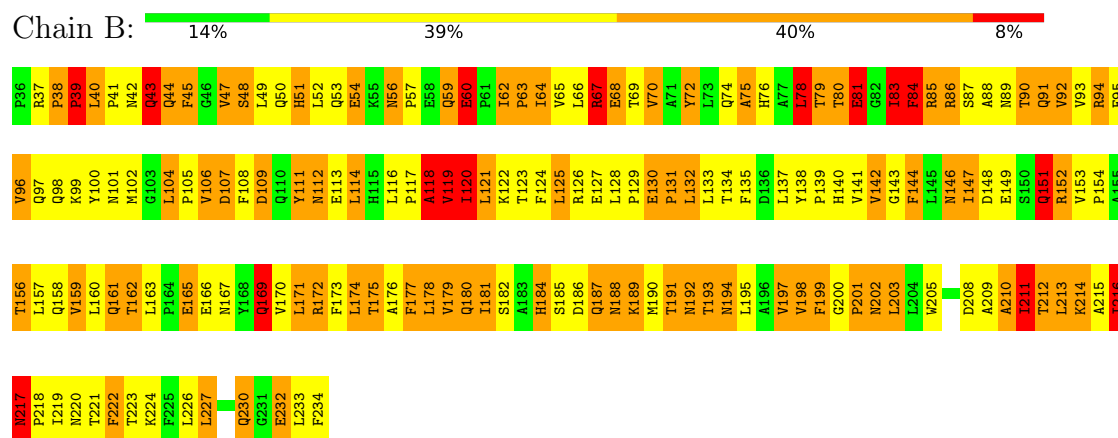
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

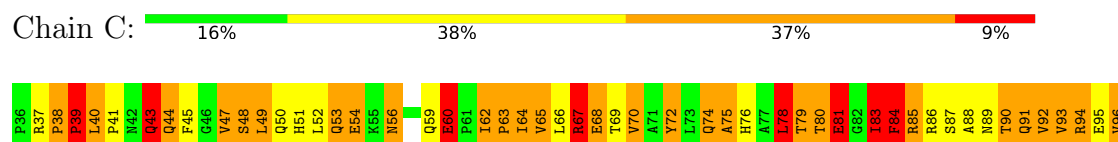
#### • Molecule 1: P50-RHOGAP

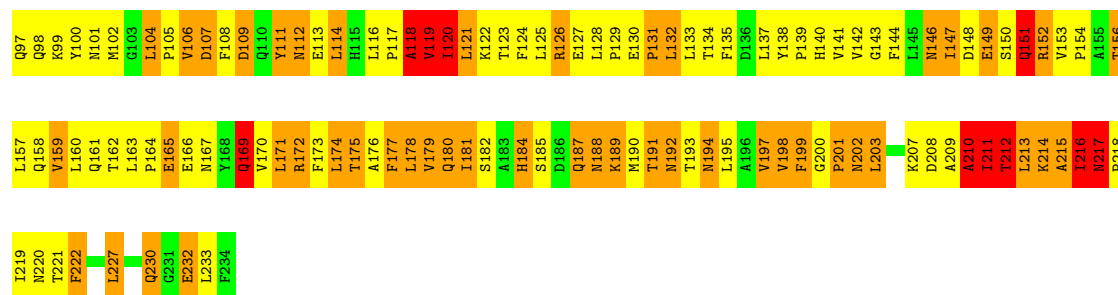


#### • Molecule 1: P50-RHOGAP

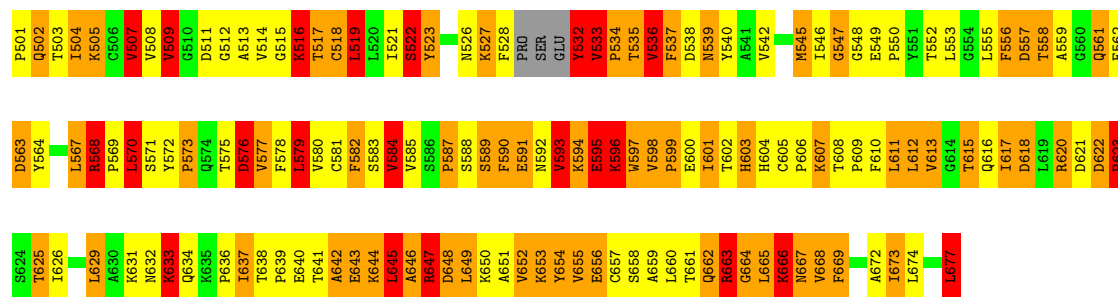
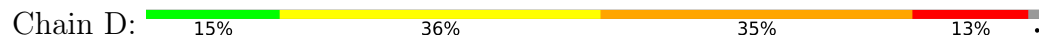


#### • Molecule 1: P50-RHOGAP

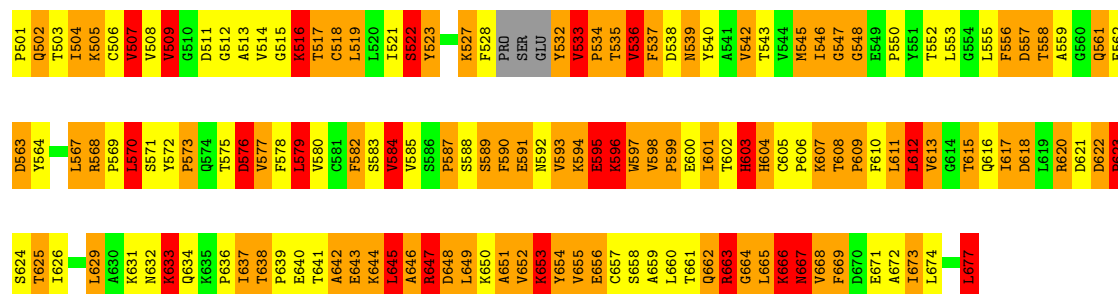




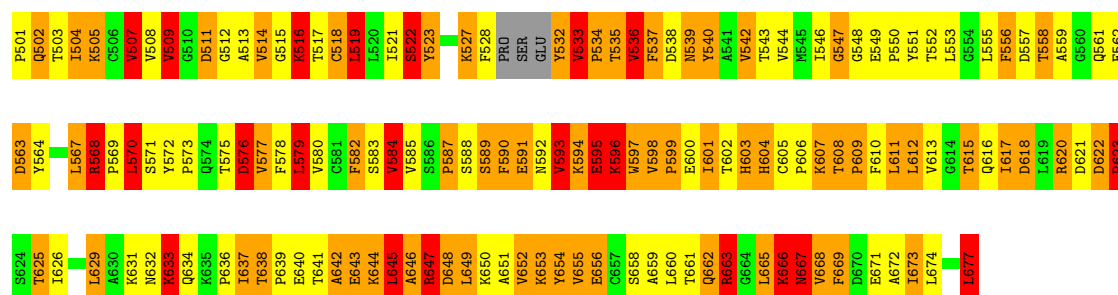
• Molecule 2: CDC42HS



• Molecule 2: CDC42HS



• Molecule 2: CDC42HS



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                        | Source    |
|----------------------------------------------------------|----------------------------------------------|-----------|
| Space group                                              | P 1                                          | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 78.11Å 78.12Å 78.10Å<br>90.01° 90.00° 90.05° | Depositor |
| Resolution (Å)                                           | 12.00 – 2.70                                 | Depositor |
| % Data completeness<br>(in resolution range)             | 96.0 (12.00-2.70)                            | Depositor |
| $R_{merge}$                                              | 0.06                                         | Depositor |
| $R_{sym}$                                                | (Not available)                              | Depositor |
| Refinement program                                       | CCP4                                         | Depositor |
| R, $R_{free}$                                            | 0.230 , 0.280                                | Depositor |
| Estimated twinning fraction                              | No twinning to report.                       | Xtriage   |
| Total number of atoms                                    | 9191                                         | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 18.0                                         | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.16         | 0/1633        | 2.78        | 165/2231 (7.4%)  |
| 1   | B     | 1.15         | 0/1633        | 2.80        | 182/2231 (8.2%)  |
| 1   | C     | 1.19         | 1/1633 (0.1%) | 2.80        | 176/2231 (7.9%)  |
| 2   | D     | 1.22         | 0/1366        | 2.78        | 133/1860 (7.2%)  |
| 2   | E     | 1.20         | 1/1366 (0.1%) | 2.77        | 144/1860 (7.7%)  |
| 2   | F     | 1.19         | 0/1366        | 2.77        | 129/1860 (6.9%)  |
| All | All   | 1.18         | 2/8997 (0.0%) | 2.78        | 929/12273 (7.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 4                   |
| 1   | B     | 0                   | 4                   |
| 1   | C     | 0                   | 4                   |
| 2   | D     | 0                   | 5                   |
| 2   | E     | 0                   | 2                   |
| 2   | F     | 0                   | 2                   |
| All | All   | 0                   | 21                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 69  | THR  | N-CA  | 5.60  | 1.53        | 1.46     |
| 2   | E     | 647 | ARG  | CD-NE | -5.10 | 1.39        | 1.46     |

All (929) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | F     | 647 | ARG  | CD-NE-CZ   | 18.83  | 150.76      | 124.40   |
| 2   | E     | 647 | ARG  | CD-NE-CZ   | 18.72  | 150.61      | 124.40   |
| 2   | D     | 647 | ARG  | CD-NE-CZ   | 18.70  | 150.58      | 124.40   |
| 2   | E     | 537 | PHE  | CA-CB-CG   | 15.20  | 129.00      | 113.80   |
| 2   | F     | 537 | PHE  | CA-CB-CG   | 15.20  | 129.00      | 113.80   |
| 2   | D     | 537 | PHE  | CA-CB-CG   | 15.10  | 128.90      | 113.80   |
| 2   | D     | 535 | THR  | CA-CB-OG1  | -14.40 | 88.00       | 109.60   |
| 2   | F     | 535 | THR  | CA-CB-OG1  | -14.22 | 88.27       | 109.60   |
| 2   | E     | 535 | THR  | CA-CB-OG1  | -13.93 | 88.71       | 109.60   |
| 1   | C     | 89  | ASN  | CA-CB-CG   | 13.17  | 125.77      | 112.60   |
| 1   | A     | 89  | ASN  | CA-CB-CG   | 13.17  | 125.77      | 112.60   |
| 1   | B     | 165 | GLU  | CA-C-N     | 11.75  | 143.99      | 121.54   |
| 1   | B     | 165 | GLU  | C-N-CA     | 11.75  | 143.99      | 121.54   |
| 1   | C     | 201 | PRO  | CA-C-N     | 11.69  | 135.95      | 120.28   |
| 1   | C     | 201 | PRO  | C-N-CA     | 11.69  | 135.95      | 120.28   |
| 1   | C     | 68  | GLU  | CA-C-O     | -11.45 | 105.92      | 119.78   |
| 1   | B     | 118 | ALA  | CA-C-O     | -11.30 | 109.14      | 121.00   |
| 1   | C     | 118 | ALA  | CA-C-O     | -11.28 | 109.15      | 121.00   |
| 1   | B     | 49  | LEU  | O-C-N      | 11.21  | 133.75      | 122.09   |
| 2   | F     | 618 | ASP  | CA-CB-CG   | 11.20  | 123.80      | 112.60   |
| 1   | A     | 62  | ILE  | O-C-N      | 11.08  | 128.35      | 121.37   |
| 1   | A     | 118 | ALA  | CA-C-O     | -11.01 | 109.44      | 121.00   |
| 1   | A     | 165 | GLU  | CA-C-N     | 11.01  | 142.57      | 121.54   |
| 1   | A     | 165 | GLU  | C-N-CA     | 11.01  | 142.57      | 121.54   |
| 1   | B     | 89  | ASN  | CA-CB-CG   | 10.97  | 123.57      | 112.60   |
| 1   | C     | 165 | GLU  | CA-C-N     | 10.89  | 142.34      | 121.54   |
| 1   | C     | 165 | GLU  | C-N-CA     | 10.89  | 142.34      | 121.54   |
| 2   | D     | 535 | THR  | N-CA-C     | 10.83  | 124.50      | 110.53   |
| 2   | D     | 665 | LEU  | CA-C-O     | -10.78 | 109.12      | 120.55   |
| 2   | E     | 615 | THR  | CA-C-O     | -10.76 | 108.99      | 121.68   |
| 2   | D     | 590 | PHE  | CA-CB-CG   | 10.74  | 124.54      | 113.80   |
| 1   | A     | 201 | PRO  | CA-C-N     | 10.71  | 134.64      | 120.28   |
| 1   | A     | 201 | PRO  | C-N-CA     | 10.71  | 134.64      | 120.28   |
| 1   | A     | 49  | LEU  | O-C-N      | 10.66  | 133.06      | 122.07   |
| 1   | B     | 68  | GLU  | CA-C-O     | -10.65 | 106.89      | 119.78   |
| 2   | D     | 615 | THR  | CA-C-O     | -10.65 | 109.00      | 121.46   |
| 1   | C     | 91  | GLN  | CB-CG-CD   | 10.62  | 130.65      | 112.60   |
| 1   | C     | 92  | VAL  | CA-C-O     | -10.60 | 110.25      | 121.27   |
| 1   | A     | 68  | GLU  | CA-C-O     | -10.58 | 106.98      | 119.78   |
| 2   | E     | 623 | PRO  | CA-C-N     | 10.56  | 134.44      | 120.28   |
| 2   | E     | 623 | PRO  | C-N-CA     | 10.56  | 134.44      | 120.28   |
| 1   | B     | 64  | ILE  | CB-CG1-CD1 | 10.54  | 135.92      | 113.80   |
| 1   | A     | 64  | ILE  | CB-CG1-CD1 | 10.49  | 135.82      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | E     | 644 | LYS  | CA-C-N     | 10.48  | 136.54      | 120.82   |
| 2   | E     | 644 | LYS  | C-N-CA     | 10.48  | 136.54      | 120.82   |
| 1   | B     | 91  | GLN  | CB-CG-CD   | 10.47  | 130.39      | 112.60   |
| 2   | F     | 615 | THR  | CA-C-O     | -10.46 | 109.22      | 121.46   |
| 1   | B     | 81  | GLU  | CA-CB-CG   | 10.45  | 135.00      | 114.10   |
| 1   | A     | 91  | GLN  | CB-CG-CD   | 10.43  | 130.34      | 112.60   |
| 1   | C     | 172 | ARG  | CD-NE-CZ   | 10.39  | 138.95      | 124.40   |
| 2   | E     | 590 | PHE  | CA-CB-CG   | 10.38  | 124.18      | 113.80   |
| 2   | F     | 665 | LEU  | CA-C-O     | -10.29 | 109.64      | 120.55   |
| 2   | F     | 535 | THR  | N-CA-C     | 10.28  | 124.42      | 110.55   |
| 1   | A     | 92  | VAL  | CA-C-O     | -10.23 | 110.78      | 121.41   |
| 2   | E     | 534 | PRO  | CA-C-O     | 10.23  | 134.73      | 121.95   |
| 1   | C     | 49  | LEU  | O-C-N      | 10.20  | 132.69      | 122.09   |
| 1   | C     | 230 | GLN  | OE1-CD-NE2 | -10.19 | 112.41      | 122.60   |
| 2   | D     | 534 | PRO  | CA-C-O     | 10.18  | 134.09      | 121.67   |
| 2   | E     | 535 | THR  | N-CA-C     | 10.12  | 124.22      | 110.55   |
| 1   | C     | 76  | HIS  | CA-CB-CG   | -10.08 | 103.72      | 113.80   |
| 2   | D     | 623 | PRO  | CA-C-N     | 10.08  | 134.60      | 120.29   |
| 2   | D     | 623 | PRO  | C-N-CA     | 10.08  | 134.60      | 120.29   |
| 2   | D     | 618 | ASP  | CA-CB-CG   | 10.05  | 122.65      | 112.60   |
| 2   | E     | 532 | TYR  | CA-CB-CG   | -10.05 | 95.80       | 113.90   |
| 2   | D     | 644 | LYS  | CA-C-N     | 10.04  | 135.88      | 120.82   |
| 2   | D     | 644 | LYS  | C-N-CA     | 10.04  | 135.88      | 120.82   |
| 2   | E     | 618 | ASP  | CA-CB-CG   | 10.02  | 122.62      | 112.60   |
| 1   | B     | 92  | VAL  | CA-C-O     | -9.99  | 111.02      | 121.41   |
| 2   | F     | 623 | PRO  | CA-C-N     | 9.99   | 134.48      | 120.29   |
| 2   | F     | 623 | PRO  | C-N-CA     | 9.99   | 134.48      | 120.29   |
| 2   | E     | 665 | LEU  | CA-C-O     | -9.92  | 109.90      | 120.42   |
| 1   | A     | 159 | VAL  | O-C-N      | 9.92   | 131.95      | 122.23   |
| 1   | C     | 81  | GLU  | CA-CB-CG   | 9.85   | 133.79      | 114.10   |
| 2   | F     | 532 | TYR  | CA-CB-CG   | -9.83  | 96.20       | 113.90   |
| 2   | D     | 532 | TYR  | CA-CB-CG   | -9.83  | 96.21       | 113.90   |
| 2   | D     | 517 | THR  | CA-CB-OG1  | -9.82  | 94.86       | 109.60   |
| 1   | B     | 76  | HIS  | CA-CB-CG   | -9.79  | 104.01      | 113.80   |
| 1   | B     | 230 | GLN  | OE1-CD-NE2 | -9.79  | 112.81      | 122.60   |
| 1   | A     | 81  | GLU  | CA-CB-CG   | 9.78   | 133.65      | 114.10   |
| 1   | A     | 76  | HIS  | CA-CB-CG   | -9.74  | 104.06      | 113.80   |
| 2   | E     | 582 | PHE  | CA-CB-CG   | 9.72   | 123.52      | 113.80   |
| 2   | F     | 517 | THR  | CA-CB-OG1  | -9.69  | 95.07       | 109.60   |
| 2   | F     | 534 | PRO  | CA-C-O     | 9.67   | 134.46      | 122.08   |
| 1   | B     | 159 | VAL  | O-C-N      | 9.65   | 131.69      | 122.23   |
| 1   | C     | 119 | VAL  | N-CA-CB    | 9.63   | 121.20      | 110.51   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | F     | 590 | PHE  | CA-CB-CG   | 9.61  | 123.41      | 113.80   |
| 2   | D     | 570 | LEU  | CA-C-N     | 9.59  | 138.37      | 122.54   |
| 2   | D     | 570 | LEU  | C-N-CA     | 9.59  | 138.37      | 122.54   |
| 1   | C     | 159 | VAL  | O-C-N      | 9.59  | 131.63      | 122.23   |
| 1   | C     | 109 | ASP  | CB-CA-C    | 9.49  | 125.49      | 109.55   |
| 2   | F     | 655 | VAL  | CA-C-O     | 9.49  | 131.29      | 120.67   |
| 1   | B     | 60  | GLU  | CA-CB-CG   | 9.47  | 133.04      | 114.10   |
| 2   | D     | 582 | PHE  | CA-CB-CG   | 9.43  | 123.23      | 113.80   |
| 2   | F     | 582 | PHE  | CA-CB-CG   | 9.43  | 123.22      | 113.80   |
| 1   | A     | 67  | ARG  | CD-NE-CZ   | 9.42  | 137.59      | 124.40   |
| 2   | D     | 655 | VAL  | CA-C-O     | 9.40  | 131.20      | 120.67   |
| 1   | C     | 64  | ILE  | CB-CG1-CD1 | 9.39  | 133.51      | 113.80   |
| 1   | B     | 179 | VAL  | CA-C-N     | 9.37  | 136.61      | 120.68   |
| 1   | B     | 179 | VAL  | C-N-CA     | 9.37  | 136.61      | 120.68   |
| 2   | F     | 644 | LYS  | CA-C-N     | 9.35  | 134.84      | 120.82   |
| 2   | F     | 644 | LYS  | C-N-CA     | 9.35  | 134.84      | 120.82   |
| 2   | E     | 655 | VAL  | CA-C-O     | 9.25  | 131.03      | 120.67   |
| 1   | A     | 60  | GLU  | CA-CB-CG   | 9.21  | 132.51      | 114.10   |
| 2   | D     | 535 | THR  | CA-CB-CG2  | 9.18  | 126.10      | 110.50   |
| 2   | F     | 535 | THR  | CA-CB-CG2  | 9.14  | 126.04      | 110.50   |
| 1   | A     | 230 | GLN  | OE1-CD-NE2 | -9.08 | 113.52      | 122.60   |
| 2   | E     | 644 | LYS  | CA-C-O     | 9.06  | 133.46      | 120.51   |
| 1   | A     | 109 | ASP  | CB-CA-C    | 9.05  | 124.76      | 109.55   |
| 2   | D     | 507 | VAL  | CA-C-O     | 8.99  | 129.83      | 120.39   |
| 1   | B     | 67  | ARG  | CD-NE-CZ   | 8.96  | 136.94      | 124.40   |
| 1   | C     | 199 | PHE  | CA-CB-CG   | -8.95 | 104.85      | 113.80   |
| 2   | E     | 535 | THR  | CA-CB-CG2  | 8.90  | 125.63      | 110.50   |
| 1   | C     | 120 | ILE  | CA-C-N     | 8.85  | 132.34      | 120.65   |
| 1   | C     | 120 | ILE  | C-N-CA     | 8.85  | 132.34      | 120.65   |
| 1   | C     | 60  | GLU  | CA-CB-CG   | 8.83  | 131.76      | 114.10   |
| 1   | B     | 62  | ILE  | O-C-N      | 8.83  | 127.82      | 121.55   |
| 1   | B     | 109 | ASP  | CB-CA-C    | 8.81  | 124.36      | 109.55   |
| 1   | B     | 201 | PRO  | CA-C-N     | 8.80  | 132.07      | 120.28   |
| 1   | B     | 201 | PRO  | C-N-CA     | 8.80  | 132.07      | 120.28   |
| 1   | A     | 172 | ARG  | CD-NE-CZ   | 8.77  | 136.68      | 124.40   |
| 1   | C     | 48  | SER  | CA-C-N     | 8.75  | 132.35      | 120.54   |
| 1   | C     | 48  | SER  | C-N-CA     | 8.75  | 132.35      | 120.54   |
| 1   | B     | 120 | ILE  | CA-C-N     | 8.75  | 131.81      | 120.44   |
| 1   | B     | 120 | ILE  | C-N-CA     | 8.75  | 131.81      | 120.44   |
| 1   | C     | 148 | ASP  | CA-CB-CG   | 8.75  | 121.35      | 112.60   |
| 1   | B     | 148 | ASP  | CA-CB-CG   | 8.74  | 121.34      | 112.60   |
| 1   | C     | 169 | GLN  | CB-CG-CD   | 8.72  | 127.43      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 119 | VAL  | N-CA-CB    | 8.68  | 121.32      | 110.47   |
| 1   | B     | 48  | SER  | CA-C-N     | 8.68  | 132.25      | 120.54   |
| 1   | B     | 48  | SER  | C-N-CA     | 8.68  | 132.25      | 120.54   |
| 2   | E     | 642 | ALA  | N-CA-C     | -8.62 | 102.35      | 113.12   |
| 1   | B     | 119 | VAL  | N-CA-CB    | 8.59  | 121.21      | 110.47   |
| 1   | B     | 104 | LEU  | CB-CA-C    | 8.59  | 122.19      | 108.87   |
| 2   | D     | 615 | THR  | O-C-N      | 8.56  | 134.59      | 123.11   |
| 2   | D     | 673 | ILE  | CA-C-O     | -8.53 | 111.58      | 120.71   |
| 2   | F     | 556 | PHE  | CA-CB-CG   | 8.52  | 122.31      | 113.80   |
| 2   | D     | 642 | ALA  | N-CA-C     | -8.50 | 102.49      | 113.12   |
| 2   | E     | 621 | ASP  | N-CA-C     | -8.46 | 100.00      | 110.65   |
| 1   | A     | 173 | PHE  | CA-CB-CG   | 8.42  | 122.22      | 113.80   |
| 1   | A     | 48  | SER  | CA-C-N     | 8.40  | 131.36      | 120.44   |
| 1   | A     | 48  | SER  | C-N-CA     | 8.40  | 131.36      | 120.44   |
| 2   | F     | 642 | ALA  | N-CA-C     | -8.39 | 102.64      | 113.12   |
| 1   | A     | 169 | GLN  | CB-CG-CD   | 8.36  | 126.81      | 112.60   |
| 1   | B     | 169 | GLN  | CB-CG-CD   | 8.32  | 126.75      | 112.60   |
| 1   | C     | 166 | GLU  | CA-CB-CG   | 8.32  | 130.73      | 114.10   |
| 1   | C     | 104 | LEU  | CB-CA-C    | 8.31  | 121.75      | 108.87   |
| 1   | A     | 120 | ILE  | CA-C-N     | 8.30  | 131.61      | 120.65   |
| 1   | A     | 120 | ILE  | C-N-CA     | 8.30  | 131.61      | 120.65   |
| 1   | B     | 222 | PHE  | O-C-N      | 8.26  | 130.58      | 122.07   |
| 1   | A     | 199 | PHE  | CA-CB-CG   | -8.21 | 105.59      | 113.80   |
| 2   | D     | 621 | ASP  | N-CA-C     | -8.21 | 100.31      | 110.65   |
| 2   | D     | 509 | VAL  | CA-C-O     | -8.21 | 113.30      | 121.67   |
| 2   | E     | 673 | ILE  | CA-C-O     | -8.18 | 111.96      | 120.71   |
| 1   | C     | 175 | THR  | O-C-N      | 8.17  | 130.49      | 122.07   |
| 1   | C     | 222 | PHE  | O-C-N      | 8.16  | 130.48      | 122.07   |
| 2   | D     | 514 | VAL  | CA-C-N     | 8.14  | 133.00      | 122.00   |
| 2   | D     | 514 | VAL  | C-N-CA     | 8.14  | 133.00      | 122.00   |
| 2   | E     | 600 | GLU  | CB-CG-CD   | 8.14  | 126.43      | 112.60   |
| 1   | A     | 120 | ILE  | CB-CA-C    | 8.13  | 123.11      | 112.14   |
| 1   | B     | 91  | GLN  | OE1-CD-NE2 | -8.13 | 114.47      | 122.60   |
| 2   | F     | 514 | VAL  | CA-C-N     | 8.12  | 133.84      | 122.63   |
| 2   | F     | 514 | VAL  | C-N-CA     | 8.12  | 133.84      | 122.63   |
| 2   | F     | 509 | VAL  | CA-C-O     | -8.12 | 113.39      | 121.67   |
| 2   | F     | 673 | ILE  | CA-C-O     | -8.11 | 112.03      | 120.71   |
| 2   | D     | 588 | SER  | CA-C-N     | 8.10  | 131.47      | 120.38   |
| 2   | D     | 588 | SER  | C-N-CA     | 8.10  | 131.47      | 120.38   |
| 2   | E     | 570 | LEU  | CA-C-N     | 8.09  | 135.89      | 122.54   |
| 2   | E     | 570 | LEU  | C-N-CA     | 8.09  | 135.89      | 122.54   |
| 2   | F     | 570 | LEU  | CA-C-N     | 8.08  | 135.88      | 122.54   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | F     | 570 | LEU  | C-N-CA     | 8.08  | 135.88      | 122.54   |
| 2   | E     | 517 | THR  | CA-CB-OG1  | -8.06 | 97.50       | 109.60   |
| 2   | F     | 621 | ASP  | N-CA-C     | -8.06 | 100.49      | 110.65   |
| 2   | E     | 556 | PHE  | CA-CB-CG   | 8.03  | 121.83      | 113.80   |
| 1   | C     | 179 | VAL  | CA-C-N     | 8.03  | 134.32      | 120.68   |
| 1   | C     | 179 | VAL  | C-N-CA     | 8.03  | 134.32      | 120.68   |
| 1   | A     | 202 | ASN  | O-C-N      | 8.02  | 130.62      | 122.12   |
| 1   | A     | 104 | LEU  | CB-CA-C    | 8.01  | 121.28      | 108.87   |
| 2   | D     | 608 | THR  | CA-C-O     | 8.01  | 125.25      | 119.32   |
| 1   | B     | 88  | ALA  | CA-C-N     | 7.99  | 136.79      | 121.54   |
| 1   | B     | 88  | ALA  | C-N-CA     | 7.99  | 136.79      | 121.54   |
| 1   | C     | 76  | HIS  | N-CA-C     | 7.99  | 121.14      | 111.40   |
| 1   | B     | 199 | PHE  | CA-CB-CG   | -7.98 | 105.82      | 113.80   |
| 2   | F     | 615 | THR  | O-C-N      | 7.98  | 133.80      | 123.11   |
| 1   | A     | 76  | HIS  | N-CA-C     | 7.95  | 121.10      | 111.40   |
| 2   | E     | 588 | SER  | CA-C-N     | 7.93  | 131.25      | 120.38   |
| 2   | E     | 588 | SER  | C-N-CA     | 7.93  | 131.25      | 120.38   |
| 1   | B     | 98  | GLN  | OE1-CD-NE2 | -7.92 | 114.68      | 122.60   |
| 1   | C     | 127 | GLU  | N-CA-C     | 7.90  | 121.73      | 112.72   |
| 2   | D     | 557 | ASP  | CA-CB-CG   | 7.90  | 120.50      | 112.60   |
| 1   | B     | 76  | HIS  | N-CA-C     | 7.90  | 121.03      | 111.40   |
| 2   | D     | 665 | LEU  | O-C-N      | 7.89  | 130.48      | 122.12   |
| 2   | E     | 514 | VAL  | CA-C-N     | 7.87  | 133.49      | 122.63   |
| 2   | E     | 514 | VAL  | C-N-CA     | 7.87  | 133.49      | 122.63   |
| 1   | A     | 91  | GLN  | OE1-CD-NE2 | -7.87 | 114.73      | 122.60   |
| 1   | C     | 85  | ARG  | NE-CZ-NH1  | 7.85  | 129.35      | 121.50   |
| 2   | F     | 644 | LYS  | CA-C-O     | 7.84  | 131.72      | 120.51   |
| 1   | C     | 120 | ILE  | CB-CA-C    | 7.82  | 122.69      | 112.14   |
| 1   | C     | 62  | ILE  | O-C-N      | 7.81  | 127.55      | 121.46   |
| 1   | C     | 67  | ARG  | CD-NE-CZ   | 7.80  | 135.32      | 124.40   |
| 2   | D     | 649 | LEU  | CB-CA-C    | 7.77  | 123.43      | 109.29   |
| 1   | C     | 88  | ALA  | CA-C-N     | 7.77  | 136.38      | 121.54   |
| 1   | C     | 88  | ALA  | C-N-CA     | 7.77  | 136.38      | 121.54   |
| 1   | C     | 202 | ASN  | O-C-N      | 7.77  | 130.36      | 122.12   |
| 2   | D     | 600 | GLU  | CB-CG-CD   | 7.77  | 125.81      | 112.60   |
| 2   | E     | 557 | ASP  | CA-CB-CG   | 7.77  | 120.37      | 112.60   |
| 1   | A     | 179 | VAL  | CA-C-N     | 7.74  | 134.69      | 121.14   |
| 1   | A     | 179 | VAL  | C-N-CA     | 7.74  | 134.69      | 121.14   |
| 1   | A     | 148 | ASP  | CA-CB-CG   | 7.73  | 120.33      | 112.60   |
| 1   | A     | 88  | ALA  | CA-C-N     | 7.72  | 136.29      | 121.54   |
| 1   | A     | 88  | ALA  | C-N-CA     | 7.72  | 136.29      | 121.54   |
| 2   | F     | 669 | PHE  | CB-CA-C    | 7.69  | 124.77      | 110.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 98  | GLN  | OE1-CD-NE2 | -7.68 | 114.92      | 122.60   |
| 2   | D     | 556 | PHE  | CA-CB-CG   | 7.68  | 121.48      | 113.80   |
| 1   | B     | 166 | GLU  | CA-CB-CG   | 7.67  | 129.45      | 114.10   |
| 2   | E     | 649 | LEU  | CB-CA-C    | 7.67  | 123.25      | 109.29   |
| 1   | A     | 80  | THR  | CA-C-O     | 7.66  | 129.78      | 121.05   |
| 2   | F     | 507 | VAL  | CA-C-O     | 7.63  | 128.40      | 120.39   |
| 2   | E     | 608 | THR  | CA-C-O     | 7.62  | 124.96      | 119.32   |
| 1   | B     | 172 | ARG  | CD-NE-CZ   | 7.61  | 135.05      | 124.40   |
| 2   | D     | 536 | VAL  | CB-CA-C    | 7.58  | 123.72      | 111.29   |
| 2   | F     | 519 | LEU  | CA-CB-CG   | 7.58  | 142.81      | 116.30   |
| 2   | E     | 669 | PHE  | CB-CA-C    | 7.57  | 124.56      | 110.70   |
| 2   | F     | 665 | LEU  | O-C-N      | 7.56  | 130.13      | 122.12   |
| 2   | F     | 536 | VAL  | CA-C-O     | -7.55 | 111.34      | 120.78   |
| 2   | E     | 519 | LEU  | CA-CB-CG   | 7.55  | 142.72      | 116.30   |
| 1   | C     | 78  | LEU  | O-C-N      | 7.53  | 130.76      | 122.11   |
| 1   | B     | 221 | THR  | CA-C-N     | 7.52  | 130.21      | 120.44   |
| 1   | B     | 221 | THR  | C-N-CA     | 7.52  | 130.21      | 120.44   |
| 1   | B     | 132 | LEU  | CA-C-O     | -7.50 | 112.82      | 121.07   |
| 1   | C     | 98  | GLN  | OE1-CD-NE2 | -7.50 | 115.10      | 122.60   |
| 1   | C     | 173 | PHE  | CA-CB-CG   | 7.49  | 121.29      | 113.80   |
| 2   | E     | 615 | THR  | O-C-N      | 7.48  | 133.63      | 122.94   |
| 2   | E     | 536 | VAL  | CB-CA-C    | 7.47  | 123.55      | 111.29   |
| 1   | A     | 163 | LEU  | O-C-N      | 7.47  | 128.75      | 121.28   |
| 1   | B     | 120 | ILE  | CB-CA-C    | 7.46  | 122.21      | 112.14   |
| 2   | E     | 518 | CYS  | CB-CA-C    | 7.46  | 122.59      | 110.88   |
| 1   | A     | 132 | LEU  | CA-C-O     | -7.46 | 112.87      | 121.07   |
| 1   | B     | 202 | ASN  | O-C-N      | 7.45  | 130.02      | 122.12   |
| 2   | F     | 536 | VAL  | CB-CA-C    | 7.45  | 123.51      | 111.29   |
| 1   | C     | 132 | LEU  | CA-C-O     | -7.45 | 112.88      | 121.07   |
| 2   | F     | 588 | SER  | CA-C-N     | 7.43  | 130.56      | 120.38   |
| 2   | F     | 588 | SER  | C-N-CA     | 7.43  | 130.56      | 120.38   |
| 1   | A     | 78  | LEU  | O-C-N      | 7.42  | 129.81      | 122.09   |
| 2   | D     | 536 | VAL  | CA-C-O     | -7.42 | 111.50      | 120.78   |
| 2   | D     | 517 | THR  | O-C-N      | 7.41  | 129.74      | 122.03   |
| 1   | A     | 232 | GLU  | CA-C-O     | -7.40 | 110.94      | 119.60   |
| 1   | A     | 166 | GLU  | CA-CB-CG   | 7.40  | 128.90      | 114.10   |
| 1   | B     | 54  | GLU  | N-CA-C     | -7.39 | 102.60      | 111.69   |
| 2   | E     | 584 | VAL  | CA-C-O     | -7.38 | 111.56      | 120.78   |
| 2   | F     | 600 | GLU  | CB-CG-CD   | 7.38  | 125.14      | 112.60   |
| 1   | C     | 221 | THR  | CA-C-N     | 7.37  | 130.02      | 120.44   |
| 1   | C     | 221 | THR  | C-N-CA     | 7.37  | 130.02      | 120.44   |
| 2   | F     | 584 | VAL  | CA-C-O     | -7.36 | 111.58      | 120.78   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 96  | VAL  | O-C-N      | 7.34  | 129.28      | 121.94   |
| 2   | E     | 509 | VAL  | CA-C-O     | -7.29 | 114.24      | 121.67   |
| 1   | A     | 107 | ASP  | CB-CA-C    | 7.28  | 122.46      | 110.74   |
| 2   | D     | 584 | VAL  | CA-C-O     | -7.25 | 111.71      | 120.78   |
| 1   | A     | 98  | GLN  | N-CA-C     | -7.25 | 103.41      | 112.90   |
| 1   | C     | 112 | ASN  | CA-CB-CG   | 7.24  | 119.84      | 112.60   |
| 1   | B     | 98  | GLN  | N-CA-C     | -7.24 | 103.42      | 112.90   |
| 1   | B     | 173 | PHE  | CA-CB-CG   | 7.24  | 121.04      | 113.80   |
| 2   | F     | 563 | ASP  | CA-C-O     | 7.23  | 128.22      | 120.55   |
| 2   | E     | 517 | THR  | O-C-N      | 7.22  | 129.54      | 122.03   |
| 1   | A     | 221 | THR  | CA-C-N     | 7.22  | 129.83      | 120.44   |
| 1   | A     | 221 | THR  | C-N-CA     | 7.22  | 129.83      | 120.44   |
| 2   | D     | 519 | LEU  | CA-CB-CG   | 7.21  | 141.53      | 116.30   |
| 1   | C     | 80  | THR  | CA-C-O     | 7.21  | 129.26      | 121.05   |
| 1   | B     | 217 | ASN  | CA-CB-CG   | -7.20 | 105.40      | 112.60   |
| 2   | F     | 660 | LEU  | CA-C-O     | 7.20  | 128.56      | 121.00   |
| 1   | C     | 68  | GLU  | N-CA-CB    | 7.20  | 121.43      | 110.42   |
| 1   | B     | 49  | LEU  | CA-C-O     | -7.19 | 113.21      | 120.90   |
| 2   | E     | 536 | VAL  | CA-C-O     | -7.19 | 111.80      | 120.78   |
| 1   | A     | 175 | THR  | O-C-N      | 7.18  | 129.47      | 122.07   |
| 1   | C     | 91  | GLN  | OE1-CD-NE2 | -7.18 | 115.42      | 122.60   |
| 1   | A     | 219 | ILE  | CB-CA-C    | 7.18  | 121.78      | 111.65   |
| 2   | F     | 516 | LYS  | CA-C-N     | 7.18  | 130.13      | 120.65   |
| 2   | F     | 516 | LYS  | C-N-CA     | 7.18  | 130.13      | 120.65   |
| 2   | F     | 608 | THR  | CA-C-O     | 7.18  | 124.63      | 119.32   |
| 1   | C     | 107 | ASP  | CB-CA-C    | 7.17  | 122.29      | 110.74   |
| 1   | B     | 188 | ASN  | CA-CB-CG   | 7.17  | 119.77      | 112.60   |
| 2   | D     | 518 | CYS  | CB-CA-C    | 7.17  | 122.87      | 110.68   |
| 1   | A     | 131 | PRO  | CA-C-N     | 7.16  | 130.75      | 120.79   |
| 1   | A     | 131 | PRO  | C-N-CA     | 7.16  | 130.75      | 120.79   |
| 1   | A     | 188 | ASN  | CA-CB-CG   | 7.16  | 119.76      | 112.60   |
| 1   | B     | 54  | GLU  | CA-CB-CG   | 7.15  | 128.41      | 114.10   |
| 1   | A     | 217 | ASN  | CA-CB-CG   | -7.14 | 105.46      | 112.60   |
| 2   | E     | 647 | ARG  | CG-CD-NE   | 7.14  | 127.70      | 112.00   |
| 2   | F     | 647 | ARG  | CG-CD-NE   | 7.12  | 127.66      | 112.00   |
| 1   | C     | 85  | ARG  | CB-CA-C    | 7.11  | 118.33      | 109.16   |
| 1   | B     | 131 | PRO  | CA-C-N     | 7.10  | 130.66      | 120.79   |
| 1   | B     | 131 | PRO  | C-N-CA     | 7.10  | 130.66      | 120.79   |
| 1   | C     | 111 | TYR  | CA-C-O     | 7.10  | 128.17      | 120.43   |
| 2   | F     | 518 | CYS  | CB-CA-C    | 7.10  | 122.75      | 110.68   |
| 2   | F     | 625 | THR  | N-CA-C     | -7.10 | 103.47      | 111.07   |
| 1   | A     | 230 | GLN  | O-C-N      | 7.10  | 131.88      | 122.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D     | 647 | ARG  | CG-CD-NE   | 7.10  | 127.61      | 112.00   |
| 1   | A     | 87  | SER  | CA-C-N     | 7.09  | 130.94      | 120.87   |
| 1   | A     | 87  | SER  | C-N-CA     | 7.09  | 130.94      | 120.87   |
| 2   | D     | 597 | TRP  | CA-C-O     | -7.08 | 113.61      | 120.90   |
| 2   | D     | 669 | PHE  | CB-CA-C    | 7.07  | 123.64      | 110.70   |
| 1   | A     | 112 | ASN  | CA-CB-CG   | 7.07  | 119.67      | 112.60   |
| 1   | A     | 222 | PHE  | O-C-N      | 7.06  | 129.34      | 122.07   |
| 1   | B     | 85  | ARG  | CB-CA-C    | 7.05  | 118.66      | 109.28   |
| 1   | B     | 122 | LYS  | O-C-N      | 7.05  | 130.18      | 122.15   |
| 1   | A     | 122 | LYS  | O-C-N      | 7.04  | 130.18      | 122.15   |
| 1   | A     | 68  | GLU  | N-CA-CB    | 7.03  | 121.18      | 110.42   |
| 1   | C     | 54  | GLU  | CA-CB-CG   | 7.03  | 128.16      | 114.10   |
| 1   | B     | 112 | ASN  | CA-CB-CG   | 7.03  | 119.63      | 112.60   |
| 1   | B     | 85  | ARG  | NE-CZ-NH1  | 7.03  | 128.53      | 121.50   |
| 1   | B     | 86  | ARG  | CA-C-N     | -7.03 | 112.81      | 122.30   |
| 1   | B     | 86  | ARG  | C-N-CA     | -7.03 | 112.81      | 122.30   |
| 1   | B     | 127 | GLU  | N-CA-C     | 7.00  | 120.70      | 112.72   |
| 1   | B     | 232 | GLU  | CA-C-O     | -7.00 | 111.41      | 119.60   |
| 2   | E     | 562 | GLU  | CA-C-O     | -6.99 | 113.08      | 120.63   |
| 1   | C     | 98  | GLN  | N-CA-C     | -6.98 | 103.75      | 112.90   |
| 1   | C     | 151 | GLN  | CA-C-N     | 6.97  | 130.19      | 120.29   |
| 1   | C     | 151 | GLN  | C-N-CA     | 6.97  | 130.19      | 120.29   |
| 1   | B     | 84  | PHE  | CA-CB-CG   | -6.96 | 106.84      | 113.80   |
| 2   | F     | 582 | PHE  | O-C-N      | 6.96  | 131.59      | 123.17   |
| 1   | B     | 68  | GLU  | N-CA-CB    | 6.95  | 121.06      | 110.42   |
| 1   | C     | 219 | ILE  | CB-CA-C    | 6.95  | 121.44      | 111.65   |
| 2   | F     | 532 | TYR  | CA-C-O     | -6.94 | 109.00      | 120.80   |
| 1   | C     | 146 | ASN  | CA-CB-CG   | 6.94  | 119.54      | 112.60   |
| 2   | F     | 662 | GLN  | OE1-CD-NE2 | 6.94  | 129.54      | 122.60   |
| 1   | A     | 84  | PHE  | CA-CB-CG   | -6.92 | 106.88      | 113.80   |
| 2   | D     | 660 | LEU  | CA-C-O     | 6.92  | 128.27      | 121.00   |
| 1   | A     | 54  | GLU  | CA-CB-CG   | 6.92  | 127.94      | 114.10   |
| 2   | E     | 660 | LEU  | CA-C-O     | 6.92  | 128.26      | 121.00   |
| 1   | C     | 194 | ASN  | CA-C-N     | 6.91  | 129.84      | 120.44   |
| 1   | C     | 194 | ASN  | C-N-CA     | 6.91  | 129.84      | 120.44   |
| 1   | C     | 202 | ASN  | CA-C-O     | -6.89 | 113.24      | 120.55   |
| 1   | B     | 208 | ASP  | CA-CB-CG   | 6.89  | 119.49      | 112.60   |
| 2   | E     | 665 | LEU  | O-C-N      | 6.87  | 129.98      | 122.15   |
| 1   | B     | 87  | SER  | CA-C-N     | 6.86  | 130.61      | 120.87   |
| 1   | B     | 87  | SER  | C-N-CA     | 6.86  | 130.61      | 120.87   |
| 2   | D     | 662 | GLN  | OE1-CD-NE2 | 6.86  | 129.46      | 122.60   |
| 1   | B     | 107 | ASP  | CB-CA-C    | 6.85  | 121.77      | 110.74   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 111 | TYR  | CA-C-O    | 6.85  | 127.90      | 120.43   |
| 2   | F     | 517 | THR  | O-C-N     | 6.85  | 129.15      | 122.03   |
| 2   | E     | 535 | THR  | O-C-N     | 6.81  | 130.61      | 122.85   |
| 2   | F     | 621 | ASP  | CB-CA-C   | 6.81  | 121.07      | 111.74   |
| 2   | E     | 621 | ASP  | CB-CA-C   | 6.81  | 121.07      | 111.74   |
| 2   | F     | 580 | VAL  | N-CA-CB   | 6.81  | 119.18      | 111.21   |
| 1   | A     | 49  | LEU  | CA-C-O    | -6.81 | 113.67      | 120.82   |
| 2   | F     | 538 | ASP  | CA-CB-CG  | 6.78  | 119.38      | 112.60   |
| 1   | B     | 121 | LEU  | O-C-N     | 6.78  | 129.05      | 122.07   |
| 2   | F     | 535 | THR  | O-C-N     | 6.77  | 130.56      | 122.85   |
| 1   | C     | 188 | ASN  | CA-CB-CG  | 6.76  | 119.36      | 112.60   |
| 1   | B     | 78  | LEU  | O-C-N     | 6.76  | 129.88      | 122.11   |
| 2   | F     | 649 | LEU  | CB-CA-C   | 6.76  | 123.27      | 109.55   |
| 1   | C     | 96  | VAL  | N-CA-C    | -6.75 | 103.27      | 110.36   |
| 1   | C     | 122 | LYS  | O-C-N     | 6.73  | 129.82      | 122.15   |
| 1   | B     | 128 | LEU  | O-C-N     | 6.72  | 128.82      | 121.36   |
| 1   | C     | 232 | GLU  | CA-C-O    | -6.72 | 111.73      | 119.60   |
| 1   | C     | 158 | GLN  | CB-CG-CD  | 6.72  | 124.03      | 112.60   |
| 1   | C     | 54  | GLU  | N-CA-C    | -6.72 | 103.42      | 111.69   |
| 1   | A     | 85  | ARG  | CB-CA-C   | 6.69  | 117.79      | 109.16   |
| 1   | C     | 191 | THR  | N-CA-C    | -6.69 | 101.90      | 110.53   |
| 1   | B     | 175 | THR  | O-C-N     | 6.68  | 128.95      | 122.07   |
| 2   | E     | 654 | TYR  | O-C-N     | 6.67  | 130.81      | 123.27   |
| 1   | A     | 96  | VAL  | O-C-N     | 6.66  | 128.60      | 121.94   |
| 1   | A     | 106 | VAL  | CA-CB-CG2 | 6.66  | 121.72      | 110.40   |
| 1   | C     | 123 | THR  | CB-CA-C   | 6.66  | 121.50      | 110.92   |
| 1   | C     | 217 | ASN  | CA-CB-CG  | -6.64 | 105.96      | 112.60   |
| 1   | A     | 217 | ASN  | N-CA-C    | 6.64  | 124.49      | 109.81   |
| 1   | B     | 96  | VAL  | N-CA-C    | -6.64 | 103.39      | 110.36   |
| 1   | C     | 135 | PHE  | CA-C-N    | 6.63  | 130.07      | 120.38   |
| 1   | C     | 135 | PHE  | C-N-CA    | 6.63  | 130.07      | 120.38   |
| 2   | D     | 582 | PHE  | CA-C-O    | -6.63 | 113.91      | 121.40   |
| 2   | D     | 621 | ASP  | CB-CA-C   | 6.63  | 120.83      | 111.74   |
| 1   | A     | 128 | LEU  | CA-C-O    | -6.63 | 114.22      | 119.66   |
| 1   | C     | 163 | LEU  | O-C-N     | 6.62  | 127.90      | 121.28   |
| 2   | F     | 552 | THR  | N-CA-CB   | 6.61  | 119.84      | 110.46   |
| 1   | A     | 85  | ARG  | NE-CZ-NH1 | 6.60  | 128.10      | 121.50   |
| 1   | C     | 169 | GLN  | CA-CB-CG  | 6.60  | 127.30      | 114.10   |
| 2   | D     | 537 | PHE  | CA-C-N    | -6.58 | 113.52      | 122.86   |
| 2   | D     | 537 | PHE  | C-N-CA    | -6.58 | 113.52      | 122.86   |
| 1   | C     | 191 | THR  | CA-CB-CG2 | 6.58  | 121.68      | 110.50   |
| 1   | A     | 96  | VAL  | N-CA-C    | -6.58 | 103.46      | 110.36   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | D     | 582 | PHE  | O-C-N     | 6.57  | 131.12      | 123.17   |
| 1   | B     | 214 | LYS  | O-C-N     | 6.57  | 129.18      | 122.09   |
| 2   | E     | 537 | PHE  | CA-C-N    | -6.55 | 113.55      | 122.86   |
| 2   | E     | 537 | PHE  | C-N-CA    | -6.55 | 113.55      | 122.86   |
| 1   | B     | 96  | VAL  | O-C-N     | 6.55  | 128.49      | 121.94   |
| 1   | C     | 84  | PHE  | CA-CB-CG  | -6.55 | 107.25      | 113.80   |
| 1   | A     | 202 | ASN  | CA-C-O    | -6.55 | 113.61      | 120.55   |
| 1   | C     | 49  | LEU  | CA-C-O    | -6.55 | 113.89      | 120.90   |
| 1   | B     | 158 | GLN  | CB-CG-CD  | 6.53  | 123.70      | 112.60   |
| 1   | A     | 158 | GLN  | CB-CG-CD  | 6.53  | 123.69      | 112.60   |
| 1   | B     | 159 | VAL  | CA-C-O    | -6.53 | 112.94      | 119.20   |
| 1   | B     | 194 | ASN  | CA-C-N    | 6.53  | 129.32      | 120.44   |
| 1   | B     | 194 | ASN  | C-N-CA    | 6.53  | 129.32      | 120.44   |
| 2   | E     | 507 | VAL  | CA-C-O    | 6.53  | 127.24      | 120.39   |
| 1   | C     | 203 | LEU  | CA-CB-CG  | 6.52  | 139.12      | 116.30   |
| 1   | B     | 230 | GLN  | O-C-N     | 6.51  | 131.10      | 122.30   |
| 1   | A     | 159 | VAL  | CA-C-O    | -6.51 | 112.95      | 119.20   |
| 1   | B     | 106 | VAL  | CA-CB-CG2 | 6.51  | 121.47      | 110.40   |
| 2   | D     | 568 | ARG  | CD-NE-CZ  | -6.50 | 115.29      | 124.40   |
| 1   | C     | 217 | ASN  | N-CA-C    | 6.49  | 124.15      | 109.81   |
| 2   | F     | 568 | ARG  | CD-NE-CZ  | -6.49 | 115.31      | 124.40   |
| 2   | D     | 605 | CYS  | O-C-N     | 6.48  | 126.68      | 121.17   |
| 1   | A     | 111 | TYR  | CA-C-O    | 6.48  | 127.49      | 120.43   |
| 1   | C     | 211 | ILE  | N-CA-CB   | -6.47 | 100.55      | 111.23   |
| 1   | A     | 191 | THR  | N-CA-C    | -6.46 | 102.20      | 110.53   |
| 2   | D     | 597 | TRP  | O-C-N     | 6.45  | 129.00      | 122.03   |
| 2   | E     | 582 | PHE  | O-C-N     | 6.45  | 130.97      | 123.17   |
| 2   | F     | 677 | LEU  | CB-CA-C   | 6.45  | 122.35      | 110.10   |
| 1   | A     | 194 | ASN  | CA-C-N    | 6.44  | 129.20      | 120.44   |
| 1   | A     | 194 | ASN  | C-N-CA    | 6.44  | 129.20      | 120.44   |
| 2   | D     | 552 | THR  | N-CA-CB   | 6.44  | 119.60      | 110.46   |
| 1   | A     | 54  | GLU  | N-CA-C    | -6.44 | 103.77      | 111.69   |
| 2   | D     | 563 | ASP  | CA-C-O    | 6.43  | 127.37      | 120.55   |
| 2   | E     | 542 | VAL  | N-CA-CB   | -6.42 | 104.38      | 112.15   |
| 2   | D     | 595 | GLU  | CG-CD-OE1 | 6.41  | 133.14      | 118.40   |
| 1   | A     | 211 | ILE  | N-CA-CB   | -6.40 | 100.67      | 111.23   |
| 2   | E     | 580 | VAL  | N-CA-CB   | 6.40  | 118.69      | 111.21   |
| 2   | F     | 542 | VAL  | N-CA-CB   | -6.40 | 104.41      | 112.15   |
| 2   | D     | 538 | ASP  | CA-CB-CG  | 6.38  | 118.98      | 112.60   |
| 2   | D     | 509 | VAL  | O-C-N     | 6.37  | 130.01      | 123.00   |
| 1   | B     | 203 | LEU  | CA-CB-CG  | 6.37  | 138.59      | 116.30   |
| 1   | A     | 146 | ASN  | O-C-N     | 6.37  | 128.85      | 122.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 194 | ASN  | N-CA-C    | 6.37  | 119.03      | 111.33   |
| 1   | A     | 146 | ASN  | CA-CB-CG  | 6.36  | 118.96      | 112.60   |
| 2   | D     | 597 | TRP  | CA-CB-CG  | -6.36 | 101.52      | 113.60   |
| 2   | D     | 625 | THR  | N-CA-C    | -6.36 | 104.27      | 111.07   |
| 1   | C     | 128 | LEU  | O-C-N     | 6.36  | 128.41      | 121.36   |
| 2   | F     | 509 | VAL  | O-C-N     | 6.34  | 129.98      | 123.00   |
| 1   | A     | 38  | PRO  | CA-C-N    | 6.34  | 127.77      | 119.84   |
| 1   | A     | 38  | PRO  | C-N-CA    | 6.34  | 127.77      | 119.84   |
| 1   | A     | 203 | LEU  | CA-CB-CG  | 6.34  | 138.49      | 116.30   |
| 1   | C     | 194 | ASN  | N-CA-C    | 6.34  | 119.00      | 111.33   |
| 2   | D     | 580 | VAL  | N-CA-CB   | 6.34  | 119.33      | 111.41   |
| 2   | F     | 537 | PHE  | CA-C-N    | -6.32 | 113.88      | 122.86   |
| 2   | F     | 537 | PHE  | C-N-CA    | -6.32 | 113.88      | 122.86   |
| 1   | C     | 109 | ASP  | N-CA-CB   | -6.30 | 101.38      | 110.65   |
| 2   | E     | 655 | VAL  | O-C-N     | -6.30 | 116.36      | 123.10   |
| 2   | F     | 618 | ASP  | O-C-N     | 6.29  | 128.64      | 122.09   |
| 2   | E     | 516 | LYS  | CA-C-N    | 6.29  | 128.96      | 120.65   |
| 2   | E     | 516 | LYS  | C-N-CA    | 6.29  | 128.96      | 120.65   |
| 1   | B     | 202 | ASN  | CA-C-O    | -6.29 | 113.88      | 120.55   |
| 2   | F     | 582 | PHE  | CA-C-O    | -6.29 | 114.30      | 121.40   |
| 2   | D     | 592 | ASN  | CA-CB-CG  | -6.28 | 106.32      | 112.60   |
| 1   | C     | 178 | LEU  | N-CA-C    | 6.28  | 119.11      | 111.82   |
| 1   | B     | 191 | THR  | N-CA-C    | -6.28 | 102.43      | 110.53   |
| 1   | A     | 149 | GLU  | CG-CD-OE2 | 6.27  | 132.83      | 118.40   |
| 2   | D     | 629 | LEU  | CB-CA-C   | 6.27  | 119.55      | 109.02   |
| 1   | B     | 217 | ASN  | N-CA-C    | 6.27  | 123.66      | 109.81   |
| 2   | E     | 552 | THR  | N-CA-CB   | 6.27  | 119.36      | 110.46   |
| 2   | F     | 557 | ASP  | CA-CB-CG  | 6.25  | 118.85      | 112.60   |
| 2   | F     | 579 | LEU  | CA-CB-CG  | 6.25  | 138.18      | 116.30   |
| 1   | B     | 220 | ASN  | CA-C-N    | 6.25  | 128.65      | 120.28   |
| 1   | B     | 220 | ASN  | C-N-CA    | 6.25  | 128.65      | 120.28   |
| 2   | E     | 618 | ASP  | O-C-N     | 6.25  | 128.59      | 122.09   |
| 2   | E     | 625 | THR  | N-CA-C    | -6.24 | 104.39      | 111.07   |
| 2   | D     | 655 | VAL  | O-C-N     | -6.24 | 116.42      | 123.10   |
| 1   | A     | 169 | GLN  | CA-CB-CG  | 6.24  | 126.58      | 114.10   |
| 1   | B     | 80  | THR  | CA-C-O    | 6.24  | 128.16      | 121.05   |
| 2   | D     | 656 | GLU  | CA-CB-CG  | 6.21  | 126.53      | 114.10   |
| 1   | B     | 163 | LEU  | O-C-N     | 6.21  | 127.50      | 121.28   |
| 1   | B     | 38  | PRO  | CA-C-N    | 6.21  | 127.61      | 119.84   |
| 1   | B     | 38  | PRO  | C-N-CA    | 6.21  | 127.61      | 119.84   |
| 1   | A     | 127 | GLU  | N-CA-C    | 6.21  | 119.80      | 112.72   |
| 1   | B     | 169 | GLN  | CA-CB-CG  | 6.20  | 126.51      | 114.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | F     | 576 | ASP  | CA-C-O    | -6.20 | 112.63      | 119.95   |
| 2   | D     | 579 | LEU  | CA-CB-CG  | 6.18  | 137.94      | 116.30   |
| 2   | F     | 534 | PRO  | O-C-N     | -6.18 | 115.46      | 123.00   |
| 1   | C     | 65  | VAL  | O-C-N     | 6.17  | 128.11      | 121.87   |
| 2   | F     | 608 | THR  | CA-CB-OG1 | -6.17 | 100.34      | 109.60   |
| 2   | F     | 547 | GLY  | CA-C-N    | 6.17  | 133.50      | 121.41   |
| 2   | F     | 547 | GLY  | C-N-CA    | 6.17  | 133.50      | 121.41   |
| 2   | F     | 667 | ASN  | CA-C-O    | -6.17 | 114.01      | 120.55   |
| 1   | B     | 149 | GLU  | CG-CD-OE2 | 6.16  | 132.58      | 118.40   |
| 1   | A     | 123 | THR  | CB-CA-C   | 6.16  | 120.72      | 110.92   |
| 1   | A     | 135 | PHE  | CA-C-N    | 6.16  | 129.37      | 120.38   |
| 1   | A     | 135 | PHE  | C-N-CA    | 6.16  | 129.37      | 120.38   |
| 2   | F     | 656 | GLU  | CA-CB-CG  | 6.16  | 126.41      | 114.10   |
| 2   | D     | 599 | PRO  | CA-C-N    | 6.15  | 130.53      | 120.63   |
| 2   | D     | 599 | PRO  | C-N-CA    | 6.15  | 130.53      | 120.63   |
| 2   | E     | 563 | ASP  | CA-C-O    | 6.15  | 127.07      | 120.55   |
| 1   | A     | 194 | ASN  | N-CA-C    | 6.14  | 118.76      | 111.33   |
| 1   | A     | 39  | PRO  | N-CA-C    | 6.14  | 125.11      | 112.47   |
| 1   | A     | 214 | LYS  | O-C-N     | 6.14  | 128.72      | 122.09   |
| 2   | E     | 677 | LEU  | CB-CA-C   | 6.14  | 121.76      | 110.10   |
| 1   | C     | 227 | LEU  | CB-CA-C   | 6.14  | 121.93      | 110.70   |
| 1   | A     | 109 | ASP  | N-CA-CB   | -6.13 | 101.63      | 110.65   |
| 1   | C     | 152 | ARG  | CG-CD-NE  | 6.13  | 125.50      | 112.00   |
| 2   | F     | 595 | GLU  | CG-CD-OE1 | 6.13  | 132.50      | 118.40   |
| 2   | D     | 504 | ILE  | O-C-N     | 6.13  | 130.23      | 122.57   |
| 2   | E     | 656 | GLU  | CA-CB-CG  | 6.12  | 126.34      | 114.10   |
| 2   | E     | 669 | PHE  | CA-C-N    | 6.12  | 128.80      | 120.54   |
| 2   | E     | 669 | PHE  | C-N-CA    | 6.12  | 128.80      | 120.54   |
| 1   | B     | 90  | THR  | O-C-N     | 6.11  | 129.37      | 122.22   |
| 2   | E     | 595 | GLU  | CG-CD-OE1 | 6.11  | 132.44      | 118.40   |
| 1   | C     | 67  | ARG  | NE-CZ-NH1 | 6.11  | 127.61      | 121.50   |
| 1   | B     | 39  | PRO  | N-CA-C    | 6.10  | 125.04      | 112.47   |
| 2   | F     | 504 | ILE  | O-C-N     | 6.10  | 130.20      | 122.57   |
| 1   | A     | 178 | LEU  | N-CA-C    | 6.10  | 118.89      | 111.82   |
| 1   | C     | 38  | PRO  | CA-C-N    | 6.09  | 127.45      | 119.84   |
| 1   | C     | 38  | PRO  | C-N-CA    | 6.09  | 127.45      | 119.84   |
| 1   | B     | 143 | GLY  | CA-C-N    | 6.09  | 128.72      | 120.38   |
| 1   | B     | 143 | GLY  | C-N-CA    | 6.09  | 128.72      | 120.38   |
| 2   | D     | 608 | THR  | CA-CB-OG1 | -6.07 | 100.49      | 109.60   |
| 2   | E     | 534 | PRO  | O-C-N     | -6.07 | 115.56      | 122.91   |
| 1   | A     | 121 | LEU  | O-C-N     | 6.07  | 128.34      | 122.03   |
| 2   | E     | 538 | ASP  | CA-CB-CG  | 6.06  | 118.66      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 86  | ARG  | CA-C-N     | -6.06 | 112.93      | 121.72   |
| 1   | C     | 86  | ARG  | C-N-CA     | -6.06 | 112.93      | 121.72   |
| 1   | B     | 173 | PHE  | CA-C-O     | -6.06 | 114.40      | 121.07   |
| 2   | F     | 597 | TRP  | CA-CB-CG   | -6.06 | 102.09      | 113.60   |
| 1   | C     | 63  | PRO  | CA-C-N     | 6.06  | 130.23      | 120.30   |
| 1   | C     | 63  | PRO  | C-N-CA     | 6.06  | 130.23      | 120.30   |
| 1   | A     | 182 | SER  | CA-C-N     | 6.05  | 130.29      | 120.60   |
| 1   | A     | 182 | SER  | C-N-CA     | 6.05  | 130.29      | 120.60   |
| 1   | A     | 161 | GLN  | OE1-CD-NE2 | -6.05 | 116.55      | 122.60   |
| 2   | F     | 654 | TYR  | O-C-N      | 6.05  | 130.11      | 123.27   |
| 2   | E     | 591 | GLU  | CB-CG-CD   | 6.04  | 122.87      | 112.60   |
| 1   | C     | 230 | GLN  | O-C-N      | 6.04  | 130.45      | 122.30   |
| 1   | A     | 143 | GLY  | CA-C-N     | 6.02  | 128.63      | 120.38   |
| 1   | A     | 143 | GLY  | C-N-CA     | 6.02  | 128.63      | 120.38   |
| 2   | E     | 518 | CYS  | CA-C-O     | -6.02 | 114.50      | 120.82   |
| 1   | C     | 149 | GLU  | CB-CG-CD   | 6.02  | 122.83      | 112.60   |
| 2   | E     | 658 | SER  | CA-C-O     | -6.01 | 114.20      | 120.70   |
| 1   | C     | 106 | VAL  | CA-CB-CG2  | 6.01  | 120.62      | 110.40   |
| 1   | C     | 159 | VAL  | CA-C-O     | -6.01 | 113.43      | 119.20   |
| 1   | B     | 43  | GLN  | CB-CG-CD   | 6.01  | 122.81      | 112.60   |
| 1   | A     | 86  | ARG  | CA-C-N     | -6.01 | 113.01      | 121.72   |
| 1   | A     | 86  | ARG  | C-N-CA     | -6.01 | 113.01      | 121.72   |
| 2   | F     | 597 | TRP  | CA-C-O     | -5.99 | 114.73      | 120.90   |
| 1   | B     | 211 | ILE  | N-CA-CB    | -5.99 | 101.34      | 111.23   |
| 2   | D     | 535 | THR  | O-C-N      | 5.99  | 130.02      | 122.65   |
| 1   | C     | 44  | GLN  | O-C-N      | 5.99  | 130.56      | 122.59   |
| 1   | B     | 174 | LEU  | O-C-N      | 5.99  | 129.22      | 122.22   |
| 2   | F     | 655 | VAL  | O-C-N      | -5.98 | 116.70      | 123.10   |
| 1   | A     | 44  | GLN  | OE1-CD-NE2 | 5.97  | 128.57      | 122.60   |
| 1   | B     | 44  | GLN  | O-C-N      | 5.97  | 130.53      | 122.59   |
| 2   | E     | 597 | TRP  | CA-CB-CG   | -5.97 | 102.26      | 113.60   |
| 1   | C     | 90  | THR  | O-C-N      | 5.96  | 129.20      | 122.22   |
| 1   | C     | 192 | ASN  | CB-CA-C    | 5.96  | 120.69      | 110.79   |
| 2   | F     | 636 | PRO  | CA-C-O     | -5.96 | 114.23      | 121.03   |
| 1   | B     | 63  | PRO  | CA-C-N     | 5.96  | 130.07      | 120.30   |
| 1   | B     | 63  | PRO  | C-N-CA     | 5.96  | 130.07      | 120.30   |
| 1   | B     | 135 | PHE  | CA-C-N     | 5.95  | 130.21      | 120.63   |
| 1   | B     | 135 | PHE  | C-N-CA     | 5.95  | 130.21      | 120.63   |
| 1   | B     | 63  | PRO  | CB-CA-C    | 5.95  | 119.55      | 110.75   |
| 1   | C     | 182 | SER  | CA-C-N     | 5.95  | 130.12      | 120.60   |
| 1   | C     | 182 | SER  | C-N-CA     | 5.95  | 130.12      | 120.60   |
| 1   | A     | 63  | PRO  | CB-CA-C    | 5.95  | 119.55      | 110.75   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 219 | ILE  | CB-CA-C   | 5.94  | 120.02      | 111.65   |
| 2   | D     | 677 | LEU  | CB-CA-C   | 5.93  | 121.38      | 110.10   |
| 1   | C     | 120 | ILE  | O-C-N     | -5.92 | 116.13      | 121.87   |
| 1   | B     | 149 | GLU  | CB-CG-CD  | 5.92  | 122.66      | 112.60   |
| 1   | C     | 60  | GLU  | CB-CA-C   | -5.91 | 103.11      | 109.85   |
| 2   | E     | 568 | ARG  | CD-NE-CZ  | -5.91 | 116.13      | 124.40   |
| 2   | E     | 579 | LEU  | CA-CB-CG  | 5.91  | 136.98      | 116.30   |
| 1   | A     | 220 | ASN  | CA-C-N    | 5.90  | 128.19      | 120.28   |
| 1   | A     | 220 | ASN  | C-N-CA    | 5.90  | 128.19      | 120.28   |
| 1   | C     | 68  | GLU  | CA-C-N    | -5.89 | 112.38      | 120.28   |
| 1   | C     | 68  | GLU  | C-N-CA    | -5.89 | 112.38      | 120.28   |
| 1   | B     | 146 | ASN  | CA-CB-CG  | 5.89  | 118.49      | 112.60   |
| 2   | F     | 629 | LEU  | CB-CA-C   | 5.88  | 118.91      | 109.02   |
| 1   | B     | 70  | VAL  | CA-C-O    | -5.88 | 114.36      | 121.18   |
| 2   | F     | 511 | ASP  | N-CA-C    | 5.87  | 118.87      | 110.24   |
| 1   | C     | 39  | PRO  | N-CA-C    | 5.87  | 124.56      | 112.47   |
| 2   | F     | 631 | LYS  | N-CA-C    | -5.86 | 104.83      | 113.61   |
| 1   | B     | 182 | SER  | CA-C-N    | 5.84  | 129.95      | 120.60   |
| 1   | B     | 182 | SER  | C-N-CA    | 5.84  | 129.95      | 120.60   |
| 1   | A     | 60  | GLU  | CB-CA-C   | -5.84 | 103.19      | 109.85   |
| 2   | E     | 578 | PHE  | CA-C-N    | 5.84  | 131.36      | 122.95   |
| 2   | E     | 578 | PHE  | C-N-CA    | 5.84  | 131.36      | 122.95   |
| 2   | E     | 613 | VAL  | N-CA-C    | 5.84  | 116.01      | 106.72   |
| 1   | A     | 126 | ARG  | CB-CG-CD  | 5.83  | 124.72      | 111.30   |
| 2   | E     | 562 | GLU  | CA-CB-CG  | 5.83  | 125.77      | 114.10   |
| 1   | B     | 166 | GLU  | CA-C-O    | 5.83  | 128.85      | 120.51   |
| 1   | A     | 43  | GLN  | CB-CG-CD  | 5.83  | 122.51      | 112.60   |
| 2   | D     | 516 | LYS  | CA-C-N    | 5.82  | 128.33      | 120.65   |
| 2   | D     | 516 | LYS  | C-N-CA    | 5.82  | 128.33      | 120.65   |
| 2   | E     | 558 | THR  | CA-C-O    | 5.81  | 128.23      | 121.49   |
| 1   | A     | 211 | ILE  | CA-C-O    | -5.80 | 113.53      | 120.78   |
| 1   | B     | 144 | PHE  | CA-C-O    | -5.80 | 114.36      | 120.63   |
| 2   | E     | 568 | ARG  | N-CA-C    | 5.80  | 122.63      | 109.81   |
| 1   | B     | 227 | LEU  | CB-CA-C   | 5.80  | 122.21      | 110.38   |
| 2   | E     | 636 | PRO  | CA-C-O    | -5.80 | 114.42      | 121.03   |
| 1   | C     | 84  | PHE  | N-CA-CB   | -5.79 | 100.70      | 110.49   |
| 2   | E     | 664 | GLY  | O-C-N     | 5.78  | 128.21      | 122.77   |
| 1   | A     | 192 | ASN  | CB-CA-C   | 5.75  | 120.34      | 110.79   |
| 2   | D     | 562 | GLU  | CG-CD-OE1 | 5.75  | 131.64      | 118.40   |
| 2   | E     | 672 | ALA  | N-CA-C    | -5.75 | 106.31      | 113.38   |
| 1   | C     | 211 | ILE  | CA-C-O    | -5.75 | 113.60      | 120.78   |
| 2   | E     | 599 | PRO  | CA-C-N    | 5.74  | 129.87      | 120.63   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | E     | 599 | PRO  | C-N-CA    | 5.74  | 129.87      | 120.63   |
| 1   | C     | 174 | LEU  | O-C-N     | 5.73  | 128.92      | 122.22   |
| 1   | A     | 90  | THR  | O-C-N     | 5.73  | 128.92      | 122.22   |
| 1   | A     | 152 | ARG  | NE-CZ-NH2 | 5.73  | 124.35      | 119.20   |
| 1   | B     | 176 | ALA  | CA-C-O    | -5.73 | 114.81      | 120.82   |
| 1   | B     | 59  | GLN  | CA-C-N    | 5.72  | 130.75      | 121.83   |
| 1   | B     | 59  | GLN  | C-N-CA    | 5.72  | 130.75      | 121.83   |
| 1   | C     | 199 | PHE  | O-C-N     | 5.71  | 130.02      | 122.36   |
| 2   | D     | 558 | THR  | CA-C-O    | 5.71  | 127.74      | 121.40   |
| 2   | E     | 511 | ASP  | N-CA-C    | 5.71  | 118.64      | 110.24   |
| 1   | A     | 199 | PHE  | O-C-N     | 5.71  | 130.01      | 122.36   |
| 2   | E     | 547 | GLY  | CA-C-N    | 5.71  | 132.60      | 121.41   |
| 2   | E     | 547 | GLY  | C-N-CA    | 5.71  | 132.60      | 121.41   |
| 1   | B     | 84  | PHE  | N-CA-CB   | -5.70 | 100.85      | 110.49   |
| 1   | C     | 121 | LEU  | O-C-N     | 5.70  | 127.96      | 122.03   |
| 1   | C     | 83  | ILE  | N-CA-CB   | 5.70  | 120.64      | 111.23   |
| 1   | C     | 87  | SER  | CA-C-N    | 5.70  | 128.96      | 120.87   |
| 1   | C     | 87  | SER  | C-N-CA    | 5.70  | 128.96      | 120.87   |
| 2   | F     | 652 | VAL  | N-CA-C    | -5.70 | 104.95      | 110.42   |
| 2   | D     | 618 | ASP  | O-C-N     | 5.70  | 128.01      | 122.09   |
| 2   | D     | 648 | ASP  | CA-CB-CG  | 5.70  | 118.30      | 112.60   |
| 2   | D     | 576 | ASP  | CA-C-O    | -5.69 | 113.23      | 119.95   |
| 1   | C     | 176 | ALA  | CA-C-O    | -5.69 | 114.84      | 120.82   |
| 1   | C     | 70  | VAL  | CA-C-O    | -5.69 | 114.58      | 121.18   |
| 2   | E     | 645 | LEU  | O-C-N     | 5.69  | 128.65      | 122.11   |
| 1   | C     | 152 | ARG  | NE-CZ-NH2 | 5.69  | 124.32      | 119.20   |
| 2   | E     | 504 | ILE  | O-C-N     | 5.68  | 129.67      | 122.57   |
| 2   | F     | 597 | TRP  | O-C-N     | 5.68  | 128.17      | 122.03   |
| 2   | D     | 591 | GLU  | CB-CG-CD  | 5.68  | 122.25      | 112.60   |
| 1   | C     | 56  | ASN  | O-C-N     | 5.68  | 128.09      | 121.10   |
| 2   | D     | 638 | THR  | CA-CB-OG1 | -5.68 | 101.08      | 109.60   |
| 1   | A     | 68  | GLU  | N-CA-C    | -5.67 | 106.03      | 113.12   |
| 2   | E     | 523 | TYR  | N-CA-C    | 5.67  | 117.14      | 111.07   |
| 2   | E     | 579 | LEU  | CA-C-O    | -5.67 | 112.64      | 120.52   |
| 2   | D     | 636 | PRO  | CA-C-O    | -5.67 | 114.57      | 121.03   |
| 1   | A     | 149 | GLU  | CB-CG-CD  | 5.66  | 122.23      | 112.60   |
| 2   | D     | 511 | ASP  | N-CA-C    | 5.66  | 118.56      | 110.24   |
| 2   | D     | 652 | VAL  | N-CA-C    | -5.66 | 104.99      | 110.42   |
| 1   | B     | 202 | ASN  | CB-CG-ND2 | 5.66  | 124.89      | 116.40   |
| 1   | A     | 127 | GLU  | CB-CG-CD  | 5.66  | 122.22      | 112.60   |
| 2   | D     | 538 | ASP  | CA-C-O    | 5.65  | 126.43      | 120.33   |
| 2   | E     | 605 | CYS  | O-C-N     | 5.64  | 126.45      | 121.37   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | E     | 597 | TRP  | O-C-N     | 5.64  | 128.12      | 122.03   |
| 1   | B     | 69  | THR  | CA-C-O    | 5.63  | 126.52      | 120.55   |
| 2   | E     | 602 | THR  | N-CA-C    | -5.63 | 106.54      | 113.41   |
| 1   | B     | 123 | THR  | CB-CA-C   | 5.63  | 119.87      | 110.92   |
| 1   | B     | 162 | THR  | CA-CB-OG1 | -5.63 | 101.16      | 109.60   |
| 2   | E     | 629 | LEU  | CB-CA-C   | 5.62  | 118.46      | 109.02   |
| 2   | E     | 631 | LYS  | N-CA-C    | -5.62 | 105.18      | 113.61   |
| 1   | A     | 44  | GLN  | O-C-N     | 5.62  | 130.06      | 122.59   |
| 1   | B     | 202 | ASN  | CB-CG-OD1 | -5.62 | 109.57      | 120.80   |
| 1   | C     | 126 | ARG  | N-CA-CB   | 5.62  | 119.71      | 110.39   |
| 1   | C     | 220 | ASN  | CA-C-N    | 5.61  | 127.80      | 120.28   |
| 1   | C     | 220 | ASN  | C-N-CA    | 5.61  | 127.80      | 120.28   |
| 1   | C     | 173 | PHE  | CA-C-O    | -5.61 | 114.90      | 121.07   |
| 1   | B     | 68  | GLU  | CA-C-N    | -5.61 | 112.77      | 120.28   |
| 1   | B     | 68  | GLU  | C-N-CA    | -5.61 | 112.77      | 120.28   |
| 2   | D     | 631 | LYS  | N-CA-C    | -5.60 | 105.21      | 113.61   |
| 2   | D     | 667 | ASN  | N-CA-C    | 5.60  | 117.39      | 111.28   |
| 2   | E     | 666 | LYS  | CG-CD-CE  | 5.60  | 124.17      | 111.30   |
| 1   | C     | 131 | PRO  | CA-C-N    | 5.60  | 128.57      | 120.79   |
| 1   | C     | 131 | PRO  | C-N-CA    | 5.60  | 128.57      | 120.79   |
| 2   | D     | 669 | PHE  | CA-C-N    | 5.59  | 128.56      | 120.79   |
| 2   | D     | 669 | PHE  | C-N-CA    | 5.59  | 128.56      | 120.79   |
| 1   | B     | 192 | ASN  | CB-CA-C   | 5.59  | 120.07      | 110.79   |
| 1   | C     | 43  | GLN  | CB-CG-CD  | 5.59  | 122.10      | 112.60   |
| 2   | D     | 587 | PRO  | N-CA-C    | 5.59  | 120.91      | 114.03   |
| 2   | F     | 638 | THR  | CA-CB-OG1 | -5.59 | 101.22      | 109.60   |
| 1   | B     | 221 | THR  | N-CA-CB   | 5.58  | 118.33      | 110.12   |
| 1   | B     | 191 | THR  | CA-CB-CG2 | 5.58  | 119.98      | 110.50   |
| 2   | F     | 663 | ARG  | N-CA-CB   | 5.57  | 118.84      | 109.94   |
| 2   | F     | 663 | ARG  | CD-NE-CZ  | 5.56  | 132.19      | 124.40   |
| 2   | D     | 645 | LEU  | O-C-N     | 5.56  | 128.50      | 122.11   |
| 2   | E     | 536 | VAL  | CA-CB-CG1 | -5.56 | 100.95      | 110.40   |
| 2   | D     | 654 | TYR  | O-C-N     | 5.56  | 129.55      | 123.27   |
| 2   | D     | 663 | ARG  | N-CA-CB   | 5.56  | 118.83      | 109.94   |
| 1   | B     | 60  | GLU  | CB-CA-C   | -5.56 | 103.52      | 109.85   |
| 2   | D     | 547 | GLY  | CA-C-N    | 5.55  | 132.29      | 121.41   |
| 2   | D     | 547 | GLY  | C-N-CA    | 5.55  | 132.29      | 121.41   |
| 2   | D     | 568 | ARG  | N-CA-C    | 5.55  | 122.07      | 109.81   |
| 1   | B     | 83  | ILE  | N-CA-CB   | 5.54  | 120.38      | 111.23   |
| 1   | C     | 69  | THR  | N-CA-CB   | 5.54  | 118.27      | 110.12   |
| 1   | A     | 210 | ALA  | CA-C-N    | 5.54  | 131.94      | 121.97   |
| 1   | A     | 210 | ALA  | C-N-CA    | 5.54  | 131.94      | 121.97   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 62  | ILE  | N-CA-C     | 5.54  | 112.60      | 107.56   |
| 1   | B     | 169 | GLN  | OE1-CD-NE2 | -5.54 | 117.06      | 122.60   |
| 2   | F     | 605 | CYS  | O-C-N      | 5.53  | 126.35      | 121.37   |
| 2   | F     | 568 | ARG  | N-CA-C     | 5.53  | 122.03      | 109.81   |
| 2   | F     | 562 | GLU  | CG-CD-OE1  | 5.53  | 131.11      | 118.40   |
| 2   | E     | 509 | VAL  | O-C-N      | 5.52  | 129.07      | 123.00   |
| 1   | C     | 135 | PHE  | CB-CA-C    | 5.52  | 119.95      | 110.79   |
| 2   | D     | 536 | VAL  | CA-CB-CG1  | -5.51 | 101.02      | 110.40   |
| 1   | C     | 202 | ASN  | CB-CG-OD1  | -5.51 | 109.77      | 120.80   |
| 1   | B     | 169 | GLN  | N-CA-C     | -5.51 | 105.35      | 111.36   |
| 2   | D     | 538 | ASP  | CB-CA-C    | 5.51  | 118.94      | 110.62   |
| 2   | F     | 591 | GLU  | CB-CG-CD   | 5.51  | 121.97      | 112.60   |
| 1   | C     | 50  | GLN  | CA-C-N     | 5.50  | 127.92      | 120.44   |
| 1   | C     | 50  | GLN  | C-N-CA     | 5.50  | 127.92      | 120.44   |
| 2   | D     | 573 | PRO  | CA-C-N     | 5.49  | 130.37      | 122.40   |
| 2   | D     | 573 | PRO  | C-N-CA     | 5.49  | 130.37      | 122.40   |
| 2   | E     | 663 | ARG  | N-CA-CB    | 5.49  | 118.72      | 109.94   |
| 1   | B     | 68  | GLU  | O-C-N      | 5.48  | 130.21      | 122.20   |
| 1   | A     | 202 | ASN  | CB-CG-OD1  | -5.48 | 109.84      | 120.80   |
| 1   | A     | 84  | PHE  | N-CA-CB    | -5.48 | 101.23      | 110.49   |
| 2   | D     | 658 | SER  | CA-C-O     | -5.48 | 114.78      | 120.70   |
| 1   | C     | 146 | ASN  | O-C-N      | 5.47  | 127.90      | 122.10   |
| 2   | D     | 656 | GLU  | CG-CD-OE2  | -5.47 | 105.83      | 118.40   |
| 1   | B     | 194 | ASN  | CA-CB-CG   | -5.46 | 107.14      | 112.60   |
| 1   | C     | 143 | GLY  | CA-C-N     | 5.46  | 127.86      | 120.38   |
| 1   | C     | 143 | GLY  | C-N-CA     | 5.46  | 127.86      | 120.38   |
| 1   | B     | 152 | ARG  | CG-CD-NE   | 5.46  | 124.02      | 112.00   |
| 1   | A     | 83  | ILE  | N-CA-CB    | 5.46  | 120.24      | 111.23   |
| 1   | A     | 59  | GLN  | CA-C-N     | 5.46  | 130.34      | 121.83   |
| 1   | A     | 59  | GLN  | C-N-CA     | 5.46  | 130.34      | 121.83   |
| 1   | A     | 216 | ILE  | CA-C-N     | 5.46  | 135.12      | 121.80   |
| 1   | A     | 216 | ILE  | C-N-CA     | 5.46  | 135.12      | 121.80   |
| 1   | C     | 68  | GLU  | O-C-N      | 5.46  | 130.17      | 122.20   |
| 1   | C     | 198 | VAL  | CA-C-O     | 5.46  | 123.70      | 118.90   |
| 2   | E     | 573 | PRO  | CA-C-N     | 5.45  | 130.30      | 122.40   |
| 2   | E     | 573 | PRO  | C-N-CA     | 5.45  | 130.30      | 122.40   |
| 2   | E     | 651 | ALA  | CA-C-O     | -5.45 | 115.56      | 121.44   |
| 1   | A     | 63  | PRO  | CA-C-N     | 5.44  | 129.23      | 120.30   |
| 1   | A     | 63  | PRO  | C-N-CA     | 5.44  | 129.23      | 120.30   |
| 1   | B     | 69  | THR  | N-CA-CB    | 5.44  | 118.11      | 110.12   |
| 1   | B     | 216 | ILE  | CA-C-N     | 5.43  | 135.06      | 121.80   |
| 1   | B     | 216 | ILE  | C-N-CA     | 5.43  | 135.06      | 121.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | E     | 562 | GLU  | CG-CD-OE1  | 5.43  | 130.90      | 118.40   |
| 2   | D     | 561 | GLN  | CA-CB-CG   | -5.43 | 103.24      | 114.10   |
| 1   | B     | 186 | ASP  | CA-CB-CG   | -5.43 | 107.17      | 112.60   |
| 1   | C     | 70  | VAL  | CB-CA-C    | 5.42  | 118.86      | 111.87   |
| 2   | E     | 669 | PHE  | N-CA-CB    | -5.41 | 102.13      | 110.20   |
| 1   | B     | 160 | LEU  | CA-C-N     | 5.41  | 127.97      | 120.29   |
| 1   | B     | 160 | LEU  | C-N-CA     | 5.41  | 127.97      | 120.29   |
| 1   | B     | 234 | PHE  | CA-C-O     | -5.40 | 111.62      | 120.80   |
| 1   | A     | 208 | ASP  | CB-CA-C    | 5.40  | 121.16      | 110.42   |
| 1   | A     | 135 | PHE  | CB-CA-C    | 5.39  | 119.74      | 110.79   |
| 2   | E     | 580 | VAL  | CA-C-O     | -5.39 | 114.71      | 120.59   |
| 2   | F     | 625 | THR  | O-C-N      | 5.39  | 127.62      | 122.07   |
| 2   | F     | 592 | ASN  | CA-CB-CG   | -5.39 | 107.21      | 112.60   |
| 2   | D     | 519 | LEU  | CA-C-O     | -5.38 | 113.78      | 119.97   |
| 1   | A     | 169 | GLN  | N-CA-C     | -5.38 | 105.50      | 111.36   |
| 2   | D     | 579 | LEU  | CA-C-O     | -5.37 | 113.05      | 120.52   |
| 2   | F     | 587 | PRO  | N-CA-C     | 5.37  | 120.64      | 114.03   |
| 2   | D     | 644 | LYS  | CA-C-O     | 5.37  | 128.19      | 120.51   |
| 2   | D     | 511 | ASP  | CA-C-O     | -5.37 | 115.11      | 120.96   |
| 2   | F     | 543 | THR  | CA-C-O     | 5.37  | 127.40      | 121.39   |
| 2   | D     | 669 | PHE  | N-CA-CB    | -5.37 | 102.20      | 110.20   |
| 2   | D     | 534 | PRO  | O-C-N      | -5.36 | 116.46      | 123.06   |
| 2   | D     | 615 | THR  | CA-CB-OG1  | -5.36 | 101.56      | 109.60   |
| 1   | C     | 59  | GLN  | CA-C-N     | 5.36  | 130.19      | 121.83   |
| 1   | C     | 59  | GLN  | C-N-CA     | 5.36  | 130.19      | 121.83   |
| 1   | C     | 68  | GLU  | N-CA-C     | -5.36 | 106.43      | 113.12   |
| 1   | B     | 184 | HIS  | O-C-N      | 5.35  | 129.17      | 121.95   |
| 1   | A     | 120 | ILE  | CB-CG1-CD1 | 5.35  | 125.03      | 113.80   |
| 1   | C     | 149 | GLU  | CG-CD-OE2  | 5.35  | 130.70      | 118.40   |
| 1   | A     | 152 | ARG  | CG-CD-NE   | 5.34  | 123.76      | 112.00   |
| 2   | E     | 603 | HIS  | N-CA-C     | -5.34 | 106.71      | 113.18   |
| 2   | F     | 602 | THR  | N-CA-C     | -5.34 | 106.89      | 113.41   |
| 1   | B     | 68  | GLU  | N-CA-C     | -5.34 | 106.44      | 113.12   |
| 2   | E     | 576 | ASP  | CA-CB-CG   | 5.34  | 117.94      | 112.60   |
| 1   | B     | 98  | GLN  | CA-CB-CG   | 5.34  | 124.78      | 114.10   |
| 2   | E     | 654 | TYR  | CA-C-O     | -5.34 | 114.61      | 120.43   |
| 1   | C     | 54  | GLU  | N-CA-CB    | 5.34  | 118.15      | 110.20   |
| 2   | D     | 535 | THR  | N-CA-CB    | -5.33 | 102.81      | 110.44   |
| 1   | A     | 148 | ASP  | O-C-N      | 5.33  | 129.68      | 122.59   |
| 1   | A     | 176 | ALA  | CA-C-O     | -5.33 | 115.22      | 120.82   |
| 2   | D     | 522 | SER  | CA-C-O     | -5.33 | 115.20      | 120.90   |
| 2   | D     | 549 | GLU  | CA-C-O     | 5.33  | 127.09      | 120.54   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 227 | LEU  | CB-CA-C    | 5.32  | 121.24      | 110.38   |
| 2   | F     | 666 | LYS  | CG-CD-CE   | 5.32  | 123.54      | 111.30   |
| 1   | B     | 178 | LEU  | N-CA-C     | 5.32  | 117.99      | 111.82   |
| 2   | E     | 543 | THR  | CA-C-O     | 5.32  | 127.35      | 121.39   |
| 1   | C     | 72  | TYR  | CA-CB-CG   | -5.32 | 104.33      | 113.90   |
| 2   | F     | 604 | HIS  | CA-CB-CG   | -5.32 | 108.48      | 113.80   |
| 2   | E     | 587 | PRO  | N-CA-C     | 5.31  | 120.57      | 114.03   |
| 2   | E     | 667 | ASN  | N-CA-C     | 5.31  | 117.07      | 111.28   |
| 2   | E     | 667 | ASN  | CA-C-O     | -5.31 | 114.92      | 120.55   |
| 1   | C     | 50  | GLN  | OE1-CD-NE2 | -5.31 | 117.29      | 122.60   |
| 1   | C     | 215 | ALA  | O-C-N      | 5.31  | 128.84      | 122.79   |
| 2   | E     | 658 | SER  | O-C-N      | 5.30  | 130.12      | 123.23   |
| 1   | C     | 214 | LYS  | O-C-N      | 5.30  | 127.82      | 122.09   |
| 1   | A     | 68  | GLU  | CA-C-N     | -5.29 | 113.19      | 120.28   |
| 1   | A     | 68  | GLU  | C-N-CA     | -5.29 | 113.19      | 120.28   |
| 1   | C     | 120 | ILE  | N-CA-CB    | -5.28 | 103.36      | 110.54   |
| 2   | E     | 662 | GLN  | OE1-CD-NE2 | 5.28  | 127.88      | 122.60   |
| 1   | B     | 184 | HIS  | CA-C-O     | -5.27 | 115.12      | 121.34   |
| 2   | E     | 652 | VAL  | N-CA-C     | -5.27 | 105.36      | 110.42   |
| 1   | B     | 109 | ASP  | N-CA-C     | -5.27 | 106.87      | 113.72   |
| 1   | C     | 127 | GLU  | CB-CG-CD   | 5.27  | 121.56      | 112.60   |
| 1   | B     | 208 | ASP  | CB-CA-C    | 5.27  | 120.90      | 110.42   |
| 2   | F     | 578 | PHE  | CA-C-N     | 5.26  | 130.53      | 122.95   |
| 2   | F     | 578 | PHE  | C-N-CA     | 5.26  | 130.53      | 122.95   |
| 1   | A     | 48  | SER  | CA-C-O     | 5.26  | 126.98      | 121.19   |
| 1   | B     | 198 | VAL  | CA-C-O     | 5.26  | 123.53      | 118.90   |
| 2   | E     | 638 | THR  | CA-CB-OG1  | -5.26 | 101.71      | 109.60   |
| 1   | C     | 166 | GLU  | CA-C-O     | 5.26  | 128.03      | 120.51   |
| 2   | D     | 666 | LYS  | CG-CD-CE   | 5.25  | 123.39      | 111.30   |
| 2   | E     | 546 | ILE  | N-CA-CB    | 5.25  | 119.90      | 111.23   |
| 1   | B     | 201 | PRO  | O-C-N      | 5.25  | 128.53      | 122.23   |
| 1   | B     | 217 | ASN  | OD1-CG-ND2 | 5.25  | 127.85      | 122.60   |
| 1   | B     | 120 | ILE  | O-C-N      | -5.25 | 116.78      | 121.87   |
| 2   | F     | 551 | TYR  | CA-C-O     | -5.24 | 114.67      | 120.33   |
| 1   | B     | 45  | PHE  | CB-CA-C    | 5.24  | 121.24      | 110.40   |
| 1   | B     | 54  | GLU  | N-CA-CB    | 5.24  | 118.00      | 110.20   |
| 1   | A     | 169 | GLN  | OE1-CD-NE2 | -5.23 | 117.37      | 122.60   |
| 1   | B     | 120 | ILE  | CB-CG1-CD1 | 5.23  | 124.79      | 113.80   |
| 1   | C     | 210 | ALA  | CA-C-N     | 5.23  | 131.38      | 121.97   |
| 1   | C     | 210 | ALA  | C-N-CA     | 5.23  | 131.38      | 121.97   |
| 1   | A     | 74  | GLN  | N-CA-CB    | 5.23  | 117.77      | 109.82   |
| 1   | C     | 53  | GLN  | CB-CG-CD   | 5.23  | 121.49      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 214 | LYS  | CA-C-O    | -5.23 | 115.32      | 120.70   |
| 2   | E     | 656 | GLU  | N-CA-CB   | -5.23 | 102.28      | 110.69   |
| 2   | E     | 582 | PHE  | CA-C-O    | -5.22 | 115.50      | 121.40   |
| 2   | E     | 608 | THR  | CA-CB-OG1 | -5.22 | 101.76      | 109.60   |
| 2   | F     | 658 | SER  | CA-C-O    | -5.22 | 115.06      | 120.70   |
| 2   | D     | 523 | TYR  | N-CA-C    | 5.22  | 116.65      | 111.07   |
| 2   | E     | 536 | VAL  | O-C-N     | 5.22  | 129.09      | 122.57   |
| 1   | C     | 79  | THR  | N-CA-C    | 5.22  | 119.77      | 113.41   |
| 2   | F     | 669 | PHE  | N-CA-CB   | -5.22 | 102.43      | 110.20   |
| 2   | E     | 671 | GLU  | CG-CD-OE1 | 5.21  | 130.39      | 118.40   |
| 2   | E     | 622 | ASP  | CB-CA-C   | 5.21  | 118.98      | 111.02   |
| 2   | F     | 672 | ALA  | N-CA-C    | -5.21 | 107.09      | 113.50   |
| 1   | A     | 194 | ASN  | CB-CA-C   | 5.20  | 119.53      | 110.68   |
| 2   | F     | 536 | VAL  | O-C-N     | 5.20  | 129.07      | 122.57   |
| 2   | F     | 669 | PHE  | CA-C-N    | 5.20  | 128.01      | 120.79   |
| 2   | F     | 669 | PHE  | C-N-CA    | 5.20  | 128.01      | 120.79   |
| 1   | A     | 221 | THR  | N-CA-CB   | 5.19  | 117.75      | 110.12   |
| 1   | B     | 151 | GLN  | CA-C-N    | 5.19  | 129.45      | 120.58   |
| 1   | B     | 151 | GLN  | C-N-CA    | 5.19  | 129.45      | 120.58   |
| 1   | C     | 63  | PRO  | CB-CA-C   | 5.18  | 118.42      | 110.75   |
| 2   | F     | 540 | TYR  | N-CA-CB   | 5.18  | 119.31      | 110.71   |
| 1   | A     | 79  | THR  | N-CA-C    | 5.18  | 119.59      | 113.12   |
| 2   | D     | 581 | CYS  | CA-C-O    | 5.18  | 126.20      | 120.71   |
| 2   | F     | 522 | SER  | CA-C-O    | -5.18 | 115.36      | 120.90   |
| 1   | B     | 67  | ARG  | NE-CZ-NH1 | 5.17  | 126.67      | 121.50   |
| 2   | F     | 590 | PHE  | O-C-N     | 5.17  | 128.96      | 122.23   |
| 1   | B     | 177 | PHE  | CA-C-O    | -5.17 | 115.07      | 120.55   |
| 1   | C     | 50  | GLN  | CB-CG-CD  | 5.17  | 121.39      | 112.60   |
| 1   | C     | 177 | PHE  | CA-C-O    | -5.17 | 115.07      | 120.55   |
| 2   | F     | 558 | THR  | CA-C-O    | 5.17  | 127.48      | 121.49   |
| 2   | E     | 604 | HIS  | CA-CB-CG  | -5.17 | 108.64      | 113.80   |
| 2   | F     | 671 | GLU  | CG-CD-OE1 | 5.17  | 130.28      | 118.40   |
| 1   | B     | 72  | TYR  | CA-CB-CG  | -5.16 | 104.61      | 113.90   |
| 1   | B     | 172 | ARG  | N-CA-C    | -5.16 | 105.55      | 111.07   |
| 2   | D     | 533 | VAL  | CA-C-O    | -5.16 | 113.04      | 119.95   |
| 2   | E     | 655 | VAL  | CB-CA-C   | 5.16  | 118.45      | 110.50   |
| 2   | E     | 648 | ASP  | CA-CB-CG  | 5.15  | 117.75      | 112.60   |
| 2   | F     | 523 | TYR  | N-CA-C    | 5.15  | 116.58      | 111.07   |
| 2   | F     | 667 | ASN  | N-CA-C    | 5.15  | 116.89      | 111.28   |
| 2   | E     | 561 | GLN  | CA-CB-CG  | -5.15 | 103.80      | 114.10   |
| 2   | E     | 538 | ASP  | CA-C-O    | 5.15  | 125.89      | 120.33   |
| 1   | C     | 74  | GLN  | N-CA-CB   | 5.15  | 117.64      | 109.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 56  | ASN  | O-C-N      | 5.15  | 127.43      | 121.10   |
| 2   | F     | 648 | ASP  | CA-CB-CG   | 5.14  | 117.75      | 112.60   |
| 1   | C     | 93  | VAL  | CA-C-O     | -5.14 | 115.92      | 121.27   |
| 1   | C     | 216 | ILE  | CA-C-N     | 5.14  | 134.34      | 121.80   |
| 1   | C     | 216 | ILE  | C-N-CA     | 5.14  | 134.34      | 121.80   |
| 2   | F     | 536 | VAL  | CA-CB-CG1  | -5.14 | 101.67      | 110.40   |
| 1   | B     | 125 | LEU  | CB-CA-C    | 5.14  | 119.03      | 110.81   |
| 2   | E     | 592 | ASN  | CA-CB-CG   | -5.13 | 107.47      | 112.60   |
| 1   | C     | 91  | GLN  | CG-CD-OE1  | 5.13  | 131.07      | 120.80   |
| 2   | E     | 597 | TRP  | CA-C-O     | -5.13 | 115.62      | 120.90   |
| 2   | E     | 588 | SER  | CB-CA-C    | 5.13  | 119.57      | 110.85   |
| 2   | E     | 592 | ASN  | CB-CA-C    | 5.13  | 119.57      | 109.72   |
| 1   | C     | 169 | GLN  | N-CA-C     | -5.13 | 105.77      | 111.36   |
| 2   | F     | 647 | ARG  | CA-C-O     | -5.13 | 113.17      | 120.51   |
| 1   | A     | 36  | PRO  | CB-CA-C    | 5.13  | 119.84      | 110.10   |
| 1   | A     | 202 | ASN  | CB-CG-ND2  | 5.12  | 124.09      | 116.40   |
| 1   | A     | 166 | GLU  | CA-C-O     | 5.12  | 127.83      | 120.51   |
| 1   | B     | 135 | PHE  | CB-CA-C    | 5.12  | 119.29      | 110.79   |
| 2   | E     | 522 | SER  | CA-C-O     | -5.12 | 115.42      | 120.90   |
| 2   | D     | 545 | MET  | CB-CA-C    | 5.12  | 118.57      | 109.72   |
| 1   | B     | 127 | GLU  | CB-CG-CD   | 5.12  | 121.30      | 112.60   |
| 2   | F     | 511 | ASP  | CA-C-O     | -5.12 | 115.38      | 120.96   |
| 1   | B     | 161 | GLN  | OE1-CD-NE2 | -5.11 | 117.49      | 122.60   |
| 2   | E     | 612 | LEU  | CB-CA-C    | 5.11  | 118.67      | 110.29   |
| 1   | A     | 54  | GLU  | N-CA-CB    | 5.11  | 117.81      | 110.20   |
| 2   | D     | 672 | ALA  | N-CA-C     | -5.11 | 107.22      | 113.50   |
| 1   | B     | 109 | ASP  | N-CA-CB    | -5.11 | 103.14      | 110.65   |
| 1   | C     | 221 | THR  | N-CA-CB    | 5.11  | 117.63      | 110.12   |
| 1   | A     | 215 | ALA  | CA-C-N     | 5.10  | 131.16      | 121.97   |
| 1   | A     | 215 | ALA  | C-N-CA     | 5.10  | 131.16      | 121.97   |
| 2   | D     | 664 | GLY  | O-C-N      | 5.10  | 127.57      | 122.77   |
| 2   | E     | 624 | SER  | N-CA-C     | 5.10  | 116.84      | 111.28   |
| 1   | C     | 148 | ASP  | O-C-N      | 5.10  | 129.37      | 122.59   |
| 2   | D     | 592 | ASN  | CB-CA-C    | 5.10  | 119.51      | 109.72   |
| 2   | F     | 658 | SER  | O-C-N      | 5.10  | 129.85      | 123.23   |
| 2   | D     | 562 | GLU  | CA-CB-CG   | 5.09  | 124.29      | 114.10   |
| 2   | E     | 545 | MET  | CB-CA-C    | 5.09  | 118.53      | 109.72   |
| 1   | A     | 68  | GLU  | O-C-N      | 5.09  | 129.63      | 122.20   |
| 2   | D     | 576 | ASP  | CA-CB-CG   | 5.09  | 117.69      | 112.60   |
| 1   | B     | 130 | GLU  | CG-CD-OE2  | -5.08 | 106.71      | 118.40   |
| 2   | D     | 613 | VAL  | N-CA-C     | 5.08  | 114.80      | 106.72   |
| 2   | F     | 599 | PRO  | CA-C-N     | 5.08  | 128.80      | 120.63   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | F     | 599 | PRO  | C-N-CA     | 5.08  | 128.80      | 120.63   |
| 1   | C     | 160 | LEU  | CA-C-N     | 5.07  | 127.50      | 120.29   |
| 1   | C     | 160 | LEU  | C-N-CA     | 5.07  | 127.50      | 120.29   |
| 2   | D     | 622 | ASP  | CB-CA-C    | 5.07  | 118.77      | 111.02   |
| 2   | E     | 582 | PHE  | N-CA-C     | -5.07 | 101.59      | 109.24   |
| 1   | C     | 215 | ALA  | CA-C-N     | 5.07  | 131.09      | 121.97   |
| 1   | C     | 215 | ALA  | C-N-CA     | 5.07  | 131.09      | 121.97   |
| 1   | A     | 56  | ASN  | O-C-N      | 5.06  | 127.33      | 121.10   |
| 2   | D     | 562 | GLU  | CA-C-O     | -5.06 | 113.28      | 120.51   |
| 2   | E     | 663 | ARG  | O-C-N      | 5.06  | 129.40      | 122.82   |
| 2   | D     | 507 | VAL  | CB-CA-C    | 5.05  | 118.11      | 110.63   |
| 1   | B     | 59  | GLN  | OE1-CD-NE2 | 5.05  | 127.66      | 122.60   |
| 1   | A     | 177 | PHE  | CA-C-O     | -5.05 | 115.51      | 120.82   |
| 2   | D     | 602 | THR  | N-CA-C     | -5.05 | 107.25      | 113.41   |
| 1   | C     | 208 | ASP  | CB-CA-C    | 5.05  | 120.47      | 110.42   |
| 2   | F     | 666 | LYS  | CA-C-O     | -5.05 | 115.07      | 120.42   |
| 1   | B     | 50  | GLN  | CB-CG-CD   | 5.05  | 121.18      | 112.60   |
| 2   | F     | 580 | VAL  | CA-C-O     | -5.05 | 115.09      | 120.59   |
| 2   | F     | 645 | LEU  | O-C-N      | 5.04  | 127.91      | 122.11   |
| 1   | A     | 191 | THR  | CA-CB-CG2  | 5.04  | 119.07      | 110.50   |
| 2   | E     | 653 | LYS  | CG-CD-CE   | 5.04  | 122.90      | 111.30   |
| 1   | A     | 45  | PHE  | CB-CA-C    | 5.04  | 120.84      | 110.40   |
| 1   | A     | 91  | GLN  | CG-CD-OE1  | 5.04  | 130.88      | 120.80   |
| 1   | C     | 74  | GLN  | N-CA-C     | -5.04 | 104.87      | 111.02   |
| 1   | B     | 199 | PHE  | N-CA-C     | -5.04 | 107.69      | 113.88   |
| 2   | F     | 622 | ASP  | CB-CA-C    | 5.04  | 118.73      | 111.02   |
| 1   | B     | 79  | THR  | N-CA-C     | 5.03  | 119.55      | 113.41   |
| 1   | A     | 65  | VAL  | O-C-N      | 5.03  | 126.95      | 121.87   |
| 1   | B     | 223 | THR  | CA-CB-CG2  | 5.03  | 119.05      | 110.50   |
| 1   | C     | 109 | ASP  | N-CA-C     | -5.03 | 107.18      | 113.72   |
| 2   | D     | 578 | PHE  | CA-C-N     | 5.03  | 130.19      | 122.95   |
| 2   | D     | 578 | PHE  | C-N-CA     | 5.03  | 130.19      | 122.95   |
| 2   | F     | 549 | GLU  | CA-C-O     | 5.02  | 126.39      | 120.41   |
| 1   | B     | 91  | GLN  | CG-CD-OE1  | 5.02  | 130.84      | 120.80   |
| 1   | B     | 64  | ILE  | N-CA-C     | 5.02  | 117.36      | 111.09   |
| 1   | B     | 121 | LEU  | CD1-CG-CD2 | -5.01 | 99.77       | 110.80   |
| 2   | F     | 592 | ASN  | CB-CA-C    | 5.01  | 119.35      | 109.72   |
| 2   | E     | 580 | VAL  | O-C-N      | 5.01  | 129.59      | 122.97   |
| 1   | C     | 184 | HIS  | O-C-N      | 5.01  | 128.72      | 121.95   |
| 1   | A     | 70  | VAL  | CB-CA-C    | 5.01  | 118.33      | 111.87   |
| 2   | D     | 647 | ARG  | CA-C-O     | -5.01 | 113.34      | 120.51   |
| 1   | B     | 90  | THR  | CA-CB-OG1  | -5.01 | 102.09      | 109.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | E     | 507 | VAL  | CB-CA-C  | 5.01  | 118.04      | 110.63   |
| 1   | A     | 53  | GLN  | CB-CG-CD | 5.00  | 121.11      | 112.60   |
| 1   | A     | 151 | GLN  | CA-C-O   | -5.00 | 113.38      | 119.43   |
| 1   | A     | 216 | ILE  | CA-C-O   | -5.00 | 114.53      | 120.78   |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 118 | ALA  | Mainchain |
| 1   | A     | 156 | THR  | Mainchain |
| 1   | A     | 193 | THR  | Mainchain |
| 1   | A     | 216 | ILE  | Mainchain |
| 1   | B     | 118 | ALA  | Mainchain |
| 1   | B     | 156 | THR  | Mainchain |
| 1   | B     | 193 | THR  | Mainchain |
| 1   | B     | 216 | ILE  | Mainchain |
| 1   | C     | 118 | ALA  | Mainchain |
| 1   | C     | 156 | THR  | Mainchain |
| 1   | C     | 193 | THR  | Mainchain |
| 1   | C     | 216 | ILE  | Mainchain |
| 2   | D     | 532 | TYR  | Mainchain |
| 2   | D     | 533 | VAL  | Mainchain |
| 2   | D     | 545 | MET  | Mainchain |
| 2   | D     | 593 | VAL  | Mainchain |
| 2   | D     | 666 | LYS  | Mainchain |
| 2   | E     | 545 | MET  | Mainchain |
| 2   | E     | 666 | LYS  | Mainchain |
| 2   | F     | 593 | VAL  | Mainchain |
| 2   | F     | 666 | LYS  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1593  | 0        | 1596     | 156     | 0            |
| 1   | B     | 1593  | 0        | 1596     | 163     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 1593  | 0        | 1596     | 154     | 0            |
| 2   | D     | 1337  | 0        | 1329     | 158     | 0            |
| 2   | E     | 1337  | 0        | 1329     | 160     | 0            |
| 2   | F     | 1337  | 0        | 1329     | 152     | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 32    | 0        | 13       | 9       | 0            |
| 4   | E     | 32    | 0        | 13       | 7       | 0            |
| 4   | F     | 32    | 0        | 13       | 7       | 0            |
| 5   | A     | 63    | 0        | 0        | 7       | 0            |
| 5   | B     | 62    | 0        | 0        | 14      | 0            |
| 5   | C     | 62    | 0        | 0        | 10      | 0            |
| 5   | D     | 36    | 0        | 0        | 9       | 0            |
| 5   | E     | 39    | 0        | 0        | 8       | 0            |
| 5   | F     | 40    | 0        | 0        | 10      | 0            |
| All | All   | 9191  | 0        | 8814     | 870     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (870) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:40:LEU:HB3   | 1:A:41:PRO:HD2   | 1.47                     | 0.97              |
| 1:C:211:ILE:HG13 | 1:C:212:THR:H    | 1.28                     | 0.97              |
| 1:A:211:ILE:HG13 | 1:A:212:THR:H    | 1.30                     | 0.96              |
| 1:B:211:ILE:HG13 | 1:B:212:THR:H    | 1.27                     | 0.96              |
| 1:B:40:LEU:HB3   | 1:B:41:PRO:HD2   | 1.48                     | 0.94              |
| 1:C:40:LEU:HB3   | 1:C:41:PRO:HD2   | 1.47                     | 0.93              |
| 2:E:535:THR:HG22 | 2:E:536:VAL:O    | 1.69                     | 0.92              |
| 2:D:535:THR:HG22 | 2:D:536:VAL:O    | 1.69                     | 0.91              |
| 2:F:535:THR:HG22 | 2:F:536:VAL:O    | 1.72                     | 0.89              |
| 2:D:655:VAL:HG23 | 2:D:668:VAL:HG22 | 1.52                     | 0.88              |
| 2:F:655:VAL:HG23 | 2:F:668:VAL:HG22 | 1.55                     | 0.88              |
| 1:C:84:PHE:HB3   | 1:C:198:VAL:HG11 | 1.53                     | 0.88              |
| 2:D:532:TYR:N    | 4:D:678:GNP:H3'  | 1.89                     | 0.88              |
| 1:C:216:ILE:HG22 | 1:C:217:ASN:H    | 1.38                     | 0.87              |
| 1:C:212:THR:HG22 | 1:C:213:LEU:HG   | 1.57                     | 0.87              |
| 1:B:84:PHE:HB3   | 1:B:198:VAL:HG11 | 1.56                     | 0.86              |
| 1:B:216:ILE:HG22 | 1:B:217:ASN:H    | 1.41                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:212:THR:HB   | 1:C:214:LYS:H    | 1.40                     | 0.86              |
| 1:A:84:PHE:HB3   | 1:A:198:VAL:HG11 | 1.57                     | 0.86              |
| 1:A:212:THR:HG22 | 1:A:213:LEU:HG   | 1.58                     | 0.86              |
| 1:A:212:THR:HB   | 1:A:214:LYS:H    | 1.41                     | 0.85              |
| 2:E:655:VAL:HG23 | 2:E:668:VAL:HG22 | 1.57                     | 0.85              |
| 2:D:508:VAL:HG22 | 2:D:579:LEU:HD12 | 1.59                     | 0.85              |
| 1:A:216:ILE:HG22 | 1:A:217:ASN:H    | 1.42                     | 0.84              |
| 1:B:212:THR:HB   | 1:B:214:LYS:H    | 1.41                     | 0.84              |
| 2:E:508:VAL:HG22 | 2:E:579:LEU:HD12 | 1.58                     | 0.83              |
| 2:F:508:VAL:HG22 | 2:F:579:LEU:HD12 | 1.59                     | 0.83              |
| 2:E:532:TYR:N    | 4:E:678:GNP:H3'  | 1.94                     | 0.83              |
| 2:E:576:ASP:O    | 2:E:577:VAL:HB   | 1.76                     | 0.82              |
| 1:B:212:THR:HG22 | 1:B:213:LEU:HG   | 1.60                     | 0.82              |
| 2:E:620:ARG:O    | 2:E:626:ILE:HD11 | 1.79                     | 0.82              |
| 1:B:126:ARG:HA   | 5:B:277:HOH:O    | 1.80                     | 0.81              |
| 2:F:576:ASP:O    | 2:F:577:VAL:HB   | 1.79                     | 0.81              |
| 1:A:210:ALA:O    | 1:A:214:LYS:HD2  | 1.81                     | 0.81              |
| 2:D:576:ASP:O    | 2:D:577:VAL:HB   | 1.79                     | 0.81              |
| 2:F:620:ARG:O    | 2:F:626:ILE:HD11 | 1.81                     | 0.81              |
| 2:D:620:ARG:O    | 2:D:626:ILE:HD11 | 1.82                     | 0.79              |
| 1:B:210:ALA:O    | 1:B:214:LYS:HD2  | 1.82                     | 0.79              |
| 2:F:532:TYR:N    | 4:F:678:GNP:H3'  | 1.98                     | 0.79              |
| 2:E:532:TYR:C    | 2:E:533:VAL:HG22 | 2.09                     | 0.78              |
| 2:F:532:TYR:O    | 2:F:533:VAL:HG13 | 1.83                     | 0.77              |
| 1:C:81:GLU:HA    | 1:C:188:ASN:HA   | 1.66                     | 0.77              |
| 1:A:147:ILE:O    | 1:A:152:ARG:NH1  | 2.18                     | 0.76              |
| 2:D:532:TYR:O    | 2:D:533:VAL:HG13 | 1.84                     | 0.76              |
| 1:A:199:PHE:HB3  | 5:A:281:HOH:O    | 1.85                     | 0.76              |
| 1:A:81:GLU:HA    | 1:A:188:ASN:HA   | 1.66                     | 0.76              |
| 1:A:37:ARG:N     | 1:A:38:PRO:HD3   | 1.99                     | 0.76              |
| 1:B:37:ARG:N     | 1:B:38:PRO:HD3   | 2.00                     | 0.76              |
| 1:B:147:ILE:O    | 1:B:152:ARG:NH1  | 2.18                     | 0.75              |
| 1:B:197:VAL:HG21 | 2:E:534:PRO:HG2  | 1.68                     | 0.75              |
| 1:A:212:THR:HG22 | 1:A:213:LEU:H    | 1.51                     | 0.75              |
| 1:C:147:ILE:O    | 1:C:152:ARG:NH1  | 2.19                     | 0.75              |
| 1:A:132:LEU:HD12 | 1:A:167:ASN:HD22 | 1.50                     | 0.75              |
| 1:B:181:ILE:HG23 | 1:B:188:ASN:HD21 | 1.50                     | 0.75              |
| 1:A:217:ASN:HB3  | 1:A:218:PRO:HD3  | 1.68                     | 0.75              |
| 1:A:181:ILE:HG23 | 1:A:188:ASN:HD21 | 1.51                     | 0.75              |
| 2:E:617:ILE:O    | 2:E:620:ARG:HB2  | 1.87                     | 0.75              |
| 1:B:81:GLU:HA    | 1:B:188:ASN:HA   | 1.68                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:37:ARG:HD3   | 1:B:101:ASN:HD21 | 1.52                     | 0.74              |
| 1:A:217:ASN:CB   | 2:D:536:VAL:HG11 | 2.18                     | 0.74              |
| 2:F:668:VAL:HG23 | 5:F:213:HOH:O    | 1.88                     | 0.74              |
| 1:C:210:ALA:O    | 1:C:214:LYS:HD2  | 1.86                     | 0.74              |
| 1:C:217:ASN:HB3  | 1:C:218:PRO:HD3  | 1.70                     | 0.73              |
| 1:B:217:ASN:HB3  | 1:B:218:PRO:HD3  | 1.71                     | 0.73              |
| 1:C:217:ASN:CB   | 2:F:536:VAL:HG11 | 2.18                     | 0.73              |
| 1:B:202:ASN:HA   | 5:B:277:HOH:O    | 1.88                     | 0.72              |
| 1:A:51:HIS:HA    | 1:A:54:GLU:HG2   | 1.71                     | 0.72              |
| 2:D:617:ILE:O    | 2:D:620:ARG:HB2  | 1.88                     | 0.72              |
| 1:B:217:ASN:HB2  | 2:E:536:VAL:HG11 | 1.72                     | 0.72              |
| 1:A:198:VAL:HG22 | 2:D:561:GLN:OE1  | 1.89                     | 0.72              |
| 1:B:217:ASN:CB   | 2:E:536:VAL:HG11 | 2.19                     | 0.72              |
| 2:F:617:ILE:O    | 2:F:620:ARG:HB2  | 1.90                     | 0.72              |
| 4:D:678:GNP:O3G  | 5:D:1:HOH:O      | 2.08                     | 0.72              |
| 1:C:197:VAL:HG21 | 2:F:534:PRO:HG2  | 1.71                     | 0.72              |
| 1:C:191:THR:HB   | 2:F:532:TYR:OH   | 1.90                     | 0.71              |
| 1:A:37:ARG:HD3   | 1:A:101:ASN:HD21 | 1.55                     | 0.71              |
| 1:C:198:VAL:HG22 | 2:F:561:GLN:OE1  | 1.90                     | 0.71              |
| 1:C:212:THR:HG22 | 1:C:213:LEU:H    | 1.55                     | 0.71              |
| 2:F:539:ASN:N    | 2:F:539:ASN:HD22 | 1.88                     | 0.71              |
| 1:A:217:ASN:HB2  | 2:D:536:VAL:HG11 | 1.71                     | 0.71              |
| 1:B:213:LEU:HD22 | 5:E:24:HOH:O     | 1.91                     | 0.71              |
| 1:B:132:LEU:HD12 | 1:B:167:ASN:HD22 | 1.55                     | 0.71              |
| 1:B:198:VAL:HG22 | 2:E:561:GLN:OE1  | 1.91                     | 0.70              |
| 1:C:141:VAL:HG22 | 1:C:222:PHE:CD1  | 2.26                     | 0.70              |
| 1:B:212:THR:HG22 | 1:B:213:LEU:H    | 1.56                     | 0.70              |
| 1:C:37:ARG:N     | 1:C:38:PRO:HD3   | 2.03                     | 0.70              |
| 1:C:217:ASN:HB2  | 2:F:536:VAL:HG11 | 1.72                     | 0.70              |
| 1:B:215:ALA:C    | 1:B:216:ILE:HD12 | 2.16                     | 0.70              |
| 2:F:569:PRO:HB3  | 2:F:604:HIS:NE2  | 2.05                     | 0.70              |
| 1:B:40:LEU:HD23  | 1:B:101:ASN:HB3  | 1.73                     | 0.70              |
| 1:A:191:THR:HB   | 2:D:532:TYR:OH   | 1.92                     | 0.70              |
| 1:A:197:VAL:HG21 | 2:D:534:PRO:HG2  | 1.72                     | 0.70              |
| 1:B:51:HIS:HA    | 1:B:54:GLU:HG2   | 1.71                     | 0.70              |
| 2:E:569:PRO:HB3  | 2:E:604:HIS:NE2  | 2.05                     | 0.70              |
| 1:C:60:GLU:HB3   | 5:C:245:HOH:O    | 1.91                     | 0.70              |
| 1:A:215:ALA:C    | 1:A:216:ILE:HD12 | 2.17                     | 0.70              |
| 2:E:539:ASN:N    | 2:E:539:ASN:HD22 | 1.90                     | 0.70              |
| 1:C:215:ALA:C    | 1:C:216:ILE:HD12 | 2.16                     | 0.70              |
| 1:B:94:ARG:HG3   | 5:B:264:HOH:O    | 1.92                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:211:ILE:HG13 | 1:B:212:THR:N    | 2.06                     | 0.70              |
| 2:D:501:PRO:HG3  | 2:D:550:PRO:HB2  | 1.74                     | 0.69              |
| 2:D:569:PRO:HB3  | 2:D:604:HIS:NE2  | 2.07                     | 0.69              |
| 1:C:217:ASN:CG   | 2:F:536:VAL:HG11 | 2.17                     | 0.69              |
| 1:C:181:ILE:HG23 | 1:C:188:ASN:HD21 | 1.56                     | 0.69              |
| 1:C:51:HIS:HA    | 1:C:54:GLU:HG2   | 1.73                     | 0.69              |
| 1:A:44:GLN:HB2   | 1:A:100:TYR:HB3  | 1.74                     | 0.69              |
| 1:B:141:VAL:HG22 | 1:B:222:PHE:CD1  | 2.27                     | 0.69              |
| 1:C:37:ARG:HD3   | 1:C:101:ASN:HD21 | 1.58                     | 0.69              |
| 1:C:44:GLN:HB2   | 1:C:100:TYR:HB3  | 1.74                     | 0.69              |
| 1:C:132:LEU:HD12 | 1:C:167:ASN:HD22 | 1.58                     | 0.69              |
| 2:F:501:PRO:HG3  | 2:F:550:PRO:HB2  | 1.74                     | 0.69              |
| 1:A:108:PHE:HD1  | 1:A:116:LEU:HD23 | 1.58                     | 0.68              |
| 1:A:141:VAL:HG22 | 1:A:222:PHE:CD2  | 2.28                     | 0.68              |
| 2:D:539:ASN:N    | 2:D:539:ASN:HD22 | 1.89                     | 0.68              |
| 2:E:617:ILE:HD11 | 2:E:656:GLU:HB3  | 1.75                     | 0.68              |
| 1:C:199:PHE:HB3  | 5:C:288:HOH:O    | 1.93                     | 0.68              |
| 2:F:617:ILE:HD11 | 2:F:656:GLU:HB3  | 1.76                     | 0.68              |
| 1:A:217:ASN:CG   | 2:D:536:VAL:HG11 | 2.18                     | 0.68              |
| 1:B:37:ARG:NH1   | 1:B:97:GLN:HB3   | 2.09                     | 0.68              |
| 1:C:40:LEU:HD23  | 1:C:101:ASN:HB3  | 1.76                     | 0.68              |
| 2:F:667:ASN:ND2  | 5:F:213:HOH:O    | 2.27                     | 0.68              |
| 4:F:678:GNP:O3G  | 5:F:3:HOH:O      | 2.10                     | 0.68              |
| 1:C:125:LEU:HD11 | 1:C:174:LEU:HD22 | 1.75                     | 0.68              |
| 2:E:646:ALA:O    | 2:E:649:LEU:N    | 2.26                     | 0.68              |
| 2:F:646:ALA:O    | 2:F:649:LEU:N    | 2.27                     | 0.68              |
| 2:E:501:PRO:HG3  | 2:E:550:PRO:HB2  | 1.76                     | 0.67              |
| 1:C:37:ARG:NH1   | 1:C:97:GLN:HB3   | 2.09                     | 0.67              |
| 1:A:200:GLY:N    | 1:A:201:PRO:HD2  | 2.10                     | 0.67              |
| 1:C:200:GLY:N    | 1:C:201:PRO:HD2  | 2.09                     | 0.67              |
| 1:B:44:GLN:HB2   | 1:B:100:TYR:HB3  | 1.76                     | 0.67              |
| 1:B:138:TYR:HA   | 5:B:267:HOH:O    | 1.94                     | 0.67              |
| 1:B:108:PHE:HD1  | 1:B:116:LEU:HD23 | 1.58                     | 0.67              |
| 1:A:40:LEU:HD23  | 1:A:101:ASN:HB3  | 1.75                     | 0.66              |
| 1:B:48:SER:OG    | 1:B:51:HIS:HB2   | 1.94                     | 0.66              |
| 1:C:108:PHE:HD1  | 1:C:116:LEU:HD23 | 1.60                     | 0.66              |
| 1:B:125:LEU:HD11 | 1:B:174:LEU:HD22 | 1.77                     | 0.66              |
| 2:E:667:ASN:ND2  | 5:E:297:HOH:O    | 2.29                     | 0.66              |
| 1:B:37:ARG:HD3   | 1:B:101:ASN:ND2  | 2.11                     | 0.66              |
| 2:D:535:THR:HG22 | 2:D:536:VAL:C    | 2.21                     | 0.66              |
| 2:D:633:LYS:HG2  | 2:D:634:GLN:HE21 | 1.61                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:217:ASN:CG   | 2:E:536:VAL:HG11 | 2.20                     | 0.66              |
| 1:B:188:ASN:O    | 1:B:189:LYS:HB2  | 1.96                     | 0.65              |
| 2:D:617:ILE:HD11 | 2:D:656:GLU:HB3  | 1.78                     | 0.65              |
| 1:A:40:LEU:HD23  | 1:A:101:ASN:CB   | 2.27                     | 0.65              |
| 1:C:211:ILE:HG13 | 1:C:212:THR:N    | 2.08                     | 0.65              |
| 2:F:606:PRO:O    | 2:F:607:LYS:HB2  | 1.96                     | 0.65              |
| 1:A:37:ARG:HD3   | 1:A:101:ASN:ND2  | 2.11                     | 0.65              |
| 1:B:212:THR:HG21 | 1:B:214:LYS:HE3  | 1.79                     | 0.65              |
| 2:E:633:LYS:HG2  | 2:E:634:GLN:HE21 | 1.62                     | 0.65              |
| 2:E:606:PRO:O    | 2:E:607:LYS:HB2  | 1.95                     | 0.65              |
| 1:C:48:SER:OG    | 1:C:51:HIS:HB2   | 1.97                     | 0.65              |
| 1:C:212:THR:HG21 | 1:C:214:LYS:HE3  | 1.79                     | 0.65              |
| 2:D:633:LYS:HG2  | 2:D:634:GLN:NE2  | 2.12                     | 0.64              |
| 1:B:99:LYS:NZ    | 1:B:111:TYR:OH   | 2.29                     | 0.64              |
| 1:B:169:GLN:HE21 | 1:B:169:GLN:HA   | 1.61                     | 0.64              |
| 1:B:191:THR:HB   | 2:E:532:TYR:OH   | 1.97                     | 0.64              |
| 1:C:99:LYS:NZ    | 1:C:111:TYR:OH   | 2.29                     | 0.64              |
| 1:C:188:ASN:O    | 1:C:189:LYS:HB2  | 1.96                     | 0.64              |
| 2:F:633:LYS:HG2  | 2:F:634:GLN:HE21 | 1.63                     | 0.64              |
| 1:A:188:ASN:O    | 1:A:189:LYS:HB2  | 1.97                     | 0.64              |
| 2:F:542:VAL:HA   | 5:F:90:HOH:O     | 1.98                     | 0.64              |
| 2:D:646:ALA:O    | 2:D:649:LEU:N    | 2.30                     | 0.64              |
| 1:A:37:ARG:NH1   | 1:A:97:GLN:HB3   | 2.13                     | 0.64              |
| 1:C:37:ARG:HD3   | 1:C:101:ASN:ND2  | 2.11                     | 0.64              |
| 1:C:40:LEU:HD23  | 1:C:101:ASN:CB   | 2.28                     | 0.63              |
| 2:D:612:LEU:HD23 | 2:D:654:TYR:HB2  | 1.80                     | 0.63              |
| 1:B:40:LEU:HD23  | 1:B:101:ASN:CB   | 2.28                     | 0.63              |
| 1:B:78:LEU:HG    | 5:B:263:HOH:O    | 1.97                     | 0.63              |
| 1:B:130:GLU:HG3  | 1:B:131:PRO:HD2  | 1.81                     | 0.63              |
| 2:E:532:TYR:O    | 2:E:533:VAL:HG13 | 1.99                     | 0.63              |
| 2:E:535:THR:HG22 | 2:E:536:VAL:C    | 2.22                     | 0.63              |
| 1:A:169:GLN:HE21 | 1:A:169:GLN:HA   | 1.63                     | 0.63              |
| 2:D:674:LEU:HD12 | 2:D:674:LEU:O    | 1.99                     | 0.63              |
| 2:E:661:THR:HG21 | 2:E:663:ARG:HB3  | 1.80                     | 0.63              |
| 1:B:47:VAL:HG13  | 1:B:52:LEU:HD21  | 1.81                     | 0.63              |
| 2:E:674:LEU:HD12 | 2:E:674:LEU:O    | 1.99                     | 0.63              |
| 2:E:532:TYR:O    | 2:E:533:VAL:HG22 | 1.98                     | 0.62              |
| 2:F:535:THR:HG22 | 2:F:536:VAL:C    | 2.22                     | 0.62              |
| 2:E:661:THR:CG2  | 2:E:663:ARG:HB3  | 2.29                     | 0.62              |
| 1:B:126:ARG:HG2  | 5:B:277:HOH:O    | 1.98                     | 0.62              |
| 2:E:633:LYS:HG2  | 2:E:634:GLN:NE2  | 2.14                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:200:GLY:N    | 1:B:201:PRO:HD2  | 2.14                     | 0.62              |
| 1:C:47:VAL:HG13  | 1:C:52:LEU:HD21  | 1.82                     | 0.62              |
| 2:D:515:GLY:HA2  | 4:D:678:GNP:H8   | 1.82                     | 0.62              |
| 1:B:216:ILE:HD13 | 2:E:537:PHE:CD1  | 2.35                     | 0.62              |
| 2:E:668:VAL:HG23 | 5:E:297:HOH:O    | 1.99                     | 0.62              |
| 2:F:503:THR:O    | 2:F:504:ILE:HG13 | 1.98                     | 0.62              |
| 1:C:180:GLN:HG3  | 5:C:270:HOH:O    | 2.00                     | 0.62              |
| 1:A:47:VAL:HG13  | 1:A:52:LEU:HD21  | 1.81                     | 0.62              |
| 2:D:503:THR:O    | 2:D:504:ILE:HG13 | 1.98                     | 0.62              |
| 2:E:668:VAL:HG12 | 2:E:669:PHE:CD2  | 2.35                     | 0.62              |
| 1:C:179:VAL:HG21 | 1:C:230:GLN:HG3  | 1.81                     | 0.62              |
| 1:A:125:LEU:HD11 | 1:A:174:LEU:HD22 | 1.82                     | 0.62              |
| 2:E:518:CYS:HB3  | 2:E:528:PHE:CE2  | 2.35                     | 0.62              |
| 1:C:169:GLN:HE21 | 1:C:169:GLN:HA   | 1.63                     | 0.62              |
| 2:F:653:LYS:HD2  | 2:F:655:VAL:HG12 | 1.82                     | 0.62              |
| 2:F:668:VAL:HG12 | 2:F:669:PHE:CD2  | 2.35                     | 0.62              |
| 2:D:668:VAL:HG12 | 2:D:669:PHE:CD2  | 2.34                     | 0.61              |
| 1:C:130:GLU:HG3  | 1:C:131:PRO:HD2  | 1.82                     | 0.61              |
| 1:C:153:VAL:N    | 1:C:154:PRO:HD2  | 2.14                     | 0.61              |
| 1:C:216:ILE:HD13 | 2:F:537:PHE:CD1  | 2.35                     | 0.61              |
| 1:A:153:VAL:N    | 1:A:154:PRO:HD2  | 2.15                     | 0.61              |
| 2:D:661:THR:CG2  | 2:D:663:ARG:HB3  | 2.30                     | 0.61              |
| 2:F:515:GLY:HA2  | 4:F:678:GNP:H8   | 1.81                     | 0.61              |
| 2:F:649:LEU:O    | 2:F:650:LYS:HB2  | 2.00                     | 0.61              |
| 2:D:606:PRO:O    | 2:D:607:LYS:HB2  | 1.99                     | 0.61              |
| 2:D:653:LYS:HD3  | 2:D:654:TYR:O    | 2.01                     | 0.61              |
| 2:D:661:THR:HG21 | 2:D:663:ARG:HB3  | 1.83                     | 0.61              |
| 2:F:653:LYS:HD3  | 2:F:654:TYR:O    | 2.01                     | 0.61              |
| 2:F:661:THR:HG21 | 2:F:663:ARG:HB3  | 1.83                     | 0.61              |
| 1:B:104:LEU:HD12 | 1:B:105:PRO:HD2  | 1.82                     | 0.61              |
| 2:F:633:LYS:HG2  | 2:F:634:GLN:NE2  | 2.15                     | 0.61              |
| 1:B:211:ILE:CG1  | 1:B:212:THR:H    | 2.09                     | 0.60              |
| 1:C:140:HIS:NE2  | 1:C:156:THR:OG1  | 2.34                     | 0.60              |
| 2:E:622:ASP:O    | 2:E:625:THR:OG1  | 2.19                     | 0.60              |
| 1:B:153:VAL:N    | 1:B:154:PRO:HD2  | 2.16                     | 0.60              |
| 2:E:553:LEU:HD22 | 2:E:673:ILE:HD11 | 1.83                     | 0.60              |
| 2:F:674:LEU:HD12 | 2:F:674:LEU:O    | 2.02                     | 0.60              |
| 2:E:515:GLY:HA2  | 4:E:678:GNP:H8   | 1.82                     | 0.60              |
| 1:C:192:ASN:OD1  | 1:C:227:LEU:HB3  | 2.02                     | 0.60              |
| 1:A:179:VAL:HG21 | 1:A:230:GLN:HG3  | 1.83                     | 0.60              |
| 2:F:508:VAL:CG2  | 2:F:579:LEU:HD12 | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:646:ALA:O    | 2:D:647:ARG:C    | 2.43                     | 0.60              |
| 1:C:184:HIS:O    | 1:C:187:GLN:HG2  | 2.02                     | 0.60              |
| 2:F:646:ALA:O    | 2:F:647:ARG:C    | 2.44                     | 0.60              |
| 2:D:518:CYS:HB3  | 2:D:528:PHE:CE2  | 2.37                     | 0.60              |
| 2:E:653:LYS:HD2  | 2:E:655:VAL:HG12 | 1.83                     | 0.60              |
| 1:A:216:ILE:HD13 | 2:D:537:PHE:CD1  | 2.36                     | 0.60              |
| 1:B:211:ILE:O    | 1:B:215:ALA:N    | 2.34                     | 0.60              |
| 2:F:661:THR:CG2  | 2:F:663:ARG:HB3  | 2.31                     | 0.60              |
| 1:A:52:LEU:O     | 1:A:56:ASN:HB2   | 2.02                     | 0.59              |
| 1:A:130:GLU:HG3  | 1:A:131:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:217:ASN:CB   | 1:A:218:PRO:HD3  | 2.33                     | 0.59              |
| 2:D:542:VAL:HA   | 5:D:52:HOH:O     | 2.02                     | 0.59              |
| 1:A:83:ILE:HD13  | 1:A:181:ILE:HD12 | 1.83                     | 0.59              |
| 2:E:653:LYS:HD3  | 2:E:654:TYR:O    | 2.02                     | 0.59              |
| 1:C:78:LEU:HG    | 5:C:270:HOH:O    | 2.00                     | 0.59              |
| 1:C:104:LEU:HD12 | 1:C:105:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:215:ALA:O    | 1:A:216:ILE:HD12 | 2.02                     | 0.59              |
| 1:C:215:ALA:O    | 1:C:216:ILE:HD12 | 2.02                     | 0.59              |
| 1:A:104:LEU:HD12 | 1:A:105:PRO:HD2  | 1.85                     | 0.59              |
| 2:D:508:VAL:CG2  | 2:D:579:LEU:HD12 | 2.32                     | 0.59              |
| 1:B:184:HIS:O    | 1:B:187:GLN:HG2  | 2.03                     | 0.59              |
| 1:A:43:GLN:HA    | 1:A:101:ASN:HA   | 1.85                     | 0.59              |
| 1:B:52:LEU:O     | 1:B:56:ASN:HB2   | 2.03                     | 0.59              |
| 1:A:119:VAL:HG23 | 1:A:120:ILE:HD13 | 1.85                     | 0.58              |
| 1:C:211:ILE:O    | 1:C:215:ALA:N    | 2.36                     | 0.58              |
| 1:A:100:TYR:CE2  | 1:A:106:VAL:HG21 | 2.38                     | 0.58              |
| 1:B:37:ARG:NH1   | 1:B:45:PHE:HB2   | 2.18                     | 0.58              |
| 2:E:503:THR:O    | 2:E:504:ILE:HG13 | 2.03                     | 0.58              |
| 2:E:649:LEU:O    | 2:E:650:LYS:HB2  | 2.04                     | 0.58              |
| 1:A:211:ILE:O    | 1:A:215:ALA:N    | 2.35                     | 0.58              |
| 1:B:197:VAL:O    | 2:E:564:TYR:HE2  | 1.86                     | 0.58              |
| 2:F:547:GLY:N    | 5:F:41:HOH:O     | 2.33                     | 0.58              |
| 1:A:181:ILE:HG23 | 1:A:188:ASN:ND2  | 2.18                     | 0.58              |
| 1:A:216:ILE:HG22 | 2:D:536:VAL:HG13 | 1.84                     | 0.58              |
| 2:F:518:CYS:HB3  | 2:F:528:PHE:CE2  | 2.38                     | 0.58              |
| 1:A:48:SER:OG    | 1:A:51:HIS:HB2   | 2.03                     | 0.58              |
| 2:E:568:ARG:O    | 2:E:571:SER:HB2  | 2.04                     | 0.58              |
| 1:A:192:ASN:OD1  | 1:A:227:LEU:HB3  | 2.03                     | 0.58              |
| 1:C:52:LEU:O     | 1:C:56:ASN:HB2   | 2.03                     | 0.58              |
| 1:C:132:LEU:HA   | 1:C:167:ASN:ND2  | 2.19                     | 0.58              |
| 1:B:179:VAL:HG21 | 1:B:230:GLN:HG3  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:197:VAL:O    | 2:F:564:TYR:HE2  | 1.86                     | 0.58              |
| 2:F:587:PRO:HG2  | 2:F:634:GLN:OE1  | 2.04                     | 0.58              |
| 1:A:37:ARG:NH1   | 1:A:45:PHE:HB2   | 2.19                     | 0.58              |
| 1:A:184:HIS:O    | 1:A:187:GLN:HG2  | 2.03                     | 0.58              |
| 2:E:590:PHE:O    | 2:E:593:VAL:HB   | 2.04                     | 0.58              |
| 1:B:43:GLN:HA    | 1:B:101:ASN:HA   | 1.85                     | 0.57              |
| 1:A:99:LYS:NZ    | 1:A:111:TYR:OH   | 2.30                     | 0.57              |
| 1:B:192:ASN:OD1  | 1:B:227:LEU:HB3  | 2.04                     | 0.57              |
| 1:B:215:ALA:O    | 1:B:216:ILE:HD12 | 2.04                     | 0.57              |
| 2:F:612:LEU:HD23 | 2:F:654:TYR:HB2  | 1.85                     | 0.57              |
| 2:F:655:VAL:CG2  | 2:F:668:VAL:HG22 | 2.32                     | 0.57              |
| 2:E:649:LEU:C    | 2:E:650:LYS:HD3  | 2.28                     | 0.57              |
| 1:C:213:LEU:HD22 | 5:F:47:HOH:O     | 2.04                     | 0.57              |
| 1:C:217:ASN:CB   | 1:C:218:PRO:HD3  | 2.33                     | 0.57              |
| 2:F:590:PHE:O    | 2:F:593:VAL:HB   | 2.04                     | 0.57              |
| 1:A:197:VAL:O    | 2:D:564:TYR:HE2  | 1.87                     | 0.57              |
| 2:D:659:ALA:HB2  | 5:D:274:HOH:O    | 2.04                     | 0.57              |
| 1:A:60:GLU:HB3   | 5:A:245:HOH:O    | 2.03                     | 0.57              |
| 1:A:132:LEU:HA   | 1:A:167:ASN:ND2  | 2.19                     | 0.57              |
| 2:D:568:ARG:O    | 2:D:571:SER:HB2  | 2.05                     | 0.57              |
| 1:B:132:LEU:HA   | 1:B:167:ASN:ND2  | 2.20                     | 0.57              |
| 1:B:181:ILE:HG23 | 1:B:188:ASN:ND2  | 2.19                     | 0.57              |
| 1:B:217:ASN:CB   | 1:B:218:PRO:HD3  | 2.33                     | 0.57              |
| 1:C:43:GLN:HA    | 1:C:101:ASN:HA   | 1.87                     | 0.57              |
| 2:F:622:ASP:O    | 2:F:625:THR:OG1  | 2.21                     | 0.57              |
| 2:D:590:PHE:O    | 2:D:593:VAL:HB   | 2.05                     | 0.57              |
| 1:B:81:GLU:CA    | 1:B:188:ASN:HA   | 2.35                     | 0.57              |
| 1:B:96:VAL:HG13  | 1:B:106:VAL:HG11 | 1.87                     | 0.57              |
| 2:D:653:LYS:HD2  | 2:D:655:VAL:HG12 | 1.86                     | 0.56              |
| 2:F:532:TYR:C    | 2:F:533:VAL:HG22 | 2.29                     | 0.56              |
| 1:A:40:LEU:HB3   | 1:A:41:PRO:CD    | 2.30                     | 0.56              |
| 1:B:96:VAL:HG13  | 1:B:106:VAL:CG1  | 2.35                     | 0.56              |
| 1:A:102:MET:SD   | 2:E:674:LEU:HD13 | 2.44                     | 0.56              |
| 1:A:106:VAL:HB   | 5:A:253:HOH:O    | 2.04                     | 0.56              |
| 2:D:503:THR:C    | 2:D:504:ILE:HG13 | 2.30                     | 0.56              |
| 2:D:509:VAL:HG12 | 2:D:558:THR:HG21 | 1.85                     | 0.56              |
| 1:B:100:TYR:CE2  | 1:B:106:VAL:HG21 | 2.39                     | 0.56              |
| 2:E:522:SER:HB3  | 2:E:665:LEU:HD21 | 1.87                     | 0.56              |
| 2:E:590:PHE:CZ   | 2:E:645:LEU:HG   | 2.41                     | 0.56              |
| 1:C:81:GLU:CA    | 1:C:188:ASN:HA   | 2.34                     | 0.56              |
| 1:C:107:ASP:C    | 1:C:109:ASP:H    | 2.14                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:597:TRP:HA   | 2:F:597:TRP:CE3  | 2.41                     | 0.56              |
| 1:A:96:VAL:HG13  | 1:A:106:VAL:HG11 | 1.87                     | 0.56              |
| 2:D:532:TYR:C    | 2:D:533:VAL:HG22 | 2.30                     | 0.56              |
| 2:D:590:PHE:CZ   | 2:D:645:LEU:HG   | 2.40                     | 0.56              |
| 1:A:157:LEU:HD21 | 1:A:232:GLU:O    | 2.05                     | 0.56              |
| 1:C:157:LEU:HD21 | 1:C:232:GLU:O    | 2.06                     | 0.56              |
| 1:C:215:ALA:HB1  | 2:F:567:LEU:HD22 | 1.87                     | 0.56              |
| 2:F:522:SER:HB3  | 2:F:665:LEU:HD21 | 1.86                     | 0.56              |
| 1:A:93:VAL:HG13  | 1:A:120:ILE:CD1  | 2.35                     | 0.56              |
| 1:A:211:ILE:HG13 | 1:A:212:THR:N    | 2.09                     | 0.56              |
| 1:A:212:THR:HG21 | 1:A:214:LYS:HE3  | 1.86                     | 0.56              |
| 2:F:503:THR:C    | 2:F:504:ILE:HG13 | 2.30                     | 0.56              |
| 2:F:610:PHE:O    | 2:F:652:VAL:HG22 | 2.06                     | 0.56              |
| 2:F:620:ARG:NH2  | 2:F:656:GLU:OE1  | 2.39                     | 0.56              |
| 2:E:508:VAL:CG2  | 2:E:579:LEU:HD12 | 2.32                     | 0.56              |
| 1:A:211:ILE:CG1  | 1:A:212:THR:H    | 2.13                     | 0.56              |
| 2:D:610:PHE:O    | 2:D:652:VAL:HG22 | 2.06                     | 0.56              |
| 2:D:649:LEU:O    | 2:D:650:LYS:HB2  | 2.05                     | 0.56              |
| 2:E:509:VAL:HG12 | 2:E:558:THR:HG21 | 1.88                     | 0.56              |
| 2:E:512:GLY:O    | 2:E:513:ALA:HB3  | 2.06                     | 0.56              |
| 2:D:655:VAL:CG2  | 2:D:668:VAL:HG22 | 2.29                     | 0.55              |
| 1:C:37:ARG:NH1   | 1:C:45:PHE:HB2   | 2.21                     | 0.55              |
| 2:F:590:PHE:CZ   | 2:F:645:LEU:HG   | 2.41                     | 0.55              |
| 1:A:44:GLN:CB    | 1:A:100:TYR:HB3  | 2.36                     | 0.55              |
| 1:A:216:ILE:CG2  | 2:D:536:VAL:HG13 | 2.36                     | 0.55              |
| 1:C:83:ILE:O     | 1:C:85:ARG:N     | 2.39                     | 0.55              |
| 1:C:216:ILE:O    | 1:C:218:PRO:HD2  | 2.06                     | 0.55              |
| 1:C:217:ASN:ND2  | 2:F:536:VAL:HG11 | 2.21                     | 0.55              |
| 2:D:522:SER:HB3  | 2:D:665:LEU:HD21 | 1.87                     | 0.55              |
| 2:D:620:ARG:NH2  | 2:D:656:GLU:OE1  | 2.39                     | 0.55              |
| 1:C:216:ILE:HG22 | 2:F:536:VAL:HG13 | 1.87                     | 0.55              |
| 2:F:568:ARG:O    | 2:F:571:SER:HB2  | 2.06                     | 0.55              |
| 1:A:81:GLU:CA    | 1:A:188:ASN:HA   | 2.34                     | 0.55              |
| 1:A:215:ALA:HB1  | 2:D:567:LEU:HD22 | 1.89                     | 0.55              |
| 2:E:613:VAL:HA   | 2:E:655:VAL:O    | 2.07                     | 0.55              |
| 1:A:178:LEU:HB3  | 1:A:195:LEU:HD13 | 1.88                     | 0.55              |
| 2:D:587:PRO:HG2  | 2:D:634:GLN:OE1  | 2.06                     | 0.55              |
| 1:B:216:ILE:HG22 | 2:E:536:VAL:HG13 | 1.87                     | 0.55              |
| 1:B:216:ILE:CG2  | 2:E:536:VAL:HG13 | 2.37                     | 0.55              |
| 1:A:41:PRO:HG3   | 2:E:548:GLY:HA3  | 1.88                     | 0.55              |
| 2:E:655:VAL:CG2  | 2:E:668:VAL:HG22 | 2.34                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:544:VAL:HG22 | 5:F:67:HOH:O     | 2.06                     | 0.55              |
| 1:B:93:VAL:HG13  | 1:B:120:ILE:CD1  | 2.36                     | 0.55              |
| 1:B:178:LEU:HB3  | 1:B:195:LEU:HD13 | 1.87                     | 0.55              |
| 2:E:597:TRP:HA   | 2:E:597:TRP:CE3  | 2.42                     | 0.55              |
| 1:C:119:VAL:HG23 | 1:C:120:ILE:HD13 | 1.89                     | 0.55              |
| 1:C:144:PHE:CZ   | 1:C:152:ARG:HD2  | 2.41                     | 0.55              |
| 1:A:94:ARG:NH2   | 5:A:248:HOH:O    | 2.40                     | 0.54              |
| 1:A:83:ILE:O     | 1:A:85:ARG:N     | 2.40                     | 0.54              |
| 1:B:107:ASP:C    | 1:B:109:ASP:H    | 2.16                     | 0.54              |
| 2:E:573:PRO:HD3  | 5:E:257:HOH:O    | 2.07                     | 0.54              |
| 1:A:217:ASN:ND2  | 2:D:536:VAL:HG11 | 2.23                     | 0.54              |
| 2:E:610:PHE:O    | 2:E:652:VAL:HG22 | 2.06                     | 0.54              |
| 2:E:645:LEU:HD13 | 2:E:649:LEU:HD12 | 1.90                     | 0.54              |
| 2:E:665:LEU:HD12 | 2:E:669:PHE:CE2  | 2.42                     | 0.54              |
| 1:C:93:VAL:HG13  | 1:C:120:ILE:CD1  | 2.37                     | 0.54              |
| 2:F:639:PRO:HA   | 2:F:654:TYR:HE2  | 1.73                     | 0.54              |
| 1:C:211:ILE:CG1  | 1:C:212:THR:H    | 2.10                     | 0.54              |
| 2:E:612:LEU:HD23 | 2:E:654:TYR:HB2  | 1.88                     | 0.54              |
| 2:F:512:GLY:O    | 2:F:513:ALA:HB3  | 2.07                     | 0.54              |
| 2:F:509:VAL:HG12 | 2:F:558:THR:HG21 | 1.89                     | 0.54              |
| 1:A:107:ASP:C    | 1:A:109:ASP:H    | 2.15                     | 0.54              |
| 2:E:540:TYR:HB2  | 2:E:555:LEU:HB2  | 1.89                     | 0.54              |
| 2:E:620:ARG:NH1  | 2:E:637:ILE:O    | 2.41                     | 0.54              |
| 2:E:653:LYS:HD2  | 2:E:655:VAL:CG1  | 2.37                     | 0.54              |
| 2:F:613:VAL:HA   | 2:F:655:VAL:O    | 2.08                     | 0.54              |
| 2:D:597:TRP:CE3  | 2:D:597:TRP:HA   | 2.43                     | 0.54              |
| 2:D:665:LEU:HD12 | 2:D:669:PHE:CE2  | 2.43                     | 0.54              |
| 1:B:44:GLN:CB    | 1:B:100:TYR:HB3  | 2.38                     | 0.54              |
| 1:C:65:VAL:HG11  | 1:C:124:PHE:HB2  | 1.90                     | 0.54              |
| 2:F:505:LYS:HB3  | 2:F:575:THR:HA   | 1.89                     | 0.54              |
| 1:A:189:LYS:HD3  | 2:D:532:TYR:CD1  | 2.43                     | 0.53              |
| 2:D:582:PHE:HE1  | 2:D:584:VAL:HA   | 1.73                     | 0.53              |
| 1:B:216:ILE:O    | 1:B:218:PRO:HD2  | 2.08                     | 0.53              |
| 2:E:646:ALA:O    | 2:E:647:ARG:C    | 2.50                     | 0.53              |
| 1:C:44:GLN:CB    | 1:C:100:TYR:HB3  | 2.36                     | 0.53              |
| 2:F:553:LEU:HD22 | 2:F:673:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:213:LEU:HD22 | 5:D:81:HOH:O     | 2.08                     | 0.53              |
| 2:D:620:ARG:NH1  | 2:D:637:ILE:O    | 2.42                     | 0.53              |
| 2:D:649:LEU:C    | 2:D:650:LYS:HD3  | 2.33                     | 0.53              |
| 1:B:144:PHE:CZ   | 1:B:152:ARG:HD2  | 2.44                     | 0.53              |
| 2:E:620:ARG:NH2  | 2:E:656:GLU:OE1  | 2.41                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:119:VAL:HG23 | 1:B:120:ILE:HD13 | 1.89                     | 0.53              |
| 2:E:587:PRO:HG2  | 2:E:634:GLN:OE1  | 2.08                     | 0.53              |
| 1:C:40:LEU:HB3   | 1:C:41:PRO:CD    | 2.30                     | 0.53              |
| 2:D:540:TYR:HB2  | 2:D:555:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:70:VAL:O     | 1:A:74:GLN:HG3   | 2.08                     | 0.53              |
| 2:E:503:THR:C    | 2:E:504:ILE:HG13 | 2.33                     | 0.53              |
| 2:E:639:PRO:HA   | 2:E:654:TYR:HE2  | 1.72                     | 0.53              |
| 1:C:116:LEU:N    | 1:C:117:PRO:CD   | 2.72                     | 0.53              |
| 2:D:582:PHE:CE1  | 2:D:584:VAL:HA   | 2.44                     | 0.53              |
| 2:D:595:GLU:O    | 2:D:596:LYS:HB2  | 2.07                     | 0.53              |
| 2:D:645:LEU:HD13 | 2:D:649:LEU:HD12 | 1.91                     | 0.53              |
| 1:B:215:ALA:HB1  | 2:E:567:LEU:HD22 | 1.91                     | 0.53              |
| 1:B:83:ILE:O     | 1:B:85:ARG:N     | 2.42                     | 0.53              |
| 2:F:568:ARG:NH2  | 5:F:279:HOH:O    | 2.34                     | 0.53              |
| 2:D:665:LEU:HD12 | 2:D:669:PHE:HE2  | 1.74                     | 0.53              |
| 1:A:144:PHE:CZ   | 1:A:152:ARG:HD2  | 2.43                     | 0.53              |
| 1:C:96:VAL:HG13  | 1:C:106:VAL:CG1  | 2.39                     | 0.53              |
| 1:C:125:LEU:CD1  | 1:C:174:LEU:HD22 | 2.39                     | 0.53              |
| 1:C:178:LEU:HB3  | 1:C:195:LEU:HD13 | 1.91                     | 0.53              |
| 2:F:572:TYR:N    | 2:F:573:PRO:HD2  | 2.23                     | 0.53              |
| 2:D:505:LYS:HB3  | 2:D:575:THR:HA   | 1.91                     | 0.52              |
| 1:A:96:VAL:HG13  | 1:A:106:VAL:CG1  | 2.38                     | 0.52              |
| 2:D:572:TYR:N    | 2:D:573:PRO:HD2  | 2.24                     | 0.52              |
| 2:D:622:ASP:O    | 2:D:625:THR:OG1  | 2.26                     | 0.52              |
| 1:C:181:ILE:HG23 | 1:C:188:ASN:ND2  | 2.23                     | 0.52              |
| 1:A:65:VAL:HG11  | 1:A:124:PHE:HB2  | 1.91                     | 0.52              |
| 1:A:140:HIS:NE2  | 1:A:156:THR:OG1  | 2.39                     | 0.52              |
| 2:D:613:VAL:HA   | 2:D:655:VAL:O    | 2.08                     | 0.52              |
| 1:B:83:ILE:HD12  | 1:B:84:PHE:CD2   | 2.44                     | 0.52              |
| 1:B:153:VAL:N    | 1:B:154:PRO:CD   | 2.73                     | 0.52              |
| 1:C:153:VAL:N    | 1:C:154:PRO:CD   | 2.72                     | 0.52              |
| 1:A:216:ILE:O    | 1:A:218:PRO:HD2  | 2.10                     | 0.52              |
| 2:D:516:LYS:HB2  | 4:D:678:GNP:O1B  | 2.09                     | 0.52              |
| 2:D:553:LEU:HD22 | 2:D:673:ILE:HD11 | 1.90                     | 0.52              |
| 2:D:561:GLN:HG3  | 5:D:1:HOH:O      | 2.09                     | 0.52              |
| 1:B:157:LEU:HD21 | 1:B:232:GLU:O    | 2.09                     | 0.52              |
| 2:E:582:PHE:CE1  | 2:E:584:VAL:HA   | 2.44                     | 0.52              |
| 2:E:643:GLU:O    | 2:E:644:LYS:C    | 2.52                     | 0.52              |
| 2:F:645:LEU:HD13 | 2:F:649:LEU:HD12 | 1.90                     | 0.52              |
| 2:D:643:GLU:O    | 2:D:644:LYS:C    | 2.52                     | 0.52              |
| 1:B:70:VAL:O     | 1:B:74:GLN:HG3   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:620:ARG:NH1  | 2:F:637:ILE:O    | 2.42                     | 0.52              |
| 2:D:512:GLY:O    | 2:D:513:ALA:HB3  | 2.09                     | 0.52              |
| 1:B:116:LEU:N    | 1:B:117:PRO:CD   | 2.72                     | 0.52              |
| 2:E:665:LEU:HD12 | 2:E:669:PHE:HE2  | 1.74                     | 0.52              |
| 1:C:211:ILE:HB   | 2:F:570:LEU:CD1  | 2.40                     | 0.52              |
| 2:F:582:PHE:CE1  | 2:F:584:VAL:HA   | 2.45                     | 0.52              |
| 1:B:40:LEU:HB3   | 1:B:41:PRO:CD    | 2.31                     | 0.52              |
| 1:A:116:LEU:N    | 1:A:117:PRO:CD   | 2.73                     | 0.52              |
| 2:D:519:LEU:HD12 | 5:D:151:HOH:O    | 2.08                     | 0.52              |
| 1:B:217:ASN:ND2  | 2:E:536:VAL:HG11 | 2.24                     | 0.52              |
| 2:E:582:PHE:HE1  | 2:E:584:VAL:HA   | 1.74                     | 0.52              |
| 1:B:65:VAL:HG11  | 1:B:124:PHE:HB2  | 1.92                     | 0.52              |
| 1:B:177:PHE:O    | 1:B:180:GLN:HG2  | 2.10                     | 0.52              |
| 2:E:595:GLU:O    | 2:E:596:LYS:HB2  | 2.10                     | 0.52              |
| 1:C:216:ILE:CG2  | 1:C:217:ASN:H    | 2.13                     | 0.52              |
| 2:F:532:TYR:N    | 2:F:533:VAL:HG22 | 2.25                     | 0.52              |
| 1:A:153:VAL:N    | 1:A:154:PRO:CD   | 2.72                     | 0.51              |
| 2:D:532:TYR:O    | 2:D:533:VAL:CG1  | 2.56                     | 0.51              |
| 2:F:582:PHE:HE1  | 2:F:584:VAL:HA   | 1.75                     | 0.51              |
| 2:E:572:TYR:N    | 2:E:573:PRO:HD2  | 2.25                     | 0.51              |
| 2:F:572:TYR:N    | 2:F:573:PRO:CD   | 2.73                     | 0.51              |
| 1:C:216:ILE:CG2  | 2:F:536:VAL:HG13 | 2.39                     | 0.51              |
| 2:F:653:LYS:HD2  | 2:F:655:VAL:CG1  | 2.40                     | 0.51              |
| 2:F:665:LEU:HD12 | 2:F:669:PHE:CE2  | 2.45                     | 0.51              |
| 1:C:70:VAL:HG22  | 1:C:177:PHE:CD2  | 2.45                     | 0.51              |
| 1:C:100:TYR:CE2  | 1:C:106:VAL:HG21 | 2.46                     | 0.51              |
| 1:A:70:VAL:HG22  | 1:A:177:PHE:CD2  | 2.46                     | 0.51              |
| 1:A:191:THR:HB   | 2:D:532:TYR:HH   | 1.75                     | 0.51              |
| 2:D:595:GLU:O    | 2:D:596:LYS:CB   | 2.58                     | 0.51              |
| 2:D:639:PRO:HA   | 2:D:654:TYR:HE2  | 1.75                     | 0.51              |
| 1:B:180:GLN:HG3  | 5:B:263:HOH:O    | 2.11                     | 0.51              |
| 2:F:649:LEU:C    | 2:F:650:LYS:HD3  | 2.35                     | 0.51              |
| 2:D:559:ALA:HB3  | 2:D:564:TYR:CB   | 2.41                     | 0.51              |
| 2:D:568:ARG:N    | 2:D:569:PRO:CD   | 2.73                     | 0.51              |
| 1:B:211:ILE:HB   | 2:E:570:LEU:CD1  | 2.41                     | 0.51              |
| 2:F:516:LYS:HB2  | 4:F:678:GNP:O1B  | 2.10                     | 0.51              |
| 2:D:508:VAL:HG12 | 2:D:516:LYS:HG2  | 1.93                     | 0.51              |
| 2:F:508:VAL:HG12 | 2:F:516:LYS:HG2  | 1.93                     | 0.51              |
| 2:F:595:GLU:O    | 2:F:596:LYS:HB2  | 2.10                     | 0.51              |
| 2:E:505:LYS:HB3  | 2:E:575:THR:HA   | 1.93                     | 0.51              |
| 2:E:539:ASN:N    | 2:E:539:ASN:ND2  | 2.59                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:632:ASN:O    | 2:E:633:LYS:HD2  | 2.11                     | 0.51              |
| 1:B:70:VAL:HG22  | 1:B:177:PHE:CD2  | 2.46                     | 0.51              |
| 1:B:125:LEU:CD1  | 1:B:174:LEU:HD22 | 2.41                     | 0.51              |
| 1:C:189:LYS:HD3  | 2:F:532:TYR:CD1  | 2.46                     | 0.51              |
| 2:F:665:LEU:HD12 | 2:F:669:PHE:HE2  | 1.76                     | 0.51              |
| 2:D:559:ALA:O    | 2:D:568:ARG:NH2  | 2.43                     | 0.50              |
| 2:F:532:TYR:O    | 2:F:533:VAL:CG1  | 2.56                     | 0.50              |
| 2:F:568:ARG:N    | 2:F:569:PRO:CD   | 2.74                     | 0.50              |
| 1:A:151:GLN:HA   | 1:A:154:PRO:HG2  | 1.93                     | 0.50              |
| 1:C:70:VAL:O     | 1:C:74:GLN:HG3   | 2.10                     | 0.50              |
| 1:A:211:ILE:HB   | 2:D:570:LEU:CD1  | 2.41                     | 0.50              |
| 1:A:133:LEU:O    | 1:A:134:THR:CB   | 2.60                     | 0.50              |
| 2:D:666:LYS:HB2  | 5:D:17:HOH:O     | 2.11                     | 0.50              |
| 2:E:568:ARG:N    | 2:E:569:PRO:CD   | 2.74                     | 0.50              |
| 1:C:157:LEU:HD23 | 1:C:233:LEU:HA   | 1.93                     | 0.50              |
| 2:F:595:GLU:O    | 2:F:596:LYS:CB   | 2.60                     | 0.50              |
| 2:F:598:VAL:CB   | 2:F:599:PRO:HD3  | 2.42                     | 0.50              |
| 1:C:94:ARG:NH2   | 5:C:247:HOH:O    | 2.43                     | 0.50              |
| 2:F:653:LYS:HG2  | 2:F:654:TYR:H    | 1.76                     | 0.50              |
| 2:D:519:LEU:HB3  | 5:D:274:HOH:O    | 2.11                     | 0.50              |
| 1:B:63:PRO:O     | 1:B:67:ARG:HG3   | 2.12                     | 0.50              |
| 2:E:673:ILE:O    | 2:E:677:LEU:HG   | 2.11                     | 0.50              |
| 2:D:547:GLY:N    | 5:D:131:HOH:O    | 2.38                     | 0.50              |
| 2:F:646:ALA:O    | 2:F:650:LYS:N    | 2.44                     | 0.50              |
| 1:A:216:ILE:HG22 | 1:A:217:ASN:N    | 2.21                     | 0.49              |
| 1:B:142:VAL:HG21 | 5:B:246:HOH:O    | 2.12                     | 0.49              |
| 1:C:63:PRO:O     | 1:C:67:ARG:HG3   | 2.12                     | 0.49              |
| 1:C:84:PHE:CD1   | 1:C:118:ALA:HB1  | 2.47                     | 0.49              |
| 1:C:177:PHE:O    | 1:C:180:GLN:HG2  | 2.12                     | 0.49              |
| 1:A:45:PHE:HZ    | 1:A:120:ILE:HG23 | 1.77                     | 0.49              |
| 2:F:559:ALA:O    | 2:F:568:ARG:NH2  | 2.43                     | 0.49              |
| 1:B:217:ASN:HB3  | 1:B:218:PRO:CD   | 2.41                     | 0.49              |
| 2:E:523:TYR:HB2  | 2:E:665:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:81:GLU:HA    | 1:B:188:ASN:CA   | 2.39                     | 0.49              |
| 1:C:83:ILE:HD12  | 1:C:84:PHE:CD2   | 2.48                     | 0.49              |
| 2:F:540:TYR:HB2  | 2:F:555:LEU:HB2  | 1.94                     | 0.49              |
| 1:A:157:LEU:CD2  | 1:A:233:LEU:HA   | 2.42                     | 0.49              |
| 2:D:653:LYS:HD2  | 2:D:655:VAL:CG1  | 2.42                     | 0.49              |
| 1:C:199:PHE:O    | 1:C:202:ASN:HB2  | 2.13                     | 0.49              |
| 1:A:200:GLY:N    | 1:A:201:PRO:CD   | 2.76                     | 0.49              |
| 1:A:212:THR:CG2  | 1:A:213:LEU:H    | 2.22                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:47:VAL:CG2   | 1:B:48:SER:N     | 2.76                     | 0.49              |
| 2:F:673:ILE:O    | 2:F:677:LEU:HG   | 2.12                     | 0.49              |
| 1:A:84:PHE:CD1   | 1:A:118:ALA:HB1  | 2.46                     | 0.49              |
| 1:A:177:PHE:O    | 1:A:180:GLN:HG2  | 2.12                     | 0.49              |
| 2:D:572:TYR:N    | 2:D:573:PRO:CD   | 2.74                     | 0.49              |
| 1:C:133:LEU:O    | 1:C:134:THR:CB   | 2.61                     | 0.49              |
| 1:B:45:PHE:HZ    | 1:B:120:ILE:HG23 | 1.77                     | 0.49              |
| 1:B:92:VAL:O     | 1:B:95:GLU:N     | 2.44                     | 0.49              |
| 2:E:598:VAL:HB   | 2:E:599:PRO:HD3  | 1.95                     | 0.49              |
| 2:E:564:TYR:HD1  | 2:E:567:LEU:HD12 | 1.78                     | 0.48              |
| 2:F:501:PRO:HG3  | 2:F:550:PRO:CB   | 2.43                     | 0.48              |
| 2:D:653:LYS:HG2  | 2:D:654:TYR:H    | 1.78                     | 0.48              |
| 2:E:601:ILE:HG23 | 2:E:610:PHE:CE1  | 2.49                     | 0.48              |
| 1:A:157:LEU:HD23 | 1:A:233:LEU:HA   | 1.95                     | 0.48              |
| 2:D:523:TYR:HB2  | 2:D:665:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:66:LEU:O     | 1:B:70:VAL:HB    | 2.14                     | 0.48              |
| 1:A:83:ILE:CD1   | 1:A:181:ILE:HD12 | 2.43                     | 0.48              |
| 2:D:501:PRO:HG3  | 2:D:550:PRO:CB   | 2.43                     | 0.48              |
| 2:D:509:VAL:HG12 | 2:D:558:THR:CG2  | 2.44                     | 0.48              |
| 2:E:539:ASN:HD22 | 2:E:539:ASN:H    | 1.61                     | 0.48              |
| 2:F:532:TYR:C    | 2:F:532:TYR:CD2  | 2.91                     | 0.48              |
| 2:D:673:ILE:O    | 2:D:677:LEU:HG   | 2.13                     | 0.48              |
| 1:B:83:ILE:HD13  | 1:B:181:ILE:HD12 | 1.96                     | 0.48              |
| 1:B:194:ASN:O    | 1:B:197:VAL:HG23 | 2.13                     | 0.48              |
| 2:E:646:ALA:HA   | 2:E:651:ALA:HB3  | 1.95                     | 0.48              |
| 2:D:598:VAL:CB   | 2:D:599:PRO:HD3  | 2.44                     | 0.48              |
| 2:E:572:TYR:N    | 2:E:573:PRO:CD   | 2.76                     | 0.48              |
| 2:F:519:LEU:HD12 | 5:F:121:HOH:O    | 2.13                     | 0.48              |
| 1:A:165:GLU:OE2  | 1:A:169:GLN:OE1  | 2.31                     | 0.48              |
| 1:A:217:ASN:HB3  | 1:A:218:PRO:CD   | 2.41                     | 0.48              |
| 2:D:646:ALA:O    | 2:D:650:LYS:N    | 2.43                     | 0.48              |
| 1:A:38:PRO:HA    | 1:A:39:PRO:HD2   | 1.62                     | 0.48              |
| 1:B:104:LEU:CD1  | 1:B:105:PRO:HD2  | 2.42                     | 0.48              |
| 2:E:583:SER:N    | 2:E:589:SER:OG   | 2.43                     | 0.48              |
| 2:E:595:GLU:O    | 2:E:596:LYS:CB   | 2.61                     | 0.48              |
| 2:E:597:TRP:O    | 2:E:601:ILE:HB   | 2.14                     | 0.48              |
| 1:C:66:LEU:O     | 1:C:70:VAL:HB    | 2.14                     | 0.48              |
| 1:C:217:ASN:HB3  | 1:C:218:PRO:CD   | 2.42                     | 0.48              |
| 2:F:598:VAL:HB   | 2:F:599:PRO:HD3  | 1.94                     | 0.48              |
| 1:C:45:PHE:HZ    | 1:C:120:ILE:HG23 | 1.78                     | 0.48              |
| 2:D:583:SER:N    | 2:D:589:SER:OG   | 2.43                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:211:ILE:HG13 | 2:E:570:LEU:HD13 | 1.96                     | 0.47              |
| 2:E:516:LYS:NZ   | 4:E:678:GNP:O1G  | 2.44                     | 0.47              |
| 1:C:194:ASN:HA   | 1:C:197:VAL:HG23 | 1.95                     | 0.47              |
| 1:C:211:ILE:HG13 | 2:F:570:LEU:HD13 | 1.95                     | 0.47              |
| 2:F:622:ASP:HA   | 2:F:623:PRO:HD2  | 1.83                     | 0.47              |
| 1:B:133:LEU:O    | 1:B:134:THR:CB   | 2.62                     | 0.47              |
| 1:C:95:GLU:O     | 1:C:96:VAL:C     | 2.56                     | 0.47              |
| 1:A:81:GLU:HA    | 1:A:188:ASN:CA   | 2.39                     | 0.47              |
| 2:E:611:LEU:HD23 | 2:E:653:LYS:O    | 2.15                     | 0.47              |
| 2:F:596:LYS:HE3  | 2:F:597:TRP:CZ2  | 2.49                     | 0.47              |
| 2:F:632:ASN:O    | 2:F:633:LYS:HD2  | 2.14                     | 0.47              |
| 2:D:617:ILE:HD13 | 2:D:656:GLU:OE1  | 2.15                     | 0.47              |
| 1:B:151:GLN:HA   | 1:B:154:PRO:HG2  | 1.96                     | 0.47              |
| 1:B:185:SER:O    | 1:B:189:LYS:HA   | 2.15                     | 0.47              |
| 2:E:646:ALA:O    | 2:E:650:LYS:N    | 2.47                     | 0.47              |
| 2:F:597:TRP:O    | 2:F:601:ILE:HB   | 2.14                     | 0.47              |
| 1:A:66:LEU:O     | 1:A:70:VAL:HB    | 2.14                     | 0.47              |
| 1:B:140:HIS:NE2  | 1:B:156:THR:OG1  | 2.40                     | 0.47              |
| 1:C:104:LEU:CD1  | 1:C:105:PRO:HD2  | 2.44                     | 0.47              |
| 1:C:216:ILE:HG22 | 1:C:217:ASN:N    | 2.17                     | 0.47              |
| 2:F:516:LYS:NZ   | 4:F:678:GNP:O1G  | 2.46                     | 0.47              |
| 2:F:601:ILE:HG23 | 2:F:610:PHE:CE1  | 2.49                     | 0.47              |
| 1:B:205:TRP:HZ3  | 5:B:277:HOH:O    | 1.97                     | 0.47              |
| 2:F:569:PRO:HG2  | 5:F:224:HOH:O    | 2.13                     | 0.47              |
| 1:A:199:PHE:O    | 1:A:202:ASN:HB2  | 2.14                     | 0.47              |
| 2:D:564:TYR:HD1  | 2:D:567:LEU:HD12 | 1.80                     | 0.47              |
| 2:D:617:ILE:CD1  | 2:D:656:GLU:HB3  | 2.44                     | 0.47              |
| 2:D:642:ALA:HB3  | 2:D:654:TYR:CE2  | 2.49                     | 0.47              |
| 1:B:37:ARG:HH12  | 1:B:97:GLN:HB3   | 1.78                     | 0.47              |
| 1:B:84:PHE:CD1   | 1:B:118:ALA:HB1  | 2.50                     | 0.47              |
| 1:B:86:ARG:HG2   | 5:B:237:HOH:O    | 2.15                     | 0.47              |
| 2:E:653:LYS:HG2  | 2:E:654:TYR:H    | 1.79                     | 0.47              |
| 1:C:151:GLN:HA   | 1:C:154:PRO:HG2  | 1.95                     | 0.47              |
| 2:F:590:PHE:CE1  | 2:F:645:LEU:HG   | 2.50                     | 0.47              |
| 2:F:643:GLU:O    | 2:F:644:LYS:C    | 2.57                     | 0.47              |
| 1:A:83:ILE:HD12  | 1:A:84:PHE:CD2   | 2.49                     | 0.47              |
| 2:D:596:LYS:HE3  | 2:D:597:TRP:CZ2  | 2.50                     | 0.47              |
| 2:E:598:VAL:CB   | 2:E:599:PRO:HD3  | 2.45                     | 0.47              |
| 1:C:200:GLY:N    | 1:C:201:PRO:CD   | 2.77                     | 0.47              |
| 2:F:564:TYR:HD1  | 2:F:567:LEU:HD12 | 1.80                     | 0.47              |
| 2:F:583:SER:N    | 2:F:589:SER:OG   | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:SER:O    | 1:A:189:LYS:HA   | 2.15                     | 0.47              |
| 1:A:216:ILE:CG1  | 2:D:567:LEU:HD13 | 2.44                     | 0.47              |
| 2:E:522:SER:HB3  | 2:E:665:LEU:CD2  | 2.45                     | 0.47              |
| 2:F:539:ASN:HD22 | 2:F:539:ASN:H    | 1.59                     | 0.47              |
| 1:A:193:THR:HG22 | 1:A:224:LYS:HD2  | 1.98                     | 0.46              |
| 2:D:516:LYS:NZ   | 4:D:678:GNP:O1G  | 2.45                     | 0.46              |
| 2:D:539:ASN:HD22 | 2:D:539:ASN:H    | 1.60                     | 0.46              |
| 2:F:523:TYR:HB2  | 2:F:665:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:63:PRO:O     | 1:A:67:ARG:HG3   | 2.14                     | 0.46              |
| 1:B:169:GLN:CD   | 1:B:172:ARG:HH21 | 2.23                     | 0.46              |
| 1:C:96:VAL:HG13  | 1:C:106:VAL:HG11 | 1.96                     | 0.46              |
| 2:D:559:ALA:HB3  | 2:D:564:TYR:HB3  | 1.96                     | 0.46              |
| 1:C:81:GLU:HA    | 1:C:188:ASN:CA   | 2.38                     | 0.46              |
| 2:D:597:TRP:O    | 2:D:601:ILE:HB   | 2.16                     | 0.46              |
| 1:B:38:PRO:HA    | 1:B:39:PRO:HD2   | 1.63                     | 0.46              |
| 1:B:60:GLU:HB3   | 5:B:257:HOH:O    | 2.15                     | 0.46              |
| 1:B:113:GLU:O    | 1:B:114:LEU:HB3  | 2.14                     | 0.46              |
| 1:B:211:ILE:CG1  | 2:E:570:LEU:HD13 | 2.45                     | 0.46              |
| 2:E:559:ALA:HB3  | 2:E:564:TYR:CB   | 2.45                     | 0.46              |
| 2:E:617:ILE:HD13 | 2:E:656:GLU:OE1  | 2.15                     | 0.46              |
| 1:B:189:LYS:HD3  | 2:E:532:TYR:CD1  | 2.51                     | 0.46              |
| 1:B:216:ILE:CG1  | 2:E:567:LEU:HD13 | 2.46                     | 0.46              |
| 1:C:157:LEU:CD2  | 1:C:233:LEU:HA   | 2.45                     | 0.46              |
| 1:A:125:LEU:CD1  | 1:A:174:LEU:HD22 | 2.45                     | 0.46              |
| 1:A:175:THR:O    | 1:A:179:VAL:HG23 | 2.15                     | 0.46              |
| 2:D:539:ASN:N    | 2:D:539:ASN:ND2  | 2.59                     | 0.46              |
| 2:E:509:VAL:HG12 | 2:E:558:THR:CG2  | 2.46                     | 0.46              |
| 1:A:189:LYS:NZ   | 2:D:532:TYR:HD1  | 2.13                     | 0.46              |
| 2:D:564:TYR:O    | 2:D:568:ARG:HB2  | 2.15                     | 0.46              |
| 1:B:94:ARG:NH2   | 5:B:247:HOH:O    | 2.48                     | 0.46              |
| 1:B:133:LEU:CB   | 1:B:203:LEU:HD13 | 2.45                     | 0.46              |
| 1:B:194:ASN:HA   | 1:B:197:VAL:HG23 | 1.97                     | 0.46              |
| 2:E:559:ALA:O    | 2:E:568:ARG:NH2  | 2.46                     | 0.46              |
| 1:C:175:THR:O    | 1:C:179:VAL:HG23 | 2.16                     | 0.46              |
| 1:C:194:ASN:O    | 1:C:197:VAL:HG23 | 2.16                     | 0.46              |
| 2:F:564:TYR:O    | 2:F:568:ARG:HB2  | 2.15                     | 0.46              |
| 2:D:601:ILE:HG23 | 2:D:610:PHE:CE1  | 2.50                     | 0.46              |
| 1:C:83:ILE:HD13  | 1:C:181:ILE:HD12 | 1.96                     | 0.46              |
| 2:F:522:SER:HB3  | 2:F:665:LEU:CD2  | 2.46                     | 0.46              |
| 1:A:113:GLU:O    | 1:A:114:LEU:HB3  | 2.15                     | 0.46              |
| 1:B:95:GLU:O     | 1:B:96:VAL:C     | 2.59                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:657:CYS:HA   | 2:E:664:GLY:HA3  | 1.98                     | 0.46              |
| 1:C:169:GLN:CD   | 1:C:172:ARG:HH21 | 2.24                     | 0.46              |
| 2:F:501:PRO:O    | 2:F:502:GLN:C    | 2.59                     | 0.46              |
| 2:F:617:ILE:CD1  | 2:F:656:GLU:HB3  | 2.45                     | 0.46              |
| 1:A:104:LEU:CD1  | 1:A:105:PRO:HD2  | 2.45                     | 0.45              |
| 2:E:594:LYS:HG3  | 2:E:595:GLU:N    | 2.31                     | 0.45              |
| 1:C:37:ARG:HH12  | 1:C:97:GLN:CG    | 2.29                     | 0.45              |
| 1:C:211:ILE:CG1  | 2:F:570:LEU:HD13 | 2.46                     | 0.45              |
| 2:F:615:THR:HG22 | 2:F:616:GLN:HG3  | 1.98                     | 0.45              |
| 2:D:522:SER:HB3  | 2:D:665:LEU:CD2  | 2.45                     | 0.45              |
| 2:D:598:VAL:HB   | 2:D:599:PRO:HD3  | 1.98                     | 0.45              |
| 1:B:141:VAL:HG22 | 1:B:222:PHE:CG   | 2.51                     | 0.45              |
| 2:F:509:VAL:HG12 | 2:F:558:THR:CG2  | 2.46                     | 0.45              |
| 1:A:194:ASN:O    | 1:A:197:VAL:HG23 | 2.17                     | 0.45              |
| 2:D:509:VAL:HA   | 2:D:558:THR:OG1  | 2.15                     | 0.45              |
| 1:B:86:ARG:NH1   | 5:B:292:HOH:O    | 2.50                     | 0.45              |
| 1:C:165:GLU:OE2  | 1:C:169:GLN:OE1  | 2.34                     | 0.45              |
| 2:D:590:PHE:CE1  | 2:D:645:LEU:HG   | 2.50                     | 0.45              |
| 2:E:515:GLY:HA2  | 4:E:678:GNP:C8   | 2.46                     | 0.45              |
| 2:E:542:VAL:HA   | 5:E:50:HOH:O     | 2.16                     | 0.45              |
| 2:E:642:ALA:HB3  | 2:E:654:TYR:CE2  | 2.52                     | 0.45              |
| 2:E:666:LYS:HB2  | 5:E:53:HOH:O     | 2.16                     | 0.45              |
| 1:C:113:GLU:O    | 1:C:114:LEU:HB3  | 2.14                     | 0.45              |
| 2:F:659:ALA:HB3  | 4:F:678:GNP:O6   | 2.16                     | 0.45              |
| 1:A:72:TYR:O     | 1:A:75:ALA:HB3   | 2.17                     | 0.45              |
| 1:A:169:GLN:CD   | 1:A:172:ARG:HH21 | 2.25                     | 0.45              |
| 2:D:532:TYR:O    | 2:D:532:TYR:CD2  | 2.70                     | 0.45              |
| 1:C:216:ILE:CG1  | 2:F:567:LEU:HD13 | 2.47                     | 0.45              |
| 1:A:95:GLU:O     | 1:A:96:VAL:C     | 2.58                     | 0.45              |
| 1:A:189:LYS:HZ3  | 2:D:532:TYR:HB2  | 1.81                     | 0.45              |
| 2:D:611:LEU:HD23 | 2:D:653:LYS:O    | 2.17                     | 0.45              |
| 1:B:157:LEU:CD2  | 1:B:233:LEU:HA   | 2.46                     | 0.45              |
| 1:B:157:LEU:HD23 | 1:B:233:LEU:HA   | 1.99                     | 0.45              |
| 1:C:185:SER:O    | 1:C:189:LYS:HA   | 2.16                     | 0.45              |
| 2:F:533:VAL:H    | 2:F:534:PRO:HD3  | 1.82                     | 0.45              |
| 2:D:532:TYR:C    | 2:D:532:TYR:CD2  | 2.94                     | 0.45              |
| 1:B:116:LEU:N    | 1:B:117:PRO:HD3  | 2.31                     | 0.45              |
| 2:E:590:PHE:CE1  | 2:E:645:LEU:HG   | 2.52                     | 0.45              |
| 1:C:62:ILE:HA    | 1:C:63:PRO:HD3   | 1.82                     | 0.45              |
| 1:C:116:LEU:O    | 1:C:120:ILE:HG12 | 2.17                     | 0.45              |
| 2:F:559:ALA:HB3  | 2:F:564:TYR:CB   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:650:LYS:HD3  | 2:E:650:LYS:N    | 2.32                     | 0.45              |
| 2:E:532:TYR:O    | 2:E:533:VAL:CG2  | 2.65                     | 0.44              |
| 2:F:611:LEU:HD23 | 2:F:653:LYS:O    | 2.17                     | 0.44              |
| 1:C:106:VAL:HB   | 5:C:240:HOH:O    | 2.17                     | 0.44              |
| 1:A:40:LEU:HD23  | 1:A:101:ASN:HB2  | 1.98                     | 0.44              |
| 2:D:622:ASP:HA   | 2:D:623:PRO:HD2  | 1.87                     | 0.44              |
| 1:B:93:VAL:HG13  | 1:B:120:ILE:HD11 | 1.99                     | 0.44              |
| 2:E:501:PRO:O    | 2:E:502:GLN:C    | 2.59                     | 0.44              |
| 2:F:539:ASN:H    | 2:F:539:ASN:ND2  | 2.15                     | 0.44              |
| 2:F:642:ALA:HB3  | 2:F:654:TYR:CE2  | 2.53                     | 0.44              |
| 1:B:216:ILE:HG22 | 1:B:217:ASN:N    | 2.19                     | 0.44              |
| 2:E:532:TYR:O    | 2:E:533:VAL:CG1  | 2.65                     | 0.44              |
| 2:E:615:THR:HG22 | 2:E:616:GLN:HG3  | 2.00                     | 0.44              |
| 2:E:617:ILE:CD1  | 2:E:656:GLU:HB3  | 2.46                     | 0.44              |
| 1:C:150:SER:HA   | 5:C:272:HOH:O    | 2.17                     | 0.44              |
| 1:A:189:LYS:NZ   | 2:D:532:TYR:CD1  | 2.85                     | 0.44              |
| 1:B:181:ILE:CG2  | 1:B:188:ASN:HD21 | 2.24                     | 0.44              |
| 2:E:521:ILE:HG22 | 2:E:527:LYS:O    | 2.17                     | 0.44              |
| 2:E:596:LYS:HE3  | 2:E:597:TRP:CZ2  | 2.53                     | 0.44              |
| 2:E:661:THR:O    | 2:E:662:GLN:HB2  | 2.18                     | 0.44              |
| 1:A:86:ARG:HG2   | 5:A:236:HOH:O    | 2.17                     | 0.44              |
| 2:D:515:GLY:HA2  | 4:D:678:GNP:C8   | 2.47                     | 0.44              |
| 2:D:632:ASN:O    | 2:D:633:LYS:HD2  | 2.17                     | 0.44              |
| 1:B:165:GLU:OE2  | 1:B:169:GLN:OE1  | 2.35                     | 0.44              |
| 2:E:622:ASP:HA   | 2:E:623:PRO:HD2  | 1.82                     | 0.44              |
| 1:C:191:THR:CB   | 2:F:532:TYR:OH   | 2.63                     | 0.44              |
| 1:A:138:TYR:HB3  | 1:A:139:PRO:HD3  | 1.99                     | 0.44              |
| 2:D:594:LYS:HB3  | 2:D:649:LEU:HD11 | 1.99                     | 0.44              |
| 2:E:564:TYR:O    | 2:E:568:ARG:HB2  | 2.17                     | 0.44              |
| 1:A:47:VAL:CG2   | 1:A:48:SER:N     | 2.81                     | 0.44              |
| 2:F:509:VAL:HA   | 2:F:558:THR:OG1  | 2.17                     | 0.44              |
| 2:F:584:VAL:CG1  | 2:F:620:ARG:NH1  | 2.81                     | 0.44              |
| 1:A:79:THR:O     | 1:A:187:GLN:HG3  | 2.17                     | 0.43              |
| 1:A:93:VAL:HG13  | 1:A:120:ILE:HD11 | 1.99                     | 0.43              |
| 1:A:181:ILE:CG2  | 1:A:188:ASN:HD21 | 2.25                     | 0.43              |
| 2:E:506:CYS:SG   | 2:E:579:LEU:HG   | 2.58                     | 0.43              |
| 2:E:509:VAL:HA   | 2:E:558:THR:OG1  | 2.17                     | 0.43              |
| 2:E:561:GLN:HG3  | 5:E:2:HOH:O      | 2.18                     | 0.43              |
| 1:A:40:LEU:CB    | 1:A:41:PRO:HD2   | 2.33                     | 0.43              |
| 1:A:156:THR:O    | 1:A:157:LEU:C    | 2.61                     | 0.43              |
| 1:A:212:THR:HG22 | 1:A:213:LEU:N    | 2.28                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:568:ARG:N    | 2:E:569:PRO:HD3  | 2.33                     | 0.43              |
| 1:C:93:VAL:HG13  | 1:C:120:ILE:HD11 | 1.99                     | 0.43              |
| 1:C:167:ASN:O    | 1:C:171:LEU:HB2  | 2.18                     | 0.43              |
| 1:A:141:VAL:HG22 | 1:A:222:PHE:CG   | 2.52                     | 0.43              |
| 1:A:194:ASN:HA   | 1:A:197:VAL:HG23 | 1.99                     | 0.43              |
| 2:D:568:ARG:N    | 2:D:569:PRO:HD3  | 2.33                     | 0.43              |
| 1:B:79:THR:O     | 1:B:187:GLN:HG3  | 2.18                     | 0.43              |
| 1:C:189:LYS:NZ   | 2:F:532:TYR:HD1  | 2.17                     | 0.43              |
| 1:C:212:THR:CG2  | 1:C:213:LEU:H    | 2.26                     | 0.43              |
| 2:D:501:PRO:CG   | 2:D:550:PRO:HB2  | 2.46                     | 0.43              |
| 1:B:138:TYR:HB3  | 1:B:139:PRO:HD3  | 1.99                     | 0.43              |
| 1:B:175:THR:O    | 1:B:179:VAL:HG23 | 2.18                     | 0.43              |
| 1:C:72:TYR:O     | 1:C:75:ALA:HB3   | 2.18                     | 0.43              |
| 1:C:169:GLN:NE2  | 1:C:172:ARG:HH21 | 2.17                     | 0.43              |
| 1:C:218:PRO:HD2  | 5:C:276:HOH:O    | 2.19                     | 0.43              |
| 2:F:515:GLY:HA2  | 4:F:678:GNP:C8   | 2.47                     | 0.43              |
| 2:F:568:ARG:N    | 2:F:569:PRO:HD3  | 2.34                     | 0.43              |
| 2:F:617:ILE:HD13 | 2:F:656:GLU:OE1  | 2.18                     | 0.43              |
| 2:F:646:ALA:HA   | 2:F:651:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:189:LYS:HD3  | 2:D:532:TYR:CE1  | 2.53                     | 0.43              |
| 2:E:547:GLY:N    | 5:E:60:HOH:O     | 2.42                     | 0.43              |
| 1:C:104:LEU:CG   | 1:C:105:PRO:HD2  | 2.49                     | 0.43              |
| 1:A:37:ARG:HH12  | 1:A:97:GLN:HB3   | 1.82                     | 0.43              |
| 1:A:191:THR:CB   | 2:D:532:TYR:OH   | 2.66                     | 0.43              |
| 2:D:532:TYR:O    | 2:D:533:VAL:CB   | 2.66                     | 0.43              |
| 1:B:156:THR:O    | 1:B:157:LEU:C    | 2.61                     | 0.43              |
| 1:C:212:THR:HG22 | 1:C:213:LEU:N    | 2.29                     | 0.43              |
| 2:D:539:ASN:H    | 2:D:539:ASN:ND2  | 2.16                     | 0.43              |
| 2:D:615:THR:HG22 | 2:D:616:GLN:HG3  | 2.00                     | 0.43              |
| 1:B:167:ASN:O    | 1:B:171:LEU:HB2  | 2.19                     | 0.43              |
| 1:C:49:LEU:HA    | 1:C:52:LEU:HD12  | 2.01                     | 0.43              |
| 1:A:169:GLN:NE2  | 1:A:172:ARG:HH21 | 2.17                     | 0.43              |
| 1:A:218:PRO:HD2  | 5:A:274:HOH:O    | 2.18                     | 0.43              |
| 1:B:189:LYS:NZ   | 2:E:532:TYR:HD1  | 2.17                     | 0.43              |
| 2:E:576:ASP:O    | 2:E:577:VAL:CB   | 2.56                     | 0.43              |
| 1:C:37:ARG:HH12  | 1:C:97:GLN:HB3   | 1.80                     | 0.43              |
| 2:E:517:THR:HB   | 4:E:678:GNP:O1A  | 2.19                     | 0.42              |
| 2:E:532:TYR:O    | 2:E:533:VAL:CB   | 2.66                     | 0.42              |
| 2:E:584:VAL:CG1  | 2:E:620:ARG:NH1  | 2.82                     | 0.42              |
| 1:B:199:PHE:O    | 1:B:202:ASN:HB2  | 2.18                     | 0.42              |
| 2:E:516:LYS:HB2  | 4:E:678:GNP:O1B  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:83:ILE:H     | 1:C:83:ILE:HG13  | 1.74                     | 0.42              |
| 2:F:532:TYR:O    | 2:F:533:VAL:CB   | 2.67                     | 0.42              |
| 1:B:217:ASN:CG   | 2:E:536:VAL:HG21 | 2.44                     | 0.42              |
| 1:C:40:LEU:HD23  | 1:C:101:ASN:HB2  | 2.00                     | 0.42              |
| 1:C:138:TYR:HB3  | 1:C:139:PRO:HD3  | 2.01                     | 0.42              |
| 2:F:599:PRO:O    | 2:F:603:HIS:HB3  | 2.19                     | 0.42              |
| 2:D:584:VAL:CG1  | 2:D:620:ARG:NH1  | 2.82                     | 0.42              |
| 2:E:507:VAL:HB   | 2:E:556:PHE:HB2  | 2.00                     | 0.42              |
| 2:E:532:TYR:C    | 2:E:532:TYR:CD2  | 2.97                     | 0.42              |
| 2:E:618:ASP:C    | 2:E:620:ARG:H    | 2.27                     | 0.42              |
| 1:C:189:LYS:HD3  | 2:F:532:TYR:HD1  | 1.84                     | 0.42              |
| 1:C:156:THR:O    | 1:C:157:LEU:C    | 2.62                     | 0.42              |
| 1:C:217:ASN:CG   | 2:F:536:VAL:HG21 | 2.44                     | 0.42              |
| 2:F:521:ILE:HG22 | 2:F:527:LYS:O    | 2.18                     | 0.42              |
| 2:F:532:TYR:O    | 2:F:532:TYR:CD2  | 2.72                     | 0.42              |
| 2:F:618:ASP:C    | 2:F:620:ARG:H    | 2.27                     | 0.42              |
| 1:A:211:ILE:CG1  | 2:D:570:LEU:HD13 | 2.50                     | 0.42              |
| 1:C:92:VAL:O     | 1:C:95:GLU:N     | 2.44                     | 0.42              |
| 1:A:70:VAL:HG22  | 1:A:177:PHE:CE2  | 2.55                     | 0.42              |
| 1:B:169:GLN:NE2  | 1:B:172:ARG:HH21 | 2.17                     | 0.42              |
| 2:E:638:THR:HA   | 2:E:639:PRO:HD3  | 1.90                     | 0.42              |
| 2:F:608:THR:HA   | 2:F:609:PRO:HD2  | 1.64                     | 0.42              |
| 1:A:189:LYS:HD3  | 2:D:532:TYR:HD1  | 1.83                     | 0.42              |
| 2:D:521:ILE:HG22 | 2:D:527:LYS:O    | 2.19                     | 0.42              |
| 2:D:522:SER:O    | 2:D:526:ASN:HA   | 2.20                     | 0.42              |
| 2:D:532:TYR:O    | 2:D:533:VAL:HG22 | 2.19                     | 0.42              |
| 1:B:189:LYS:HZ3  | 2:E:532:TYR:HB2  | 1.85                     | 0.42              |
| 2:E:532:TYR:C    | 2:E:533:VAL:CG2  | 2.77                     | 0.42              |
| 2:E:659:ALA:HB3  | 4:E:678:GNP:O6   | 2.20                     | 0.42              |
| 1:C:126:ARG:CG   | 1:C:202:ASN:OD1  | 2.67                     | 0.42              |
| 1:C:140:HIS:CE1  | 1:C:222:PHE:HE1  | 2.38                     | 0.42              |
| 1:C:211:ILE:CG1  | 1:C:212:THR:N    | 2.76                     | 0.42              |
| 2:D:599:PRO:O    | 2:D:603:HIS:HB3  | 2.20                     | 0.42              |
| 2:D:659:ALA:HB3  | 4:D:678:GNP:O6   | 2.20                     | 0.42              |
| 1:B:193:THR:HG22 | 1:B:224:LYS:HD2  | 2.01                     | 0.42              |
| 2:E:599:PRO:O    | 2:E:603:HIS:HB3  | 2.20                     | 0.42              |
| 2:D:598:VAL:HG21 | 2:D:649:LEU:HD13 | 2.01                     | 0.42              |
| 1:B:191:THR:HB   | 2:E:532:TYR:HH   | 1.84                     | 0.42              |
| 1:C:116:LEU:N    | 1:C:117:PRO:HD3  | 2.35                     | 0.42              |
| 1:C:133:LEU:CB   | 1:C:203:LEU:HD13 | 2.50                     | 0.42              |
| 1:A:216:ILE:HG13 | 2:D:567:LEU:HD13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:501:PRO:O    | 2:D:502:GLN:C    | 2.62                     | 0.41              |
| 2:D:618:ASP:C    | 2:D:620:ARG:H    | 2.28                     | 0.41              |
| 1:B:104:LEU:CG   | 1:B:105:PRO:HD2  | 2.50                     | 0.41              |
| 1:C:141:VAL:HG22 | 1:C:222:PHE:CG   | 2.54                     | 0.41              |
| 2:F:661:THR:O    | 2:F:662:GLN:HB2  | 2.20                     | 0.41              |
| 1:A:133:LEU:CB   | 1:A:203:LEU:HD13 | 2.51                     | 0.41              |
| 2:E:611:LEU:HD23 | 2:E:611:LEU:HA   | 1.81                     | 0.41              |
| 1:C:79:THR:O     | 1:C:187:GLN:HG3  | 2.19                     | 0.41              |
| 1:A:167:ASN:O    | 1:A:171:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:211:ILE:HG13 | 2:D:570:LEU:HD13 | 2.02                     | 0.41              |
| 2:D:585:VAL:O    | 2:D:629:LEU:HD22 | 2.21                     | 0.41              |
| 1:B:70:VAL:HG22  | 1:B:177:PHE:CE2  | 2.54                     | 0.41              |
| 1:B:72:TYR:O     | 1:B:75:ALA:HB3   | 2.19                     | 0.41              |
| 1:B:217:ASN:ND2  | 2:E:536:VAL:HG21 | 2.35                     | 0.41              |
| 2:E:594:LYS:HB3  | 2:E:649:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:42:ASN:O     | 1:A:43:GLN:C     | 2.63                     | 0.41              |
| 1:B:42:ASN:O     | 1:B:43:GLN:C     | 2.64                     | 0.41              |
| 2:E:564:TYR:CD1  | 2:E:567:LEU:HD12 | 2.54                     | 0.41              |
| 1:C:38:PRO:HA    | 1:C:39:PRO:HD2   | 1.62                     | 0.41              |
| 2:F:501:PRO:CG   | 2:F:550:PRO:HB2  | 2.47                     | 0.41              |
| 2:F:584:VAL:HG13 | 2:F:620:ARG:NH1  | 2.35                     | 0.41              |
| 1:A:140:HIS:CE1  | 1:A:222:PHE:HE2  | 2.39                     | 0.41              |
| 2:D:507:VAL:HB   | 2:D:556:PHE:HB2  | 2.02                     | 0.41              |
| 2:D:584:VAL:HG13 | 2:D:620:ARG:NH1  | 2.36                     | 0.41              |
| 2:E:559:ALA:HB3  | 2:E:564:TYR:HB3  | 2.01                     | 0.41              |
| 1:C:207:LYS:HG3  | 5:C:239:HOH:O    | 2.20                     | 0.41              |
| 1:C:217:ASN:ND2  | 2:F:536:VAL:HG21 | 2.35                     | 0.41              |
| 2:F:654:TYR:OH   | 2:F:656:GLU:OE2  | 2.36                     | 0.41              |
| 2:D:516:LYS:HB2  | 4:D:678:GNP:O2B  | 2.20                     | 0.41              |
| 2:D:650:LYS:HD3  | 2:D:650:LYS:N    | 2.36                     | 0.41              |
| 1:B:151:GLN:C    | 1:B:154:PRO:HD2  | 2.45                     | 0.41              |
| 1:B:197:VAL:CG2  | 2:E:534:PRO:HG2  | 2.45                     | 0.41              |
| 2:E:508:VAL:HG12 | 2:E:516:LYS:HG2  | 2.03                     | 0.41              |
| 2:F:594:LYS:HB3  | 2:F:649:LEU:HD11 | 2.01                     | 0.41              |
| 2:F:643:GLU:OE2  | 2:F:654:TYR:HB3  | 2.21                     | 0.41              |
| 1:A:151:GLN:C    | 1:A:154:PRO:HD2  | 2.45                     | 0.41              |
| 1:B:83:ILE:H     | 1:B:83:ILE:HG13  | 1.74                     | 0.41              |
| 1:B:189:LYS:HZ3  | 2:E:532:TYR:HD1  | 1.62                     | 0.41              |
| 2:E:532:TYR:O    | 2:E:532:TYR:CD2  | 2.73                     | 0.41              |
| 1:C:132:LEU:HB3  | 5:C:278:HOH:O    | 2.21                     | 0.41              |
| 2:D:603:HIS:ND1  | 2:D:603:HIS:C    | 2.79                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:657:CYS:HA   | 2:D:664:GLY:HA3  | 2.02                     | 0.41              |
| 2:E:572:TYR:H    | 2:E:573:PRO:HD2  | 1.85                     | 0.41              |
| 2:F:638:THR:HA   | 2:F:639:PRO:HD3  | 1.89                     | 0.41              |
| 1:A:104:LEU:CG   | 1:A:105:PRO:HD2  | 2.50                     | 0.41              |
| 2:D:564:TYR:CD1  | 2:D:567:LEU:HD12 | 2.55                     | 0.41              |
| 2:D:646:ALA:HA   | 2:D:651:ALA:HB3  | 2.03                     | 0.41              |
| 1:B:62:ILE:HA    | 1:B:63:PRO:HD3   | 1.83                     | 0.41              |
| 1:B:81:GLU:HA    | 1:B:188:ASN:CB   | 2.51                     | 0.41              |
| 1:B:218:PRO:HD2  | 5:B:275:HOH:O    | 2.21                     | 0.41              |
| 1:B:222:PHE:CE2  | 1:B:226:LEU:HD11 | 2.56                     | 0.41              |
| 2:F:507:VAL:HB   | 2:F:556:PHE:HB2  | 2.02                     | 0.41              |
| 2:F:511:ASP:O    | 2:F:514:VAL:HG13 | 2.20                     | 0.41              |
| 1:A:189:LYS:NZ   | 2:D:532:TYR:HB2  | 2.35                     | 0.41              |
| 1:B:140:HIS:CE1  | 1:B:222:PHE:HE1  | 2.39                     | 0.41              |
| 2:E:501:PRO:HG3  | 2:E:550:PRO:CB   | 2.45                     | 0.41              |
| 2:E:606:PRO:O    | 2:E:607:LYS:CB   | 2.68                     | 0.41              |
| 2:F:585:VAL:O    | 2:F:629:LEU:HD22 | 2.21                     | 0.41              |
| 2:D:517:THR:HB   | 4:D:678:GNP:O1A  | 2.22                     | 0.40              |
| 2:D:661:THR:O    | 2:D:662:GLN:HB2  | 2.21                     | 0.40              |
| 1:B:44:GLN:CG    | 1:B:100:TYR:HB3  | 2.51                     | 0.40              |
| 2:E:608:THR:HA   | 2:E:609:PRO:HD2  | 1.61                     | 0.40              |
| 2:F:572:TYR:H    | 2:F:573:PRO:HD2  | 1.85                     | 0.40              |
| 1:A:49:LEU:HA    | 1:A:52:LEU:HD12  | 2.03                     | 0.40              |
| 1:B:96:VAL:CG1   | 1:B:106:VAL:HG11 | 2.52                     | 0.40              |
| 1:C:189:LYS:CE   | 2:F:532:TYR:HD1  | 2.35                     | 0.40              |
| 1:A:44:GLN:CG    | 1:A:100:TYR:HB3  | 2.50                     | 0.40              |
| 2:D:611:LEU:HD23 | 2:D:611:LEU:HA   | 1.77                     | 0.40              |
| 1:B:37:ARG:HH12  | 1:B:97:GLN:CG    | 2.35                     | 0.40              |
| 1:B:45:PHE:CD1   | 1:B:97:GLN:HG2   | 2.57                     | 0.40              |
| 1:B:56:ASN:HA    | 1:B:57:PRO:HD2   | 1.89                     | 0.40              |
| 2:E:585:VAL:O    | 2:E:629:LEU:HD22 | 2.22                     | 0.40              |
| 1:A:86:ARG:NH1   | 5:A:267:HOH:O    | 2.54                     | 0.40              |
| 1:B:200:GLY:N    | 1:B:201:PRO:CD   | 2.80                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|-----------|-----------|----------|-------------|---|
| 1   | A     | 197/199 (99%)   | 157 (80%) | 29 (15%)  | 11 (6%)  | 1           | 2 |
| 1   | B     | 197/199 (99%)   | 157 (80%) | 29 (15%)  | 11 (6%)  | 1           | 2 |
| 1   | C     | 197/199 (99%)   | 159 (81%) | 26 (13%)  | 12 (6%)  | 1           | 2 |
| 2   | D     | 170/177 (96%)   | 137 (81%) | 21 (12%)  | 12 (7%)  | 1           | 1 |
| 2   | E     | 170/177 (96%)   | 136 (80%) | 22 (13%)  | 12 (7%)  | 1           | 1 |
| 2   | F     | 170/177 (96%)   | 136 (80%) | 22 (13%)  | 12 (7%)  | 1           | 1 |
| All | All   | 1101/1128 (98%) | 882 (80%) | 149 (14%) | 70 (6%)  | 1           | 1 |

All (70) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 209 | ALA  |
| 1   | A     | 210 | ALA  |
| 1   | A     | 211 | ILE  |
| 1   | A     | 216 | ILE  |
| 1   | A     | 217 | ASN  |
| 2   | D     | 533 | VAL  |
| 2   | D     | 577 | VAL  |
| 2   | D     | 596 | LYS  |
| 1   | B     | 209 | ALA  |
| 1   | B     | 210 | ALA  |
| 1   | B     | 211 | ILE  |
| 1   | B     | 216 | ILE  |
| 1   | B     | 217 | ASN  |
| 2   | E     | 533 | VAL  |
| 2   | E     | 577 | VAL  |
| 2   | E     | 596 | LYS  |
| 1   | C     | 209 | ALA  |
| 1   | C     | 210 | ALA  |
| 1   | C     | 211 | ILE  |
| 1   | C     | 216 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 217 | ASN  |
| 2   | F     | 533 | VAL  |
| 2   | F     | 577 | VAL  |
| 2   | F     | 596 | LYS  |
| 1   | A     | 84  | PHE  |
| 2   | D     | 502 | GLN  |
| 2   | D     | 546 | ILE  |
| 2   | D     | 633 | LYS  |
| 1   | B     | 84  | PHE  |
| 2   | E     | 502 | GLN  |
| 2   | E     | 546 | ILE  |
| 2   | E     | 633 | LYS  |
| 1   | C     | 84  | PHE  |
| 2   | F     | 502 | GLN  |
| 2   | F     | 546 | ILE  |
| 2   | F     | 548 | GLY  |
| 2   | F     | 633 | LYS  |
| 1   | A     | 75  | ALA  |
| 2   | D     | 607 | LYS  |
| 2   | D     | 646 | ALA  |
| 1   | B     | 75  | ALA  |
| 2   | E     | 548 | GLY  |
| 2   | E     | 607 | LYS  |
| 2   | E     | 609 | PRO  |
| 2   | E     | 623 | PRO  |
| 2   | E     | 646 | ALA  |
| 1   | C     | 75  | ALA  |
| 2   | F     | 607 | LYS  |
| 2   | F     | 646 | ALA  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 212 | THR  |
| 2   | D     | 609 | PRO  |
| 2   | D     | 623 | PRO  |
| 1   | B     | 114 | LEU  |
| 1   | C     | 114 | LEU  |
| 2   | F     | 609 | PRO  |
| 2   | F     | 623 | PRO  |
| 2   | D     | 548 | GLY  |
| 1   | B     | 129 | PRO  |
| 1   | B     | 212 | THR  |
| 1   | C     | 129 | PRO  |
| 1   | C     | 212 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 129 | PRO  |
| 2   | E     | 536 | VAL  |
| 2   | F     | 536 | VAL  |
| 1   | A     | 39  | PRO  |
| 2   | D     | 536 | VAL  |
| 1   | B     | 39  | PRO  |
| 1   | C     | 39  | PRO  |
| 1   | C     | 164 | PRO  |

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

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | A     | 175/180 (97%)  | 133 (76%) | 42 (24%)  | 1           | 2 |
| 1   | B     | 175/180 (97%)  | 135 (77%) | 40 (23%)  | 1           | 2 |
| 1   | C     | 175/180 (97%)  | 135 (77%) | 40 (23%)  | 1           | 2 |
| 2   | D     | 147/157 (94%)  | 102 (69%) | 45 (31%)  | 0           | 1 |
| 2   | E     | 147/157 (94%)  | 103 (70%) | 44 (30%)  | 0           | 1 |
| 2   | F     | 147/157 (94%)  | 103 (70%) | 44 (30%)  | 0           | 1 |
| All | All   | 966/1011 (96%) | 711 (74%) | 255 (26%) | 0           | 2 |

All (255) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | LEU  |
| 1   | A     | 43  | GLN  |
| 1   | A     | 47  | VAL  |
| 1   | A     | 51  | HIS  |
| 1   | A     | 53  | GLN  |
| 1   | A     | 59  | GLN  |
| 1   | A     | 60  | GLU  |
| 1   | A     | 64  | ILE  |
| 1   | A     | 67  | ARG  |
| 1   | A     | 68  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 78  | LEU  |
| 1   | A     | 80  | THR  |
| 1   | A     | 81  | GLU  |
| 1   | A     | 83  | ILE  |
| 1   | A     | 90  | THR  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 94  | ARG  |
| 1   | A     | 102 | MET  |
| 1   | A     | 112 | ASN  |
| 1   | A     | 119 | VAL  |
| 1   | A     | 120 | ILE  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 137 | LEU  |
| 1   | A     | 142 | VAL  |
| 1   | A     | 146 | ASN  |
| 1   | A     | 147 | ILE  |
| 1   | A     | 149 | GLU  |
| 1   | A     | 151 | GLN  |
| 1   | A     | 159 | VAL  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 162 | THR  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 170 | VAL  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 181 | ILE  |
| 1   | A     | 187 | GLN  |
| 1   | A     | 189 | LYS  |
| 1   | A     | 190 | MET  |
| 1   | A     | 197 | VAL  |
| 1   | A     | 212 | THR  |
| 1   | A     | 213 | LEU  |
| 2   | D     | 505 | LYS  |
| 2   | D     | 507 | VAL  |
| 2   | D     | 509 | VAL  |
| 2   | D     | 516 | LYS  |
| 2   | D     | 519 | LEU  |
| 2   | D     | 522 | SER  |
| 2   | D     | 527 | LYS  |
| 2   | D     | 533 | VAL  |
| 2   | D     | 539 | ASN  |
| 2   | D     | 557 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 563 | ASP  |
| 2   | D     | 567 | LEU  |
| 2   | D     | 568 | ARG  |
| 2   | D     | 570 | LEU  |
| 2   | D     | 576 | ASP  |
| 2   | D     | 579 | LEU  |
| 2   | D     | 584 | VAL  |
| 2   | D     | 589 | SER  |
| 2   | D     | 591 | GLU  |
| 2   | D     | 593 | VAL  |
| 2   | D     | 594 | LYS  |
| 2   | D     | 595 | GLU  |
| 2   | D     | 596 | LYS  |
| 2   | D     | 598 | VAL  |
| 2   | D     | 601 | ILE  |
| 2   | D     | 603 | HIS  |
| 2   | D     | 611 | LEU  |
| 2   | D     | 612 | LEU  |
| 2   | D     | 617 | ILE  |
| 2   | D     | 620 | ARG  |
| 2   | D     | 623 | PRO  |
| 2   | D     | 633 | LYS  |
| 2   | D     | 637 | ILE  |
| 2   | D     | 640 | GLU  |
| 2   | D     | 641 | THR  |
| 2   | D     | 643 | GLU  |
| 2   | D     | 645 | LEU  |
| 2   | D     | 647 | ARG  |
| 2   | D     | 648 | ASP  |
| 2   | D     | 653 | LYS  |
| 2   | D     | 663 | ARG  |
| 2   | D     | 666 | LYS  |
| 2   | D     | 667 | ASN  |
| 2   | D     | 668 | VAL  |
| 2   | D     | 677 | LEU  |
| 1   | B     | 40  | LEU  |
| 1   | B     | 43  | GLN  |
| 1   | B     | 47  | VAL  |
| 1   | B     | 51  | HIS  |
| 1   | B     | 53  | GLN  |
| 1   | B     | 59  | GLN  |
| 1   | B     | 60  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 64  | ILE  |
| 1   | B     | 67  | ARG  |
| 1   | B     | 68  | GLU  |
| 1   | B     | 78  | LEU  |
| 1   | B     | 80  | THR  |
| 1   | B     | 81  | GLU  |
| 1   | B     | 83  | ILE  |
| 1   | B     | 90  | THR  |
| 1   | B     | 91  | GLN  |
| 1   | B     | 94  | ARG  |
| 1   | B     | 102 | MET  |
| 1   | B     | 112 | ASN  |
| 1   | B     | 119 | VAL  |
| 1   | B     | 120 | ILE  |
| 1   | B     | 121 | LEU  |
| 1   | B     | 137 | LEU  |
| 1   | B     | 142 | VAL  |
| 1   | B     | 146 | ASN  |
| 1   | B     | 147 | ILE  |
| 1   | B     | 151 | GLN  |
| 1   | B     | 159 | VAL  |
| 1   | B     | 161 | GLN  |
| 1   | B     | 162 | THR  |
| 1   | B     | 169 | GLN  |
| 1   | B     | 170 | VAL  |
| 1   | B     | 171 | LEU  |
| 1   | B     | 180 | GLN  |
| 1   | B     | 181 | ILE  |
| 1   | B     | 187 | GLN  |
| 1   | B     | 189 | LYS  |
| 1   | B     | 190 | MET  |
| 1   | B     | 197 | VAL  |
| 1   | B     | 213 | LEU  |
| 2   | E     | 505 | LYS  |
| 2   | E     | 507 | VAL  |
| 2   | E     | 509 | VAL  |
| 2   | E     | 516 | LYS  |
| 2   | E     | 519 | LEU  |
| 2   | E     | 522 | SER  |
| 2   | E     | 527 | LYS  |
| 2   | E     | 533 | VAL  |
| 2   | E     | 539 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 557 | ASP  |
| 2   | E     | 563 | ASP  |
| 2   | E     | 567 | LEU  |
| 2   | E     | 570 | LEU  |
| 2   | E     | 576 | ASP  |
| 2   | E     | 579 | LEU  |
| 2   | E     | 584 | VAL  |
| 2   | E     | 589 | SER  |
| 2   | E     | 591 | GLU  |
| 2   | E     | 593 | VAL  |
| 2   | E     | 594 | LYS  |
| 2   | E     | 595 | GLU  |
| 2   | E     | 596 | LYS  |
| 2   | E     | 598 | VAL  |
| 2   | E     | 601 | ILE  |
| 2   | E     | 603 | HIS  |
| 2   | E     | 611 | LEU  |
| 2   | E     | 612 | LEU  |
| 2   | E     | 617 | ILE  |
| 2   | E     | 620 | ARG  |
| 2   | E     | 623 | PRO  |
| 2   | E     | 633 | LYS  |
| 2   | E     | 637 | ILE  |
| 2   | E     | 640 | GLU  |
| 2   | E     | 641 | THR  |
| 2   | E     | 643 | GLU  |
| 2   | E     | 645 | LEU  |
| 2   | E     | 647 | ARG  |
| 2   | E     | 648 | ASP  |
| 2   | E     | 653 | LYS  |
| 2   | E     | 663 | ARG  |
| 2   | E     | 666 | LYS  |
| 2   | E     | 667 | ASN  |
| 2   | E     | 668 | VAL  |
| 2   | E     | 677 | LEU  |
| 1   | C     | 40  | LEU  |
| 1   | C     | 43  | GLN  |
| 1   | C     | 47  | VAL  |
| 1   | C     | 53  | GLN  |
| 1   | C     | 60  | GLU  |
| 1   | C     | 64  | ILE  |
| 1   | C     | 67  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 68  | GLU  |
| 1   | C     | 78  | LEU  |
| 1   | C     | 80  | THR  |
| 1   | C     | 81  | GLU  |
| 1   | C     | 83  | ILE  |
| 1   | C     | 90  | THR  |
| 1   | C     | 91  | GLN  |
| 1   | C     | 94  | ARG  |
| 1   | C     | 102 | MET  |
| 1   | C     | 112 | ASN  |
| 1   | C     | 119 | VAL  |
| 1   | C     | 120 | ILE  |
| 1   | C     | 121 | LEU  |
| 1   | C     | 137 | LEU  |
| 1   | C     | 142 | VAL  |
| 1   | C     | 146 | ASN  |
| 1   | C     | 147 | ILE  |
| 1   | C     | 149 | GLU  |
| 1   | C     | 151 | GLN  |
| 1   | C     | 159 | VAL  |
| 1   | C     | 161 | GLN  |
| 1   | C     | 162 | THR  |
| 1   | C     | 169 | GLN  |
| 1   | C     | 170 | VAL  |
| 1   | C     | 171 | LEU  |
| 1   | C     | 180 | GLN  |
| 1   | C     | 181 | ILE  |
| 1   | C     | 187 | GLN  |
| 1   | C     | 189 | LYS  |
| 1   | C     | 190 | MET  |
| 1   | C     | 197 | VAL  |
| 1   | C     | 212 | THR  |
| 1   | C     | 213 | LEU  |
| 2   | F     | 505 | LYS  |
| 2   | F     | 507 | VAL  |
| 2   | F     | 509 | VAL  |
| 2   | F     | 516 | LYS  |
| 2   | F     | 519 | LEU  |
| 2   | F     | 522 | SER  |
| 2   | F     | 527 | LYS  |
| 2   | F     | 533 | VAL  |
| 2   | F     | 539 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 563 | ASP  |
| 2   | F     | 567 | LEU  |
| 2   | F     | 568 | ARG  |
| 2   | F     | 570 | LEU  |
| 2   | F     | 576 | ASP  |
| 2   | F     | 579 | LEU  |
| 2   | F     | 584 | VAL  |
| 2   | F     | 589 | SER  |
| 2   | F     | 591 | GLU  |
| 2   | F     | 593 | VAL  |
| 2   | F     | 594 | LYS  |
| 2   | F     | 595 | GLU  |
| 2   | F     | 596 | LYS  |
| 2   | F     | 598 | VAL  |
| 2   | F     | 601 | ILE  |
| 2   | F     | 603 | HIS  |
| 2   | F     | 611 | LEU  |
| 2   | F     | 612 | LEU  |
| 2   | F     | 617 | ILE  |
| 2   | F     | 620 | ARG  |
| 2   | F     | 623 | PRO  |
| 2   | F     | 633 | LYS  |
| 2   | F     | 637 | ILE  |
| 2   | F     | 640 | GLU  |
| 2   | F     | 641 | THR  |
| 2   | F     | 643 | GLU  |
| 2   | F     | 645 | LEU  |
| 2   | F     | 647 | ARG  |
| 2   | F     | 648 | ASP  |
| 2   | F     | 653 | LYS  |
| 2   | F     | 663 | ARG  |
| 2   | F     | 666 | LYS  |
| 2   | F     | 667 | ASN  |
| 2   | F     | 668 | VAL  |
| 2   | F     | 677 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | GLN  |
| 1   | A     | 76  | HIS  |
| 1   | A     | 89  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 110 | GLN  |
| 1   | A     | 146 | ASN  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 187 | GLN  |
| 2   | D     | 539 | ASN  |
| 2   | D     | 574 | GLN  |
| 2   | D     | 592 | ASN  |
| 1   | B     | 59  | GLN  |
| 1   | B     | 76  | HIS  |
| 1   | B     | 89  | ASN  |
| 1   | B     | 146 | ASN  |
| 1   | B     | 161 | GLN  |
| 1   | B     | 167 | ASN  |
| 1   | B     | 169 | GLN  |
| 1   | B     | 187 | GLN  |
| 2   | E     | 539 | ASN  |
| 2   | E     | 574 | GLN  |
| 2   | E     | 667 | ASN  |
| 1   | C     | 59  | GLN  |
| 1   | C     | 76  | HIS  |
| 1   | C     | 89  | ASN  |
| 1   | C     | 146 | ASN  |
| 1   | C     | 161 | GLN  |
| 1   | C     | 167 | ASN  |
| 1   | C     | 169 | GLN  |
| 1   | C     | 187 | GLN  |
| 2   | F     | 539 | ASN  |
| 2   | F     | 574 | GLN  |
| 2   | F     | 667 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | GNP  | E     | 678 | 3    | 34,34,34     | 3.80 | 21 (61%) | 47,54,54    | 4.36 | 28 (59%) |
| 4   | GNP  | F     | 678 | 3    | 34,34,34     | 3.98 | 22 (64%) | 47,54,54    | 4.28 | 25 (53%) |
| 4   | GNP  | D     | 678 | 3    | 34,34,34     | 3.89 | 18 (52%) | 47,54,54    | 4.35 | 29 (61%) |

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   | GNP  | E     | 678 | 3    | -       | 8/18/38/38 | 0/3/3/3 |
| 4   | GNP  | F     | 678 | 3    | -       | 8/18/38/38 | 0/3/3/3 |
| 4   | GNP  | D     | 678 | 3    | -       | 8/18/38/38 | 0/3/3/3 |

All (61) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | D     | 678 | GNP  | PA-O3A | 12.03 | 1.72        | 1.59     |
| 4   | E     | 678 | GNP  | PA-O3A | 11.28 | 1.71        | 1.59     |
| 4   | F     | 678 | GNP  | PA-O3A | 11.14 | 1.71        | 1.59     |
| 4   | F     | 678 | GNP  | PB-O2B | -9.17 | 1.32        | 1.56     |
| 4   | F     | 678 | GNP  | PG-O1G | 8.89  | 1.59        | 1.46     |
| 4   | D     | 678 | GNP  | PB-O2B | -8.68 | 1.33        | 1.56     |
| 4   | E     | 678 | GNP  | PB-O2B | -8.41 | 1.34        | 1.56     |
| 4   | E     | 678 | GNP  | PG-O1G | 7.05  | 1.56        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 678 | GNP  | O6-C6   | 6.72  | 1.36        | 1.23     |
| 4   | D     | 678 | GNP  | PG-O1G  | 6.66  | 1.56        | 1.46     |
| 4   | E     | 678 | GNP  | O6-C6   | 6.57  | 1.36        | 1.23     |
| 4   | F     | 678 | GNP  | O6-C6   | 6.41  | 1.35        | 1.23     |
| 4   | D     | 678 | GNP  | PB-N3B  | 5.59  | 1.78        | 1.63     |
| 4   | F     | 678 | GNP  | PB-N3B  | 5.51  | 1.77        | 1.63     |
| 4   | E     | 678 | GNP  | PB-N3B  | 5.47  | 1.77        | 1.63     |
| 4   | F     | 678 | GNP  | PG-O2G  | -5.04 | 1.43        | 1.56     |
| 4   | D     | 678 | GNP  | C2-N1   | 4.99  | 1.49        | 1.37     |
| 4   | F     | 678 | GNP  | C2-N1   | 4.86  | 1.49        | 1.37     |
| 4   | D     | 678 | GNP  | PG-O2G  | -4.75 | 1.44        | 1.56     |
| 4   | E     | 678 | GNP  | C8-N9   | 4.67  | 1.48        | 1.37     |
| 4   | F     | 678 | GNP  | C8-N9   | 4.57  | 1.47        | 1.37     |
| 4   | E     | 678 | GNP  | C2-N1   | 4.46  | 1.48        | 1.37     |
| 4   | E     | 678 | GNP  | PG-O2G  | -4.24 | 1.45        | 1.56     |
| 4   | D     | 678 | GNP  | PB-O3A  | -4.10 | 1.54        | 1.59     |
| 4   | D     | 678 | GNP  | C8-N9   | 4.05  | 1.46        | 1.37     |
| 4   | F     | 678 | GNP  | O3'-C3' | 4.02  | 1.52        | 1.43     |
| 4   | E     | 678 | GNP  | C2-N3   | -3.84 | 1.23        | 1.33     |
| 4   | E     | 678 | GNP  | O3'-C3' | 3.73  | 1.52        | 1.43     |
| 4   | D     | 678 | GNP  | O3'-C3' | 3.46  | 1.51        | 1.43     |
| 4   | D     | 678 | GNP  | C6-N1   | -3.45 | 1.32        | 1.38     |
| 4   | F     | 678 | GNP  | C2-N3   | -3.39 | 1.24        | 1.33     |
| 4   | D     | 678 | GNP  | C2-N3   | -3.35 | 1.25        | 1.33     |
| 4   | E     | 678 | GNP  | PB-O3A  | -3.01 | 1.55        | 1.59     |
| 4   | E     | 678 | GNP  | C6-N1   | -2.98 | 1.33        | 1.38     |
| 4   | E     | 678 | GNP  | C2-N2   | -2.75 | 1.27        | 1.34     |
| 4   | F     | 678 | GNP  | PB-O3A  | -2.72 | 1.55        | 1.59     |
| 4   | D     | 678 | GNP  | C2-N2   | -2.68 | 1.27        | 1.34     |
| 4   | F     | 678 | GNP  | C2-N2   | -2.68 | 1.27        | 1.34     |
| 4   | D     | 678 | GNP  | C8-N7   | 2.63  | 1.39        | 1.32     |
| 4   | F     | 678 | GNP  | C6-N1   | -2.60 | 1.34        | 1.38     |
| 4   | D     | 678 | GNP  | C5-N7   | -2.50 | 1.34        | 1.39     |
| 4   | E     | 678 | GNP  | C2'-C3' | 2.47  | 1.60        | 1.53     |
| 4   | F     | 678 | GNP  | C8-N7   | 2.44  | 1.39        | 1.32     |
| 4   | F     | 678 | GNP  | C5-N7   | -2.44 | 1.34        | 1.39     |
| 4   | E     | 678 | GNP  | C8-N7   | 2.42  | 1.39        | 1.32     |
| 4   | F     | 678 | GNP  | C2'-C3' | 2.40  | 1.59        | 1.53     |
| 4   | E     | 678 | GNP  | C5-N7   | -2.39 | 1.34        | 1.39     |
| 4   | F     | 678 | GNP  | PB-O1B  | 2.38  | 1.49        | 1.46     |
| 4   | D     | 678 | GNP  | C2'-C3' | 2.26  | 1.59        | 1.53     |
| 4   | E     | 678 | GNP  | O4'-C1' | 2.23  | 1.47        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | E     | 678 | GNP  | C5-C4   | 2.23  | 1.44        | 1.38     |
| 4   | F     | 678 | GNP  | O4'-C1' | 2.20  | 1.47        | 1.42     |
| 4   | D     | 678 | GNP  | C2'-C1' | 2.18  | 1.60        | 1.53     |
| 4   | F     | 678 | GNP  | C2'-C1' | 2.13  | 1.60        | 1.53     |
| 4   | E     | 678 | GNP  | C2'-C1' | 2.11  | 1.60        | 1.53     |
| 4   | E     | 678 | GNP  | O2'-C2' | 2.11  | 1.48        | 1.43     |
| 4   | F     | 678 | GNP  | C5'-C4' | -2.09 | 1.45        | 1.51     |
| 4   | F     | 678 | GNP  | O2'-C2' | 2.08  | 1.48        | 1.43     |
| 4   | F     | 678 | GNP  | C5-C4   | 2.08  | 1.44        | 1.38     |
| 4   | E     | 678 | GNP  | PB-O1B  | 2.03  | 1.49        | 1.46     |
| 4   | D     | 678 | GNP  | O4'-C1' | 2.01  | 1.46        | 1.42     |

All (82) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4   | F     | 678 | GNP  | N9-C8-N7 | -12.43 | 90.35       | 113.40   |
| 4   | D     | 678 | GNP  | N9-C8-N7 | -12.35 | 90.50       | 113.40   |
| 4   | E     | 678 | GNP  | N9-C8-N7 | -12.34 | 90.51       | 113.40   |
| 4   | E     | 678 | GNP  | C8-N7-C5 | 11.69  | 125.09      | 104.26   |
| 4   | F     | 678 | GNP  | C8-N7-C5 | 11.57  | 124.86      | 104.26   |
| 4   | D     | 678 | GNP  | C8-N7-C5 | 11.38  | 124.54      | 104.26   |
| 4   | E     | 678 | GNP  | C6-C5-N7 | 10.97  | 150.26      | 130.29   |
| 4   | F     | 678 | GNP  | C6-C5-N7 | 10.38  | 149.19      | 130.29   |
| 4   | D     | 678 | GNP  | C6-C5-N7 | 10.35  | 149.12      | 130.29   |
| 4   | F     | 678 | GNP  | C8-N9-C4 | 7.09   | 119.32      | 106.03   |
| 4   | D     | 678 | GNP  | C8-N9-C4 | 7.08   | 119.30      | 106.03   |
| 4   | D     | 678 | GNP  | C2-N3-C4 | 7.07   | 124.47      | 112.30   |
| 4   | E     | 678 | GNP  | C6-C5-C4 | -7.07  | 108.20      | 118.83   |
| 4   | E     | 678 | GNP  | C2-N3-C4 | 6.97   | 124.31      | 112.30   |
| 4   | E     | 678 | GNP  | C8-N9-C4 | 6.90   | 118.96      | 106.03   |
| 4   | F     | 678 | GNP  | C2-N3-C4 | 6.89   | 124.17      | 112.30   |
| 4   | D     | 678 | GNP  | C6-C5-C4 | -6.58  | 108.93      | 118.83   |
| 4   | F     | 678 | GNP  | C6-C5-C4 | -6.53  | 109.00      | 118.83   |
| 4   | E     | 678 | GNP  | C4-C5-N7 | -5.84  | 101.42      | 110.67   |
| 4   | E     | 678 | GNP  | C5-C6-N1 | 5.73   | 127.83      | 113.25   |
| 4   | F     | 678 | GNP  | C4-C5-N7 | -5.68  | 101.68      | 110.67   |
| 4   | D     | 678 | GNP  | C5-C6-N1 | 5.67   | 127.68      | 113.25   |
| 4   | E     | 678 | GNP  | O6-C6-C5 | -5.65  | 111.61      | 126.53   |
| 4   | D     | 678 | GNP  | C4-C5-N7 | -5.63  | 101.74      | 110.67   |
| 4   | F     | 678 | GNP  | C5-C6-N1 | 5.51   | 127.27      | 113.25   |
| 4   | E     | 678 | GNP  | C2-N1-C6 | -5.30  | 115.50      | 125.11   |
| 4   | D     | 678 | GNP  | C2-N1-C6 | -5.24  | 115.60      | 125.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | F     | 678 | GNP  | O6-C6-C5    | -5.22 | 112.75      | 126.53   |
| 4   | D     | 678 | GNP  | O3'-C3'-C4' | -5.18 | 96.21       | 111.08   |
| 4   | F     | 678 | GNP  | C2-N1-C6    | -5.12 | 115.82      | 125.11   |
| 4   | D     | 678 | GNP  | N2-C2-N3    | 5.10  | 129.63      | 119.67   |
| 4   | D     | 678 | GNP  | O6-C6-C5    | -5.08 | 113.11      | 126.53   |
| 4   | D     | 678 | GNP  | O1G-PG-N3B  | -4.93 | 104.50      | 111.77   |
| 4   | E     | 678 | GNP  | O3'-C3'-C4' | -4.88 | 97.06       | 111.08   |
| 4   | F     | 678 | GNP  | N2-C2-N3    | 4.85  | 129.14      | 119.67   |
| 4   | F     | 678 | GNP  | O3'-C3'-C4' | -4.80 | 97.29       | 111.08   |
| 4   | E     | 678 | GNP  | O1G-PG-N3B  | -4.66 | 104.91      | 111.77   |
| 4   | E     | 678 | GNP  | N2-C2-N3    | 4.61  | 128.67      | 119.67   |
| 4   | F     | 678 | GNP  | O3'-C3'-C2' | -4.39 | 97.73       | 111.82   |
| 4   | F     | 678 | GNP  | O1G-PG-N3B  | -4.32 | 105.41      | 111.77   |
| 4   | D     | 678 | GNP  | O3G-PG-O1G  | -4.17 | 102.99      | 113.45   |
| 4   | D     | 678 | GNP  | O3'-C3'-C2' | -4.13 | 98.57       | 111.82   |
| 4   | E     | 678 | GNP  | O3'-C3'-C2' | -4.08 | 98.75       | 111.82   |
| 4   | D     | 678 | GNP  | C2'-C3'-C4' | 3.98  | 110.29      | 102.61   |
| 4   | E     | 678 | GNP  | C2'-C3'-C4' | 3.98  | 110.29      | 102.61   |
| 4   | F     | 678 | GNP  | O3G-PG-O1G  | -3.62 | 104.38      | 113.45   |
| 4   | F     | 678 | GNP  | C2'-C3'-C4' | 3.59  | 109.55      | 102.61   |
| 4   | F     | 678 | GNP  | C1'-N9-C8   | -3.44 | 116.95      | 126.73   |
| 4   | E     | 678 | GNP  | O3G-PG-O1G  | -3.44 | 104.84      | 113.45   |
| 4   | E     | 678 | GNP  | C1'-N9-C8   | -3.36 | 117.19      | 126.73   |
| 4   | D     | 678 | GNP  | C1'-N9-C8   | -3.26 | 117.48      | 126.73   |
| 4   | D     | 678 | GNP  | C4'-O4'-C1' | 3.23  | 116.59      | 109.47   |
| 4   | E     | 678 | GNP  | C4'-O4'-C1' | 3.21  | 116.55      | 109.47   |
| 4   | E     | 678 | GNP  | O2'-C2'-C1' | -3.10 | 99.42       | 110.10   |
| 4   | F     | 678 | GNP  | C4'-O4'-C1' | 2.98  | 116.04      | 109.47   |
| 4   | D     | 678 | GNP  | O2'-C2'-C1' | -2.97 | 99.89       | 110.10   |
| 4   | F     | 678 | GNP  | O2'-C2'-C1' | -2.95 | 99.95       | 110.10   |
| 4   | D     | 678 | GNP  | N1-C2-N3    | -2.88 | 118.06      | 123.32   |
| 4   | F     | 678 | GNP  | N1-C2-N3    | -2.79 | 118.22      | 123.32   |
| 4   | D     | 678 | GNP  | O2G-PG-O3G  | 2.78  | 115.06      | 107.59   |
| 4   | D     | 678 | GNP  | O2B-PB-O3A  | 2.71  | 113.67      | 104.64   |
| 4   | F     | 678 | GNP  | O2G-PG-O1G  | -2.66 | 106.77      | 113.45   |
| 4   | E     | 678 | GNP  | O4'-C4'-C3' | -2.66 | 99.87       | 105.15   |
| 4   | D     | 678 | GNP  | N9-C4-N3    | 2.59  | 131.13      | 125.95   |
| 4   | F     | 678 | GNP  | O2A-PA-O1A  | 2.57  | 124.38      | 112.44   |
| 4   | E     | 678 | GNP  | O2G-PG-O1G  | -2.56 | 107.04      | 113.45   |
| 4   | D     | 678 | GNP  | O4'-C4'-C3' | -2.55 | 100.10      | 105.15   |
| 4   | F     | 678 | GNP  | N9-C4-N3    | 2.50  | 130.96      | 125.95   |
| 4   | E     | 678 | GNP  | N9-C4-N3    | 2.47  | 130.89      | 125.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | E     | 678 | GNP  | N1-C2-N3    | -2.46 | 118.82      | 123.32   |
| 4   | E     | 678 | GNP  | O2A-PA-O1A  | 2.45  | 123.83      | 112.44   |
| 4   | D     | 678 | GNP  | O2A-PA-O1A  | 2.35  | 123.38      | 112.44   |
| 4   | E     | 678 | GNP  | O2G-PG-O3G  | 2.31  | 113.80      | 107.59   |
| 4   | D     | 678 | GNP  | O2G-PG-O1G  | -2.30 | 107.69      | 113.45   |
| 4   | F     | 678 | GNP  | O4'-C4'-C3' | -2.25 | 100.69      | 105.15   |
| 4   | E     | 678 | GNP  | O3A-PB-N3B  | 2.24  | 112.80      | 106.59   |
| 4   | D     | 678 | GNP  | C5-C4-N3    | -2.12 | 125.01      | 128.39   |
| 4   | D     | 678 | GNP  | N2-C2-N1    | -2.11 | 112.31      | 116.76   |
| 4   | D     | 678 | GNP  | O3A-PB-N3B  | 2.08  | 112.37      | 106.59   |
| 4   | E     | 678 | GNP  | C5-C4-N3    | -2.05 | 125.13      | 128.39   |
| 4   | E     | 678 | GNP  | N2-C2-N1    | -2.02 | 112.50      | 116.76   |
| 4   | F     | 678 | GNP  | C5'-C4'-C3' | 2.01  | 122.43      | 115.21   |

There are no chirality outliers.

All (24) torsion outliers are listed below:

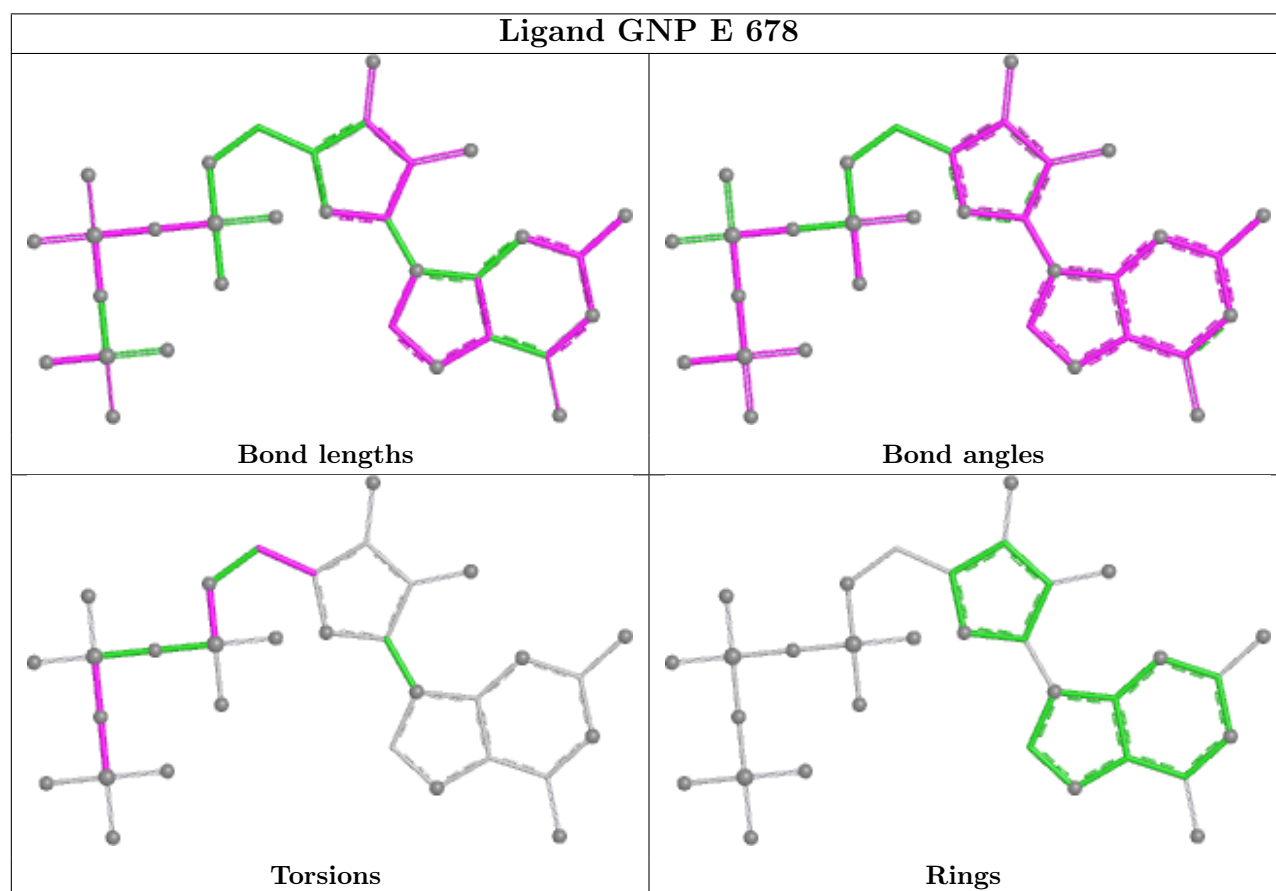
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | D     | 678 | GNP  | PB-N3B-PG-O1G   |
| 4   | D     | 678 | GNP  | PG-N3B-PB-O1B   |
| 4   | D     | 678 | GNP  | PG-N3B-PB-O3A   |
| 4   | D     | 678 | GNP  | C5'-O5'-PA-O2A  |
| 4   | D     | 678 | GNP  | O4'-C4'-C5'-O5' |
| 4   | E     | 678 | GNP  | PB-N3B-PG-O1G   |
| 4   | E     | 678 | GNP  | PG-N3B-PB-O1B   |
| 4   | E     | 678 | GNP  | PG-N3B-PB-O3A   |
| 4   | E     | 678 | GNP  | C5'-O5'-PA-O2A  |
| 4   | E     | 678 | GNP  | O4'-C4'-C5'-O5' |
| 4   | F     | 678 | GNP  | PB-N3B-PG-O1G   |
| 4   | F     | 678 | GNP  | PG-N3B-PB-O1B   |
| 4   | F     | 678 | GNP  | PG-N3B-PB-O3A   |
| 4   | F     | 678 | GNP  | C5'-O5'-PA-O2A  |
| 4   | F     | 678 | GNP  | O4'-C4'-C5'-O5' |
| 4   | D     | 678 | GNP  | C3'-C4'-C5'-O5' |
| 4   | E     | 678 | GNP  | C3'-C4'-C5'-O5' |
| 4   | F     | 678 | GNP  | C3'-C4'-C5'-O5' |
| 4   | D     | 678 | GNP  | C5'-O5'-PA-O3A  |
| 4   | D     | 678 | GNP  | C5'-O5'-PA-O1A  |
| 4   | E     | 678 | GNP  | C5'-O5'-PA-O3A  |
| 4   | E     | 678 | GNP  | C5'-O5'-PA-O1A  |
| 4   | F     | 678 | GNP  | C5'-O5'-PA-O3A  |
| 4   | F     | 678 | GNP  | C5'-O5'-PA-O1A  |

There are no ring outliers.

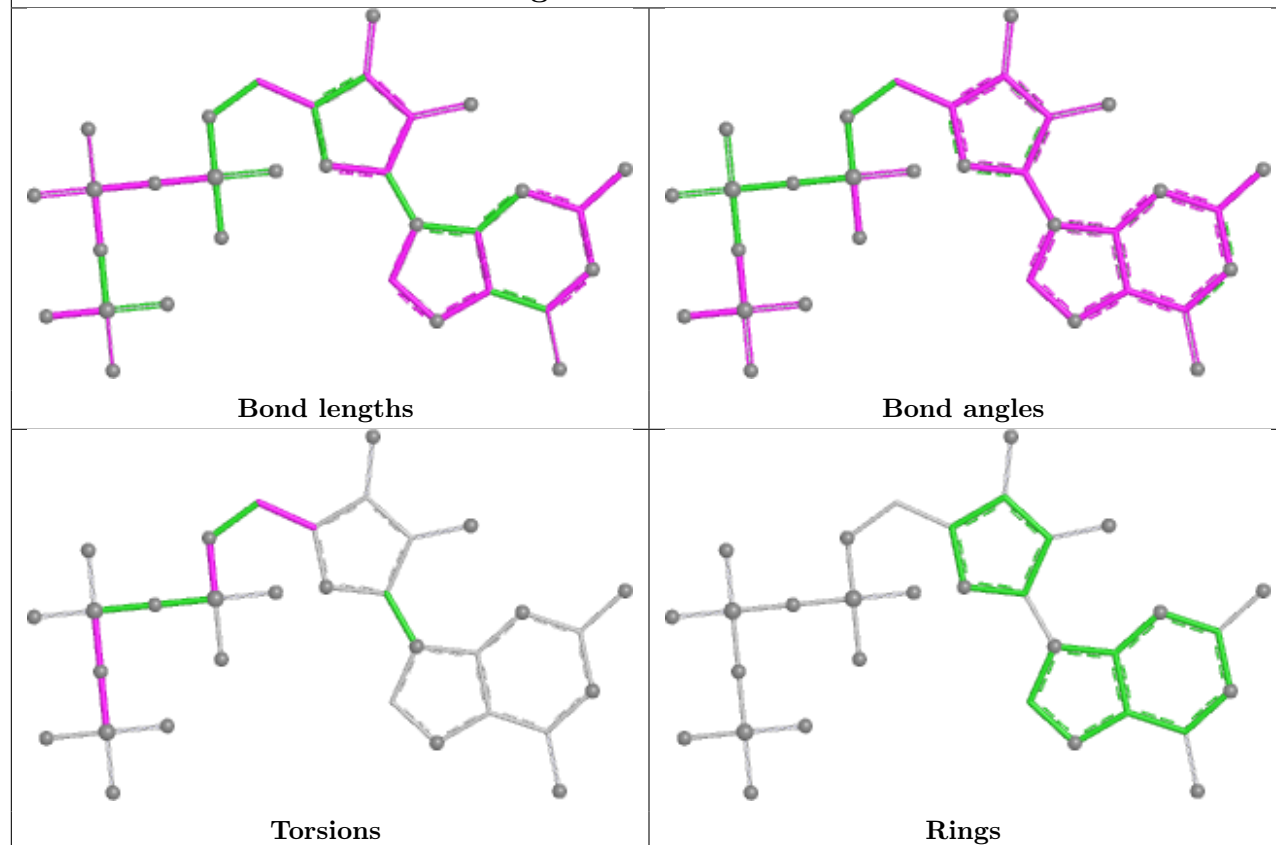
3 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | E     | 678 | GNP  | 7       | 0            |
| 4   | F     | 678 | GNP  | 7       | 0            |
| 4   | D     | 678 | GNP  | 9       | 0            |

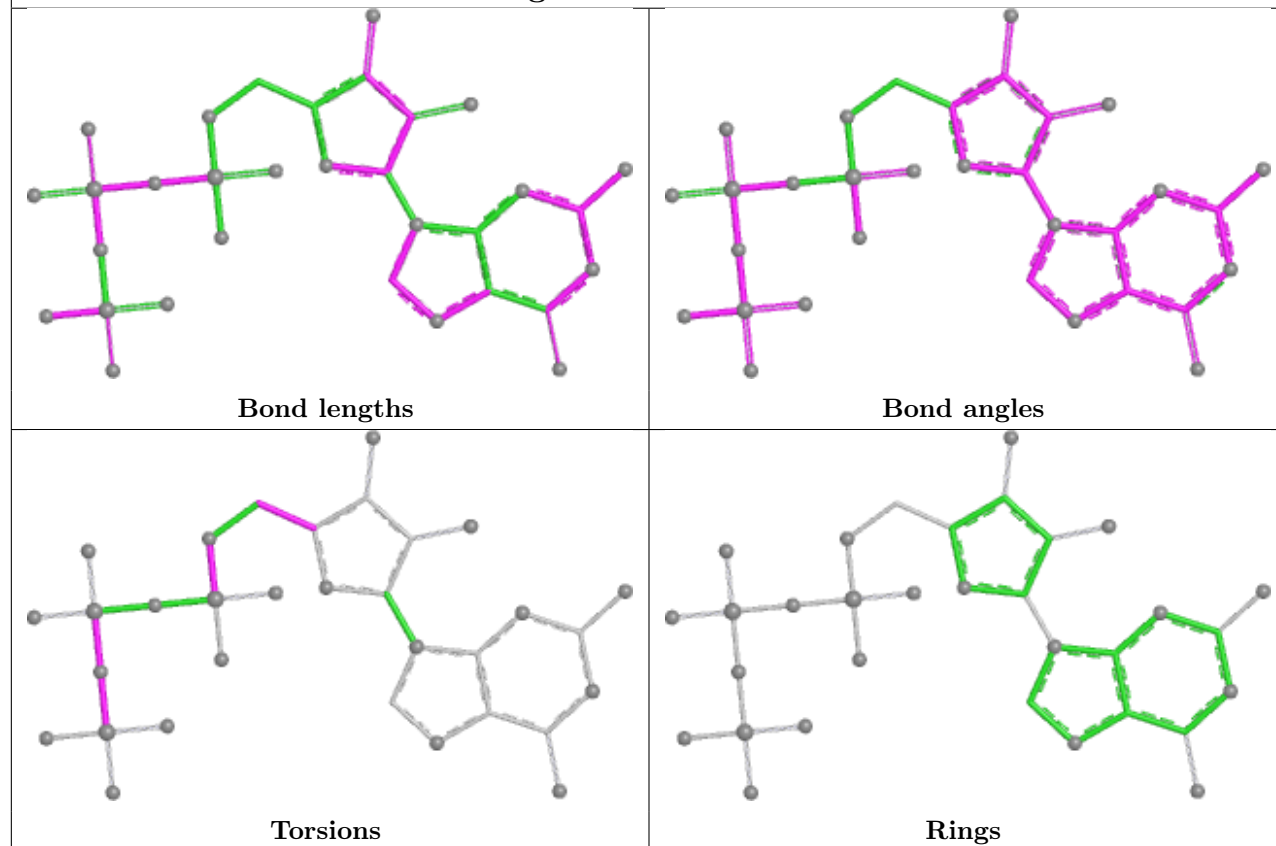
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand GNP F 678



## Ligand GNP D 678



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.