



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:57 PM UTC

PDB ID : 7P3Y / pdb\_00007p3y  
EMDB ID : EMD-13188  
Title : Homology model of the full-length AP-3 complex in an intermediate open conformation  
Authors : Schubert, E.; Raunser, S.  
Deposited on : 2021-07-09  
Resolution : 10.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

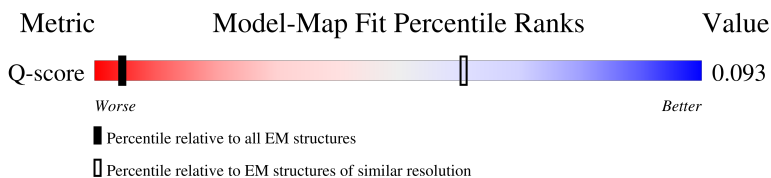
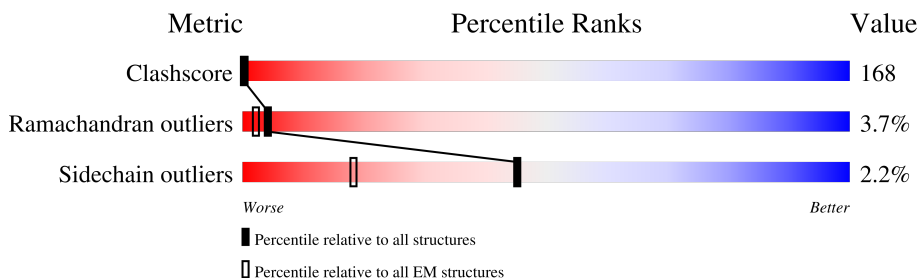
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.10 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 127 ( 9.60 - 10.60 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                       |
|-----|-------|--------|--------------------------------------------------------|
| 1   | A     | 964    | <div> <div>21%</div> <div>16% 36% 6% 40%</div> </div>  |
| 2   | B     | 809    | <div> <div>33%</div> <div>16% 53% 7% 23%</div> </div>  |
| 3   | M     | 483    | <div> <div>34%</div> <div>25% 46% 7% 18%</div> </div>  |
| 4   | S     | 194    | <div> <div>51%</div> <div>26% 48% 11% 13%</div> </div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14102 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 AP-3 complex subunit delta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 576      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4625  | 2978 | 738 | 881 | 28 |         |       |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| A     | 933     | ARG      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 934     | THR      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 935     | LEU      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 936     | GLN      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 937     | VAL      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 938     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 939     | GLY      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 940     | SER      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 941     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 942     | TYR      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 943     | LYS      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 944     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 945     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 946     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 947     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 948     | LYS      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 949     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 950     | TYR      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 951     | LYS      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 952     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 953     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 954     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 955     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 956     | LYS      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 957     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 958     | TYR      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 959     | LYS      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 960     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| A     | 961     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 962     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 963     | ASP      | -      | expression tag | UNP A0A7I9C4X2 |
| A     | 964     | LYS      | -      | expression tag | UNP A0A7I9C4X2 |

- Molecule 2 is a protein called Y55\_G0035830.mRNA.1.CDS.1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 621      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4961  | 3166 | 830 | 937 | 28 |         |       |

- Molecule 3 is a protein called AP-3 complex subunit mu.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | M     | 397      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3158  | 2018 | 516 | 612 | 12 |         |       |

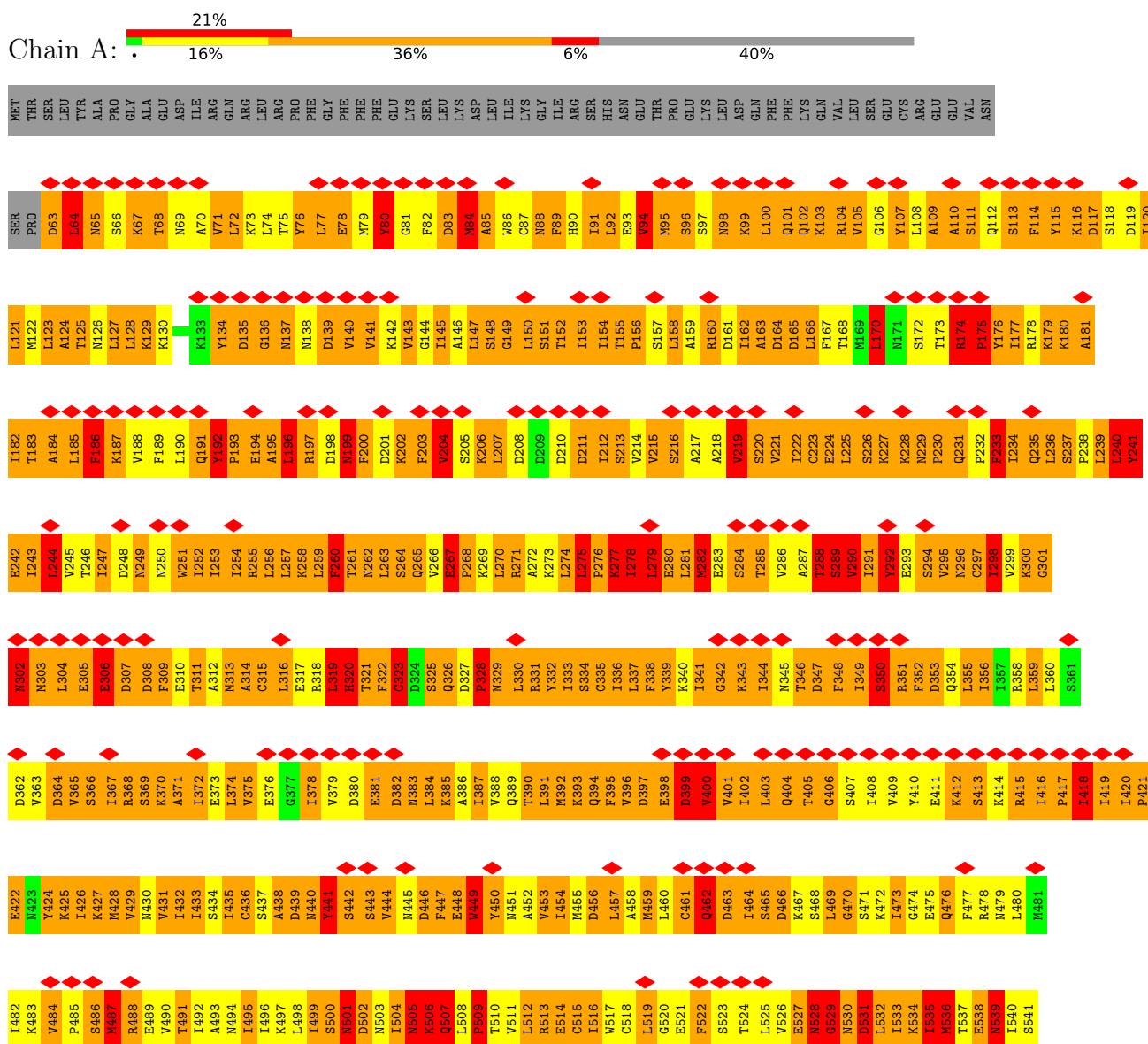
- Molecule 4 is a protein called AP complex subunit sigma.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | S     | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1358  | 867 | 215 | 272 | 4 |         |       |

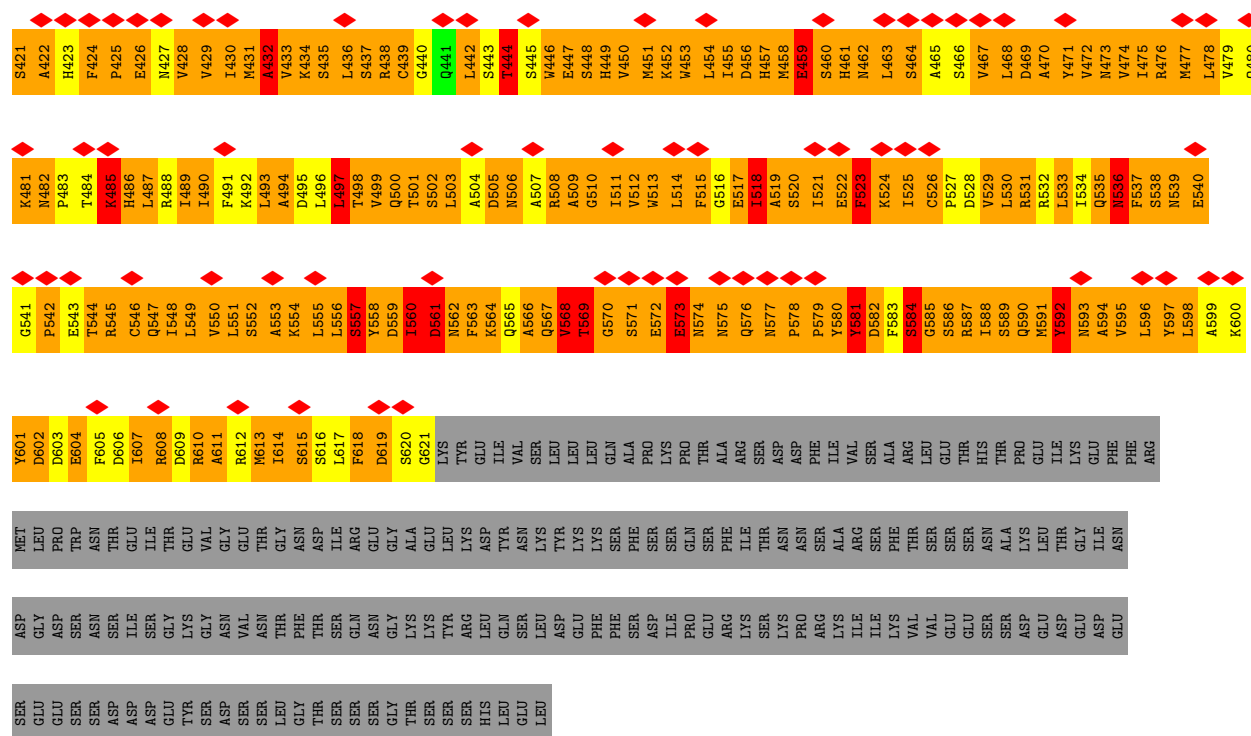
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

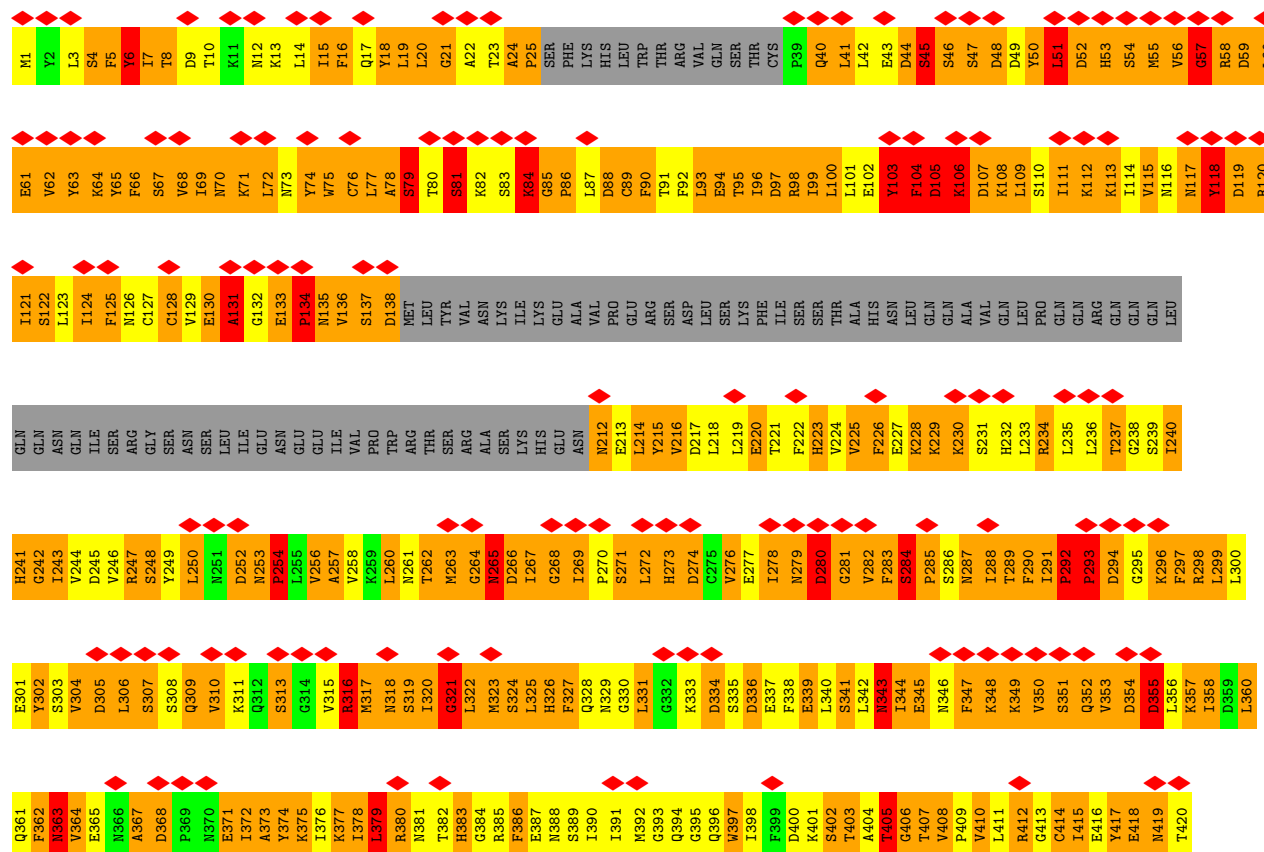
#### • Molecule 1: AP-3 complex subunit delta





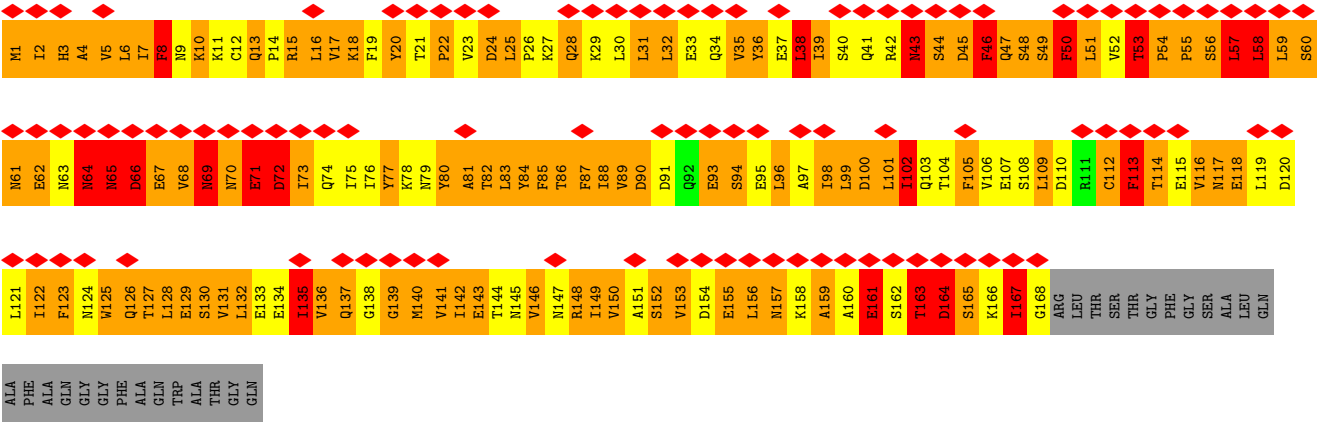


• Molecule 3: AP-3 complex subunit mu





• Molecule 4: AP complex subunit sigma



|     |
|-----|
| ALA |
| PHE |
| ALA |
| GLN |
| GLY |
| GLY |
| PHE |
| ALA |
| GLN |
| TRP |
| ALA |
| THR |
| GLY |
| GLN |

## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 19300                     | Depositor |
| Resolution determination method      | FSC 0.5 CUT-OFF           | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY       | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 81                        | Depositor |
| Minimum defocus (nm)                 | 1500                      | Depositor |
| Maximum defocus (nm)                 | 3600                      | Depositor |
| Magnification                        | 130000                    | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 0.051                     | Depositor |
| Minimum map value                    | -0.021                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.002                     | Depositor |
| Recommended contour level            | 0.018                     | Depositor |
| Map size ( $\text{\AA}$ )            | 282.48, 282.48, 282.48    | wwPDB     |
| Map dimensions                       | 264, 264, 264             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.07, 1.07, 1.07          | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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     | 2.74         | 396/4699 (8.4%)   | 4.71        | 1226/6358 (19.3%)  |
| 2   | B     | 2.57         | 381/5055 (7.5%)   | 4.28        | 1219/6852 (17.8%)  |
| 3   | M     | 3.75         | 365/3217 (11.3%)  | 4.17        | 634/4346 (14.6%)   |
| 4   | S     | 3.86         | 196/1379 (14.2%)  | 4.43        | 330/1874 (17.6%)   |
| All | All   | 3.06         | 1338/14350 (9.3%) | 4.42        | 3409/19430 (17.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 52                  |
| 2   | B     | 0                   | 32                  |
| 3   | M     | 1                   | 23                  |
| 4   | S     | 1                   | 18                  |
| All | All   | 2                   | 125                 |

All (1338) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | M     | 104 | PHE  | N-CA  | -35.34 | 1.00        | 1.46     |
| 3   | M     | 135 | ASN  | C-N   | -34.35 | 0.94        | 1.33     |
| 3   | M     | 63  | TYR  | CA-C  | -29.63 | 1.16        | 1.52     |
| 3   | M     | 65  | TYR  | CA-C  | -28.59 | 1.17        | 1.52     |
| 3   | M     | 64  | LYS  | N-CA  | -28.36 | 1.09        | 1.45     |
| 3   | M     | 136 | VAL  | N-CA  | -25.88 | 1.15        | 1.46     |
| 3   | M     | 131 | ALA  | CA-C  | -24.91 | 1.21        | 1.53     |
| 3   | M     | 107 | ASP  | N-CA  | -23.75 | 1.15        | 1.46     |
| 3   | M     | 61  | GLU  | CA-C  | -23.51 | 1.24        | 1.52     |
| 4   | S     | 48  | SER  | CA-C  | -23.23 | 1.22        | 1.52     |
| 4   | S     | 49  | SER  | N-CA  | -22.80 | 1.16        | 1.46     |
| 4   | S     | 58  | LEU  | CA-C  | -22.50 | 1.26        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | M     | 56  | VAL  | CA-C  | -22.46 | 1.25        | 1.52     |
| 4   | S     | 68  | VAL  | C-N   | 21.95  | 1.67        | 1.33     |
| 3   | M     | 135 | ASN  | CA-C  | -21.28 | 1.26        | 1.52     |
| 4   | S     | 163 | THR  | CA-C  | 21.27  | 1.81        | 1.52     |
| 2   | B     | 293 | VAL  | C-N   | -21.22 | 1.13        | 1.33     |
| 4   | S     | 46  | PHE  | CA-C  | -21.22 | 1.24        | 1.52     |
| 1   | A     | 218 | ALA  | CA-C  | -20.45 | 1.26        | 1.52     |
| 1   | A     | 438 | ALA  | CA-CB | -20.01 | 1.19        | 1.53     |
| 4   | S     | 48  | SER  | C-N   | -19.95 | 1.04        | 1.33     |
| 3   | M     | 81  | SER  | C-N   | -19.87 | 1.08        | 1.33     |
| 4   | S     | 64  | ASN  | CA-C  | 19.57  | 1.80        | 1.52     |
| 3   | M     | 132 | GLY  | CA-C  | -19.55 | 1.24        | 1.51     |
| 3   | M     | 133 | GLU  | N-CA  | -19.31 | 1.18        | 1.45     |
| 3   | M     | 64  | LYS  | CA-C  | -19.27 | 1.29        | 1.52     |
| 4   | S     | 50  | PHE  | CA-C  | -19.13 | 1.27        | 1.52     |
| 4   | S     | 53  | THR  | N-CA  | -18.97 | 1.17        | 1.45     |
| 3   | M     | 281 | GLY  | CA-C  | 18.95  | 1.78        | 1.51     |
| 3   | M     | 3   | LEU  | C-N   | -18.87 | 1.07        | 1.33     |
| 3   | M     | 66  | PHE  | N-CA  | -18.73 | 1.21        | 1.45     |
| 3   | M     | 62  | VAL  | CA-C  | -18.48 | 1.28        | 1.52     |
| 3   | M     | 282 | VAL  | N-CA  | 18.30  | 1.68        | 1.46     |
| 3   | M     | 41  | LEU  | CA-C  | -18.00 | 1.29        | 1.52     |
| 3   | M     | 63  | TYR  | N-CA  | -17.56 | 1.24        | 1.46     |
| 4   | S     | 83  | LEU  | CA-C  | 17.53  | 1.73        | 1.52     |
| 4   | S     | 63  | ASN  | CA-C  | -16.99 | 1.32        | 1.52     |
| 3   | M     | 335 | SER  | CA-C  | -16.83 | 1.31        | 1.52     |
| 3   | M     | 354 | ASP  | CA-C  | 16.81  | 1.73        | 1.52     |
| 3   | M     | 137 | SER  | N-CA  | -16.80 | 1.24        | 1.46     |
| 1   | A     | 405 | THR  | CA-C  | -16.51 | 1.31        | 1.52     |
| 1   | A     | 394 | GLN  | CA-C  | -16.48 | 1.31        | 1.52     |
| 3   | M     | 105 | ASP  | C-N   | -16.43 | 1.10        | 1.33     |
| 3   | M     | 225 | VAL  | CA-C  | -16.43 | 1.31        | 1.52     |
| 3   | M     | 80  | THR  | C-N   | -16.11 | 1.11        | 1.33     |
| 3   | M     | 52  | ASP  | C-N   | -16.00 | 1.13        | 1.33     |
| 3   | M     | 62  | VAL  | N-CA  | -15.91 | 1.25        | 1.46     |
| 3   | M     | 65  | TYR  | N-CA  | -15.81 | 1.26        | 1.45     |
| 3   | M     | 131 | ALA  | CA-CB | 15.81  | 1.78        | 1.53     |
| 1   | A     | 139 | ASP  | N-CA  | -15.72 | 1.27        | 1.46     |
| 4   | S     | 51  | LEU  | N-CA  | -15.68 | 1.27        | 1.46     |
| 2   | B     | 284 | ASN  | C-N   | -15.52 | 1.13        | 1.33     |
| 2   | B     | 337 | THR  | N-CA  | -15.45 | 1.28        | 1.46     |
| 4   | S     | 116 | VAL  | CA-C  | -15.29 | 1.33        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 407 | SER  | N-CA  | 15.20  | 1.65        | 1.45     |
| 3   | M     | 281 | GLY  | C-N   | 15.13  | 1.53        | 1.33     |
| 3   | M     | 130 | GLU  | C-N   | -15.07 | 1.12        | 1.33     |
| 1   | A     | 406 | GLY  | CA-C  | 14.98  | 1.73        | 1.51     |
| 3   | M     | 61  | GLU  | C-N   | -14.90 | 1.15        | 1.33     |
| 3   | M     | 348 | LYS  | CA-C  | 14.88  | 1.72        | 1.52     |
| 2   | B     | 212 | VAL  | C-O   | 14.65  | 1.38        | 1.24     |
| 3   | M     | 45  | SER  | CA-C  | 14.62  | 1.72        | 1.52     |
| 3   | M     | 132 | GLY  | N-CA  | -14.46 | 1.24        | 1.45     |
| 3   | M     | 136 | VAL  | CA-C  | -14.45 | 1.33        | 1.52     |
| 2   | B     | 581 | TYR  | N-CA  | -14.35 | 1.28        | 1.46     |
| 3   | M     | 21  | GLY  | C-N   | -14.34 | 1.13        | 1.33     |
| 4   | S     | 49  | SER  | C-N   | 14.30  | 1.53        | 1.33     |
| 3   | M     | 103 | TYR  | CA-C  | 14.22  | 1.72        | 1.53     |
| 2   | B     | 581 | TYR  | C-N   | -14.21 | 1.14        | 1.33     |
| 4   | S     | 71  | GLU  | N-CA  | -14.12 | 1.27        | 1.46     |
| 3   | M     | 230 | LYS  | CA-C  | 14.09  | 1.70        | 1.53     |
| 3   | M     | 351 | SER  | C-N   | -13.94 | 1.14        | 1.33     |
| 4   | S     | 143 | GLU  | CA-C  | -13.76 | 1.35        | 1.52     |
| 3   | M     | 231 | SER  | N-CA  | 13.72  | 1.63        | 1.46     |
| 1   | A     | 406 | GLY  | C-N   | 13.53  | 1.51        | 1.33     |
| 2   | B     | 185 | LYS  | N-CA  | -13.50 | 1.30        | 1.46     |
| 4   | S     | 55  | PRO  | N-CA  | 13.44  | 1.65        | 1.47     |
| 3   | M     | 131 | ALA  | N-CA  | -13.43 | 1.26        | 1.46     |
| 1   | A     | 217 | ALA  | C-N   | 13.40  | 1.51        | 1.33     |
| 3   | M     | 20  | LEU  | C-N   | -13.40 | 1.13        | 1.33     |
| 1   | A     | 440 | ASN  | N-CA  | -13.32 | 1.30        | 1.46     |
| 3   | M     | 106 | LYS  | C-N   | -13.31 | 1.14        | 1.33     |
| 1   | A     | 467 | LYS  | N-CA  | -13.17 | 1.29        | 1.46     |
| 3   | M     | 349 | LYS  | N-CA  | 13.16  | 1.63        | 1.46     |
| 3   | M     | 450 | GLU  | C-N   | -13.14 | 1.17        | 1.33     |
| 2   | B     | 329 | ALA  | CA-C  | -13.13 | 1.35        | 1.52     |
| 4   | S     | 67  | GLU  | N-CA  | -13.11 | 1.28        | 1.45     |
| 4   | S     | 115 | GLU  | CA-C  | -13.00 | 1.39        | 1.53     |
| 1   | A     | 289 | SER  | C-N   | -12.96 | 1.18        | 1.33     |
| 3   | M     | 319 | SER  | C-N   | -12.84 | 1.16        | 1.33     |
| 4   | S     | 72  | ASP  | N-CA  | -12.81 | 1.29        | 1.46     |
| 3   | M     | 282 | VAL  | CA-C  | -12.74 | 1.36        | 1.52     |
| 3   | M     | 439 | TYR  | CA-C  | -12.72 | 1.37        | 1.52     |
| 3   | M     | 55  | MET  | C-N   | 12.63  | 1.49        | 1.33     |
| 3   | M     | 348 | LYS  | C-N   | 12.61  | 1.52        | 1.33     |
| 3   | M     | 279 | ASN  | C-N   | -12.58 | 1.16        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | M     | 293 | PRO  | N-CD  | 12.57  | 1.65        | 1.47     |
| 3   | M     | 239 | SER  | N-CA  | -12.56 | 1.31        | 1.46     |
| 4   | S     | 60  | SER  | N-CA  | -12.55 | 1.30        | 1.45     |
| 4   | S     | 57  | LEU  | CA-C  | -12.54 | 1.37        | 1.53     |
| 4   | S     | 6   | LEU  | C-N   | -12.54 | 1.17        | 1.33     |
| 3   | M     | 294 | ASP  | N-CA  | -12.48 | 1.30        | 1.45     |
| 4   | S     | 140 | MET  | N-CA  | -12.46 | 1.30        | 1.46     |
| 4   | S     | 144 | THR  | N-CA  | -12.43 | 1.28        | 1.45     |
| 1   | A     | 464 | ILE  | CA-C  | -12.42 | 1.36        | 1.52     |
| 1   | A     | 71  | VAL  | CA-C  | -12.40 | 1.36        | 1.52     |
| 4   | S     | 103 | GLN  | CA-C  | -12.38 | 1.36        | 1.52     |
| 1   | A     | 378 | ILE  | C-N   | -12.33 | 1.19        | 1.33     |
| 3   | M     | 60  | LEU  | CA-C  | -12.33 | 1.36        | 1.52     |
| 3   | M     | 262 | THR  | CA-C  | -12.31 | 1.37        | 1.52     |
| 4   | S     | 22  | PRO  | C-N   | -12.27 | 1.17        | 1.33     |
| 3   | M     | 44  | ASP  | C-N   | 12.21  | 1.50        | 1.33     |
| 1   | A     | 534 | LYS  | CA-C  | -12.17 | 1.37        | 1.52     |
| 3   | M     | 134 | PRO  | C-N   | -12.09 | 1.16        | 1.33     |
| 2   | B     | 293 | VAL  | CA-C  | -12.05 | 1.37        | 1.52     |
| 3   | M     | 288 | ILE  | CA-C  | -12.03 | 1.37        | 1.52     |
| 3   | M     | 97  | ASP  | CA-C  | -12.01 | 1.37        | 1.52     |
| 3   | M     | 64  | LYS  | C-N   | -11.89 | 1.18        | 1.33     |
| 3   | M     | 59  | ASP  | N-CA  | 11.82  | 1.61        | 1.46     |
| 4   | S     | 5   | VAL  | CA-C  | 11.77  | 1.67        | 1.52     |
| 3   | M     | 283 | PHE  | N-CA  | -11.76 | 1.31        | 1.46     |
| 3   | M     | 287 | ASN  | CA-C  | 11.75  | 1.67        | 1.52     |
| 1   | A     | 415 | ARG  | C-N   | -11.73 | 1.24        | 1.33     |
| 1   | A     | 466 | ASP  | CA-C  | -11.71 | 1.40        | 1.52     |
| 3   | M     | 352 | GLN  | C-N   | -11.66 | 1.17        | 1.33     |
| 3   | M     | 136 | VAL  | C-N   | -11.65 | 1.17        | 1.33     |
| 1   | A     | 439 | ASP  | C-N   | -11.64 | 1.18        | 1.33     |
| 3   | M     | 21  | GLY  | N-CA  | -11.62 | 1.32        | 1.45     |
| 3   | M     | 62  | VAL  | C-N   | -11.58 | 1.16        | 1.33     |
| 3   | M     | 278 | ILE  | CA-C  | -11.57 | 1.38        | 1.52     |
| 2   | B     | 567 | GLN  | CA-C  | -11.55 | 1.38        | 1.52     |
| 3   | M     | 379 | LEU  | C-N   | -11.53 | 1.18        | 1.33     |
| 2   | B     | 289 | PRO  | CA-C  | -11.49 | 1.36        | 1.52     |
| 3   | M     | 108 | LYS  | CA-C  | -11.49 | 1.41        | 1.53     |
| 1   | A     | 87  | CYS  | N-CA  | -11.29 | 1.30        | 1.46     |
| 3   | M     | 91  | THR  | CA-C  | -11.27 | 1.37        | 1.52     |
| 3   | M     | 95  | THR  | N-CA  | 11.27  | 1.60        | 1.46     |
| 1   | A     | 302 | ASN  | CA-C  | -11.23 | 1.37        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2   | B     | 184 | GLY  | C-N   | -11.22 | 1.19        | 1.33     |
| 3   | M     | 453 | ASP  | C-N   | -11.21 | 1.17        | 1.33     |
| 4   | S     | 70  | ASN  | C-N   | -11.21 | 1.18        | 1.33     |
| 2   | B     | 334 | MET  | N-CA  | 11.20  | 1.61        | 1.46     |
| 4   | S     | 58  | LEU  | C-N   | 11.18  | 1.48        | 1.33     |
| 2   | B     | 522 | GLU  | CA-C  | -11.15 | 1.37        | 1.53     |
| 3   | M     | 109 | LEU  | N-CA  | -11.15 | 1.31        | 1.46     |
| 2   | B     | 582 | ASP  | N-CA  | -11.13 | 1.32        | 1.46     |
| 2   | B     | 500 | GLN  | CA-C  | -11.09 | 1.39        | 1.53     |
| 2   | B     | 260 | LEU  | N-CA  | -11.07 | 1.30        | 1.46     |
| 1   | A     | 566 | PHE  | CA-C  | -11.05 | 1.36        | 1.52     |
| 1   | A     | 388 | VAL  | CA-C  | -11.03 | 1.39        | 1.52     |
| 1   | A     | 120 | ILE  | CA-C  | -11.00 | 1.39        | 1.52     |
| 2   | B     | 334 | MET  | C-N   | -10.99 | 1.19        | 1.33     |
| 2   | B     | 187 | ASP  | CA-C  | -10.99 | 1.38        | 1.52     |
| 2   | B     | 443 | SER  | CA-C  | -10.95 | 1.39        | 1.52     |
| 1   | A     | 508 | LEU  | N-CA  | -10.92 | 1.34        | 1.46     |
| 3   | M     | 442 | GLN  | N-CA  | -10.88 | 1.31        | 1.46     |
| 4   | S     | 116 | VAL  | N-CA  | -10.86 | 1.33        | 1.46     |
| 4   | S     | 99  | LEU  | CA-C  | -10.84 | 1.38        | 1.52     |
| 4   | S     | 2   | ILE  | CA-C  | -10.81 | 1.40        | 1.52     |
| 1   | A     | 192 | TYR  | CA-C  | -10.80 | 1.39        | 1.52     |
| 3   | M     | 295 | GLY  | CA-C  | 10.78  | 1.67        | 1.51     |
| 3   | M     | 403 | THR  | C-N   | -10.78 | 1.17        | 1.33     |
| 1   | A     | 83  | ASP  | CA-C  | -10.73 | 1.39        | 1.52     |
| 4   | S     | 108 | SER  | N-CA  | -10.71 | 1.33        | 1.46     |
| 3   | M     | 261 | ASN  | CA-C  | -10.65 | 1.40        | 1.52     |
| 3   | M     | 440 | ILE  | N-CA  | -10.65 | 1.32        | 1.46     |
| 2   | B     | 485 | LYS  | CA-C  | -10.64 | 1.38        | 1.52     |
| 3   | M     | 113 | LYS  | CA-C  | -10.62 | 1.38        | 1.52     |
| 3   | M     | 296 | LYS  | CA-C  | -10.62 | 1.38        | 1.52     |
| 2   | B     | 35  | TYR  | CA-C  | -10.62 | 1.39        | 1.52     |
| 2   | B     | 285 | GLU  | N-CA  | -10.61 | 1.32        | 1.46     |
| 2   | B     | 183 | ALA  | CA-CB | -10.58 | 1.36        | 1.54     |
| 1   | A     | 138 | ASN  | CA-C  | -10.57 | 1.40        | 1.53     |
| 4   | S     | 114 | THR  | C-N   | -10.57 | 1.19        | 1.33     |
| 1   | A     | 531 | ASP  | CA-C  | -10.57 | 1.38        | 1.52     |
| 1   | A     | 387 | ILE  | CA-C  | -10.56 | 1.38        | 1.52     |
| 4   | S     | 62  | GLU  | C-N   | -10.55 | 1.19        | 1.33     |
| 4   | S     | 124 | ASN  | N-CA  | -10.50 | 1.33        | 1.46     |
| 3   | M     | 336 | ASP  | N-CA  | -10.49 | 1.33        | 1.46     |
| 4   | S     | 52  | VAL  | CA-C  | -10.46 | 1.40        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | M     | 419 | ASN  | CA-C  | -10.46 | 1.40        | 1.52     |
| 1   | A     | 348 | PHE  | CA-C  | -10.45 | 1.38        | 1.52     |
| 3   | M     | 280 | ASP  | CA-C  | -10.38 | 1.38        | 1.52     |
| 3   | M     | 344 | ILE  | CA-C  | -10.36 | 1.39        | 1.52     |
| 1   | A     | 533 | ILE  | N-CA  | -10.33 | 1.34        | 1.46     |
| 3   | M     | 82  | LYS  | C-N   | -10.32 | 1.19        | 1.33     |
| 1   | A     | 153 | ILE  | C-N   | -10.32 | 1.22        | 1.33     |
| 4   | S     | 158 | LYS  | CA-C  | -10.31 | 1.38        | 1.52     |
| 3   | M     | 6   | TYR  | C-N   | -10.30 | 1.20        | 1.33     |
| 3   | M     | 320 | ILE  | N-CA  | -10.26 | 1.33        | 1.46     |
| 3   | M     | 81  | SER  | N-CA  | -10.26 | 1.32        | 1.46     |
| 1   | A     | 465 | SER  | N-CA  | -10.23 | 1.32        | 1.45     |
| 1   | A     | 418 | ILE  | C-N   | 10.22  | 1.47        | 1.33     |
| 1   | A     | 216 | SER  | C-N   | 10.20  | 1.47        | 1.33     |
| 1   | A     | 394 | GLN  | N-CA  | -10.19 | 1.34        | 1.46     |
| 3   | M     | 267 | ILE  | CA-C  | -10.18 | 1.41        | 1.52     |
| 3   | M     | 373 | ALA  | CA-C  | -10.18 | 1.40        | 1.52     |
| 1   | A     | 242 | GLU  | CA-C  | -10.15 | 1.40        | 1.52     |
| 4   | S     | 4   | ALA  | CA-CB | 10.15  | 1.70        | 1.53     |
| 2   | B     | 219 | TYR  | C-N   | -10.07 | 1.21        | 1.33     |
| 2   | B     | 568 | VAL  | N-CA  | -10.04 | 1.33        | 1.46     |
| 4   | S     | 25  | LEU  | CA-C  | 10.00  | 1.65        | 1.52     |
| 1   | A     | 623 | MET  | CA-C  | -9.99  | 1.39        | 1.52     |
| 1   | A     | 221 | VAL  | N-CA  | 9.99   | 1.58        | 1.46     |
| 3   | M     | 70  | ASN  | C-N   | -9.99  | 1.18        | 1.33     |
| 1   | A     | 298 | ILE  | C-O   | 9.97   | 1.35        | 1.24     |
| 1   | A     | 445 | ASN  | CA-C  | -9.97  | 1.39        | 1.52     |
| 3   | M     | 83  | SER  | N-CA  | -9.97  | 1.34        | 1.47     |
| 3   | M     | 420 | THR  | N-CA  | -9.97  | 1.32        | 1.46     |
| 2   | B     | 580 | TYR  | CA-C  | -9.95  | 1.40        | 1.52     |
| 1   | A     | 378 | ILE  | CA-C  | -9.93  | 1.40        | 1.52     |
| 3   | M     | 55  | MET  | N-CA  | -9.90  | 1.32        | 1.46     |
| 1   | A     | 466 | ASP  | C-N   | -9.87  | 1.20        | 1.34     |
| 2   | B     | 329 | ALA  | N-CA  | -9.87  | 1.34        | 1.46     |
| 3   | M     | 392 | MET  | N-CA  | -9.86  | 1.33        | 1.46     |
| 2   | B     | 153 | ILE  | CA-C  | -9.85  | 1.40        | 1.52     |
| 1   | A     | 399 | ASP  | CA-C  | -9.85  | 1.40        | 1.53     |
| 2   | B     | 290 | SER  | CA-C  | -9.83  | 1.39        | 1.52     |
| 1   | A     | 218 | ALA  | CA-CB | -9.82  | 1.38        | 1.53     |
| 2   | B     | 296 | ASP  | CA-C  | -9.82  | 1.40        | 1.52     |
| 4   | S     | 115 | GLU  | C-N   | -9.81  | 1.21        | 1.33     |
| 4   | S     | 29  | LYS  | CA-C  | -9.81  | 1.39        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 515 | PHE  | CA-C  | 9.80  | 1.66        | 1.52     |
| 3   | M     | 105 | ASP  | N-CA  | -9.80 | 1.33        | 1.46     |
| 4   | S     | 60  | SER  | C-N   | -9.79 | 1.20        | 1.33     |
| 1   | A     | 384 | LEU  | CA-C  | -9.79 | 1.40        | 1.52     |
| 3   | M     | 288 | ILE  | N-CA  | 9.78  | 1.58        | 1.46     |
| 3   | M     | 263 | MET  | N-CA  | -9.74 | 1.34        | 1.46     |
| 3   | M     | 364 | VAL  | CA-C  | -9.74 | 1.40        | 1.52     |
| 1   | A     | 175 | PRO  | N-CD  | 9.73  | 1.61        | 1.47     |
| 1   | A     | 410 | TYR  | N-CA  | -9.72 | 1.33        | 1.46     |
| 3   | M     | 126 | ASN  | CA-C  | -9.68 | 1.39        | 1.52     |
| 3   | M     | 130 | GLU  | CA-C  | 9.68  | 1.66        | 1.53     |
| 4   | S     | 64  | ASN  | C-N   | 9.66  | 1.47        | 1.33     |
| 3   | M     | 377 | LYS  | C-N   | -9.65 | 1.20        | 1.33     |
| 2   | B     | 219 | TYR  | CA-C  | -9.65 | 1.39        | 1.52     |
| 3   | M     | 402 | SER  | C-N   | 9.63  | 1.46        | 1.33     |
| 3   | M     | 66  | PHE  | C-N   | -9.62 | 1.21        | 1.33     |
| 1   | A     | 444 | VAL  | N-CA  | -9.60 | 1.34        | 1.46     |
| 2   | B     | 336 | ASN  | C-N   | -9.59 | 1.21        | 1.33     |
| 4   | S     | 67  | GLU  | CA-C  | -9.59 | 1.40        | 1.53     |
| 4   | S     | 47  | GLN  | N-CA  | -9.58 | 1.34        | 1.46     |
| 2   | B     | 330 | SER  | N-CA  | -9.55 | 1.32        | 1.45     |
| 2   | B     | 422 | ALA  | CA-C  | -9.54 | 1.40        | 1.53     |
| 2   | B     | 494 | ALA  | CA-C  | -9.53 | 1.40        | 1.52     |
| 2   | B     | 582 | ASP  | C-N   | -9.51 | 1.21        | 1.33     |
| 1   | A     | 287 | ALA  | CA-CB | -9.51 | 1.37        | 1.53     |
| 1   | A     | 558 | VAL  | CA-C  | -9.50 | 1.41        | 1.52     |
| 2   | B     | 458 | MET  | C-O   | 9.50  | 1.35        | 1.24     |
| 3   | M     | 257 | ALA  | N-CA  | -9.50 | 1.34        | 1.46     |
| 3   | M     | 293 | PRO  | CA-C  | -9.49 | 1.39        | 1.52     |
| 2   | B     | 264 | THR  | CA-C  | -9.49 | 1.40        | 1.52     |
| 3   | M     | 137 | SER  | CA-C  | -9.45 | 1.40        | 1.52     |
| 3   | M     | 65  | TYR  | C-N   | -9.44 | 1.20        | 1.33     |
| 1   | A     | 244 | LEU  | C-N   | -9.43 | 1.23        | 1.34     |
| 2   | B     | 263 | PRO  | CA-C  | 9.43  | 1.61        | 1.52     |
| 2   | B     | 83  | PHE  | C-N   | 9.39  | 1.46        | 1.33     |
| 2   | B     | 169 | VAL  | CA-C  | -9.38 | 1.41        | 1.52     |
| 3   | M     | 288 | ILE  | C-N   | -9.37 | 1.20        | 1.33     |
| 4   | S     | 80  | TYR  | N-CA  | -9.36 | 1.35        | 1.46     |
| 1   | A     | 465 | SER  | CA-C  | -9.36 | 1.40        | 1.52     |
| 2   | B     | 226 | LEU  | CA-C  | -9.35 | 1.40        | 1.52     |
| 4   | S     | 108 | SER  | CA-C  | -9.35 | 1.40        | 1.52     |
| 3   | M     | 322 | LEU  | C-O   | 9.35  | 1.35        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 96  | ILE  | C-N   | 9.33  | 1.46        | 1.33     |
| 2   | B     | 274 | PRO  | N-CD  | 9.32  | 1.60        | 1.47     |
| 3   | M     | 23  | THR  | C-N   | -9.32 | 1.20        | 1.34     |
| 1   | A     | 281 | LEU  | N-CA  | 9.31  | 1.58        | 1.46     |
| 2   | B     | 576 | GLN  | C-N   | -9.31 | 1.21        | 1.34     |
| 2   | B     | 583 | PHE  | CA-C  | -9.28 | 1.41        | 1.53     |
| 4   | S     | 36  | TYR  | CA-C  | -9.24 | 1.40        | 1.52     |
| 4   | S     | 84  | TYR  | C-N   | -9.20 | 1.21        | 1.33     |
| 4   | S     | 48  | SER  | N-CA  | -9.20 | 1.34        | 1.46     |
| 1   | A     | 631 | SER  | CA-C  | -9.20 | 1.40        | 1.52     |
| 3   | M     | 20  | LEU  | CA-C  | -9.19 | 1.41        | 1.52     |
| 3   | M     | 331 | LEU  | CA-C  | -9.19 | 1.40        | 1.52     |
| 4   | S     | 70  | ASN  | CA-C  | -9.19 | 1.40        | 1.52     |
| 1   | A     | 588 | LEU  | C-N   | -9.18 | 1.21        | 1.33     |
| 3   | M     | 18  | TYR  | N-CA  | -9.18 | 1.34        | 1.46     |
| 2   | B     | 568 | VAL  | CA-C  | -9.17 | 1.41        | 1.52     |
| 3   | M     | 68  | VAL  | N-CA  | -9.16 | 1.35        | 1.46     |
| 3   | M     | 404 | ALA  | N-CA  | -9.16 | 1.34        | 1.45     |
| 1   | A     | 635 | ALA  | CA-C  | -9.15 | 1.40        | 1.52     |
| 1   | A     | 277 | LYS  | C-N   | -9.15 | 1.20        | 1.33     |
| 2   | B     | 339 | PHE  | CA-C  | -9.15 | 1.41        | 1.52     |
| 4   | S     | 105 | PHE  | CA-C  | -9.13 | 1.40        | 1.52     |
| 3   | M     | 41  | LEU  | C-N   | 9.12  | 1.45        | 1.33     |
| 3   | M     | 256 | VAL  | C-O   | 9.11  | 1.33        | 1.24     |
| 1   | A     | 303 | MET  | N-CA  | -9.09 | 1.34        | 1.46     |
| 1   | A     | 632 | PHE  | CA-C  | -9.09 | 1.41        | 1.52     |
| 1   | A     | 508 | LEU  | CA-C  | -9.08 | 1.42        | 1.53     |
| 1   | A     | 301 | GLY  | CA-C  | -9.08 | 1.40        | 1.52     |
| 1   | A     | 507 | GLN  | C-N   | -9.08 | 1.22        | 1.33     |
| 2   | B     | 284 | ASN  | CA-C  | -9.07 | 1.40        | 1.53     |
| 4   | S     | 59  | LEU  | N-CA  | -9.07 | 1.35        | 1.46     |
| 4   | S     | 167 | ILE  | C-N   | 9.07  | 1.46        | 1.33     |
| 1   | A     | 355 | LEU  | CA-C  | -9.06 | 1.40        | 1.52     |
| 1   | A     | 467 | LYS  | CA-C  | -9.04 | 1.40        | 1.52     |
| 2   | B     | 576 | GLN  | CA-C  | -9.04 | 1.41        | 1.53     |
| 3   | M     | 22  | ALA  | N-CA  | -9.04 | 1.34        | 1.46     |
| 2   | B     | 193 | LEU  | CA-C  | -9.01 | 1.44        | 1.53     |
| 1   | A     | 147 | LEU  | CA-C  | -9.01 | 1.41        | 1.52     |
| 4   | S     | 3   | HIS  | N-CA  | -8.98 | 1.34        | 1.46     |
| 1   | A     | 270 | LEU  | CA-C  | -8.97 | 1.41        | 1.52     |
| 2   | B     | 330 | SER  | C-N   | -8.97 | 1.20        | 1.33     |
| 3   | M     | 7   | ILE  | CA-C  | -8.96 | 1.41        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 138 | ASN  | C-N   | -8.93 | 1.21        | 1.33     |
| 3   | M     | 75  | TRP  | C-N   | -8.93 | 1.21        | 1.33     |
| 4   | S     | 6   | LEU  | CA-C  | 8.92  | 1.63        | 1.52     |
| 2   | B     | 275 | ARG  | C-N   | -8.91 | 1.22        | 1.33     |
| 2   | B     | 383 | VAL  | CA-C  | -8.91 | 1.39        | 1.52     |
| 3   | M     | 133 | GLU  | CA-C  | -8.90 | 1.42        | 1.53     |
| 4   | S     | 22  | PRO  | N-CA  | -8.89 | 1.36        | 1.47     |
| 3   | M     | 367 | ALA  | CA-CB | -8.88 | 1.40        | 1.53     |
| 2   | B     | 500 | GLN  | C-N   | -8.85 | 1.21        | 1.33     |
| 3   | M     | 323 | MET  | N-CA  | -8.82 | 1.35        | 1.46     |
| 1   | A     | 362 | ASP  | C-N   | -8.81 | 1.24        | 1.34     |
| 3   | M     | 61  | GLU  | N-CA  | -8.80 | 1.35        | 1.46     |
| 2   | B     | 572 | GLU  | CA-C  | -8.76 | 1.41        | 1.52     |
| 3   | M     | 394 | GLN  | CA-C  | 8.76  | 1.63        | 1.52     |
| 1   | A     | 214 | VAL  | CA-C  | -8.75 | 1.41        | 1.52     |
| 1   | A     | 522 | PHE  | CA-C  | -8.75 | 1.39        | 1.52     |
| 4   | S     | 83  | LEU  | N-CA  | -8.74 | 1.35        | 1.45     |
| 1   | A     | 567 | GLN  | CA-C  | -8.74 | 1.41        | 1.52     |
| 2   | B     | 337 | THR  | CA-C  | -8.72 | 1.41        | 1.52     |
| 2   | B     | 460 | SER  | CA-C  | -8.72 | 1.40        | 1.52     |
| 1   | A     | 84  | MET  | N-CA  | -8.72 | 1.34        | 1.46     |
| 3   | M     | 365 | GLU  | N-CA  | -8.71 | 1.35        | 1.46     |
| 3   | M     | 228 | LYS  | C-N   | -8.71 | 1.22        | 1.33     |
| 1   | A     | 221 | VAL  | CA-C  | -8.71 | 1.42        | 1.52     |
| 2   | B     | 66  | ILE  | CA-C  | -8.71 | 1.41        | 1.52     |
| 2   | B     | 486 | HIS  | CA-C  | -8.70 | 1.41        | 1.52     |
| 3   | M     | 441 | GLY  | C-N   | -8.69 | 1.22        | 1.33     |
| 2   | B     | 425 | PRO  | CA-C  | -8.69 | 1.42        | 1.52     |
| 2   | B     | 526 | CYS  | CA-C  | -8.69 | 1.41        | 1.52     |
| 2   | B     | 382 | TYR  | N-CA  | -8.68 | 1.35        | 1.46     |
| 1   | A     | 367 | ILE  | CA-C  | -8.67 | 1.40        | 1.52     |
| 3   | M     | 262 | THR  | N-CA  | -8.65 | 1.35        | 1.46     |
| 1   | A     | 263 | LEU  | N-CA  | -8.64 | 1.34        | 1.46     |
| 3   | M     | 223 | HIS  | C-N   | -8.63 | 1.21        | 1.33     |
| 2   | B     | 528 | ASP  | CA-C  | -8.63 | 1.41        | 1.52     |
| 3   | M     | 354 | ASP  | C-N   | -8.63 | 1.21        | 1.33     |
| 3   | M     | 372 | ILE  | CA-C  | -8.60 | 1.45        | 1.52     |
| 1   | A     | 143 | VAL  | CA-C  | -8.57 | 1.42        | 1.52     |
| 3   | M     | 50  | TYR  | C-N   | -8.56 | 1.21        | 1.33     |
| 3   | M     | 272 | LEU  | CA-C  | 8.56  | 1.62        | 1.52     |
| 1   | A     | 241 | TYR  | N-CA  | -8.56 | 1.35        | 1.46     |
| 3   | M     | 440 | ILE  | C-N   | -8.56 | 1.21        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 444 | VAL  | CA-C  | -8.54 | 1.43        | 1.52     |
| 4   | S     | 144 | THR  | C-N   | -8.54 | 1.21        | 1.33     |
| 3   | M     | 14  | LEU  | C-N   | -8.53 | 1.23        | 1.33     |
| 1   | A     | 257 | LEU  | CA-C  | -8.52 | 1.41        | 1.52     |
| 1   | A     | 242 | GLU  | C-O   | -8.52 | 1.13        | 1.23     |
| 3   | M     | 350 | VAL  | CA-C  | -8.50 | 1.43        | 1.52     |
| 2   | B     | 222 | HIS  | N-CA  | 8.50  | 1.57        | 1.46     |
| 2   | B     | 265 | VAL  | CA-C  | -8.48 | 1.42        | 1.52     |
| 4   | S     | 38  | LEU  | CA-C  | -8.48 | 1.41        | 1.52     |
| 1   | A     | 85  | ALA  | C-N   | 8.48  | 1.45        | 1.33     |
| 1   | A     | 162 | ILE  | CA-C  | -8.47 | 1.42        | 1.52     |
| 2   | B     | 115 | LEU  | CA-C  | -8.47 | 1.41        | 1.52     |
| 1   | A     | 496 | ILE  | CA-C  | -8.46 | 1.42        | 1.52     |
| 2   | B     | 559 | ASP  | CA-C  | -8.46 | 1.40        | 1.52     |
| 1   | A     | 177 | ILE  | CA-C  | -8.45 | 1.42        | 1.52     |
| 1   | A     | 341 | ILE  | CA-C  | -8.45 | 1.41        | 1.52     |
| 1   | A     | 217 | ALA  | CA-C  | -8.45 | 1.41        | 1.52     |
| 3   | M     | 408 | VAL  | N-CA  | -8.44 | 1.38        | 1.46     |
| 2   | B     | 355 | ASN  | CA-C  | -8.43 | 1.42        | 1.52     |
| 1   | A     | 453 | VAL  | N-CA  | -8.40 | 1.36        | 1.46     |
| 4   | S     | 83  | LEU  | C-N   | -8.40 | 1.21        | 1.33     |
| 3   | M     | 115 | VAL  | N-CA  | -8.39 | 1.36        | 1.46     |
| 2   | B     | 82  | TYR  | N-CA  | -8.39 | 1.35        | 1.46     |
| 1   | A     | 260 | PHE  | C-N   | -8.39 | 1.23        | 1.33     |
| 2   | B     | 601 | TYR  | N-CA  | -8.36 | 1.35        | 1.46     |
| 1   | A     | 304 | LEU  | N-CA  | -8.36 | 1.36        | 1.46     |
| 1   | A     | 400 | VAL  | CA-C  | -8.36 | 1.42        | 1.52     |
| 1   | A     | 304 | LEU  | CA-C  | 8.35  | 1.63        | 1.52     |
| 3   | M     | 284 | SER  | C-N   | -8.35 | 1.24        | 1.33     |
| 3   | M     | 292 | PRO  | CA-C  | 8.35  | 1.59        | 1.52     |
| 1   | A     | 464 | ILE  | C-N   | -8.35 | 1.22        | 1.33     |
| 1   | A     | 285 | THR  | CA-C  | -8.34 | 1.42        | 1.52     |
| 3   | M     | 426 | LYS  | C-N   | -8.34 | 1.22        | 1.33     |
| 2   | B     | 328 | LEU  | CA-C  | -8.34 | 1.41        | 1.52     |
| 2   | B     | 73  | ASP  | CA-C  | -8.33 | 1.42        | 1.53     |
| 4   | S     | 81  | ALA  | CA-CB | -8.33 | 1.39        | 1.53     |
| 4   | S     | 104 | THR  | CA-C  | -8.33 | 1.41        | 1.52     |
| 1   | A     | 596 | VAL  | CA-C  | -8.32 | 1.42        | 1.52     |
| 3   | M     | 82  | LYS  | CA-C  | 8.32  | 1.63        | 1.52     |
| 1   | A     | 392 | MET  | N-CA  | -8.32 | 1.36        | 1.46     |
| 1   | A     | 424 | TYR  | CA-C  | -8.31 | 1.41        | 1.52     |
| 2   | B     | 501 | THR  | N-CA  | -8.31 | 1.35        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 391 | ILE  | CA-C  | -8.30 | 1.42        | 1.52     |
| 1   | A     | 162 | ILE  | N-CA  | -8.30 | 1.36        | 1.46     |
| 1   | A     | 237 | SER  | CA-C  | -8.30 | 1.42        | 1.52     |
| 3   | M     | 67  | SER  | CA-C  | -8.30 | 1.42        | 1.52     |
| 4   | S     | 47  | GLN  | CA-C  | -8.29 | 1.41        | 1.52     |
| 2   | B     | 290 | SER  | N-CA  | -8.27 | 1.35        | 1.46     |
| 2   | B     | 238 | LYS  | CA-C  | 8.27  | 1.63        | 1.52     |
| 4   | S     | 138 | GLY  | C-N   | 8.25  | 1.44        | 1.33     |
| 1   | A     | 364 | ASP  | CA-C  | -8.23 | 1.42        | 1.52     |
| 3   | M     | 280 | ASP  | C-N   | -8.23 | 1.21        | 1.33     |
| 2   | B     | 381 | PHE  | CA-C  | -8.22 | 1.41        | 1.52     |
| 1   | A     | 401 | VAL  | CA-C  | -8.22 | 1.42        | 1.52     |
| 1   | A     | 607 | LEU  | CA-C  | -8.20 | 1.42        | 1.52     |
| 3   | M     | 99  | ILE  | CA-C  | -8.20 | 1.40        | 1.52     |
| 1   | A     | 303 | MET  | CA-C  | -8.20 | 1.42        | 1.52     |
| 3   | M     | 439 | TYR  | C-N   | -8.19 | 1.23        | 1.33     |
| 4   | S     | 93  | GLU  | CA-C  | -8.19 | 1.42        | 1.52     |
| 4   | S     | 143 | GLU  | C-N   | -8.18 | 1.21        | 1.33     |
| 3   | M     | 406 | GLY  | N-CA  | -8.18 | 1.33        | 1.45     |
| 4   | S     | 141 | VAL  | CA-C  | -8.18 | 1.42        | 1.52     |
| 4   | S     | 66  | ASP  | CA-C  | 8.17  | 1.63        | 1.52     |
| 4   | S     | 42  | ARG  | C-N   | -8.17 | 1.22        | 1.33     |
| 4   | S     | 130 | SER  | CA-C  | -8.17 | 1.42        | 1.52     |
| 4   | S     | 28  | GLN  | CA-C  | -8.16 | 1.41        | 1.52     |
| 2   | B     | 150 | LEU  | N-CA  | -8.14 | 1.35        | 1.46     |
| 1   | A     | 281 | LEU  | C-N   | -8.14 | 1.22        | 1.34     |
| 2   | B     | 415 | LEU  | CA-C  | -8.14 | 1.41        | 1.52     |
| 1   | A     | 306 | GLU  | C-N   | -8.13 | 1.22        | 1.33     |
| 1   | A     | 188 | VAL  | CA-C  | -8.13 | 1.43        | 1.52     |
| 4   | S     | 55  | PRO  | CA-C  | -8.12 | 1.37        | 1.52     |
| 1   | A     | 602 | GLU  | C-N   | 8.12  | 1.44        | 1.33     |
| 3   | M     | 425 | THR  | CA-C  | 8.11  | 1.62        | 1.52     |
| 2   | B     | 352 | ASN  | C-N   | -8.09 | 1.23        | 1.33     |
| 3   | M     | 58  | ARG  | N-CA  | -8.08 | 1.36        | 1.46     |
| 1   | A     | 220 | SER  | C-N   | 8.06  | 1.44        | 1.33     |
| 2   | B     | 458 | MET  | C-N   | 8.06  | 1.45        | 1.33     |
| 1   | A     | 323 | CYS  | CA-C  | 8.05  | 1.64        | 1.52     |
| 3   | M     | 129 | VAL  | C-O   | -8.04 | 1.13        | 1.24     |
| 3   | M     | 8   | THR  | CA-C  | -8.04 | 1.42        | 1.52     |
| 3   | M     | 110 | SER  | CA-C  | -8.02 | 1.41        | 1.53     |
| 2   | B     | 363 | ILE  | N-CA  | -8.01 | 1.36        | 1.46     |
| 3   | M     | 296 | LYS  | N-CA  | 8.01  | 1.56        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | S     | 69  | ASN  | CA-C  | -8.00 | 1.41        | 1.52     |
| 1   | A     | 611 | LEU  | CA-C  | -8.00 | 1.42        | 1.52     |
| 2   | B     | 428 | VAL  | CA-C  | -8.00 | 1.40        | 1.52     |
| 4   | S     | 72  | ASP  | C-N   | 8.00  | 1.44        | 1.33     |
| 3   | M     | 310 | VAL  | N-CA  | -7.99 | 1.36        | 1.46     |
| 2   | B     | 264 | THR  | C-N   | -7.98 | 1.24        | 1.33     |
| 3   | M     | 309 | GLN  | CA-C  | -7.98 | 1.42        | 1.52     |
| 4   | S     | 8   | PHE  | C-N   | -7.97 | 1.21        | 1.33     |
| 3   | M     | 355 | ASP  | CA-C  | 7.96  | 1.63        | 1.52     |
| 3   | M     | 276 | VAL  | C-N   | 7.95  | 1.44        | 1.33     |
| 1   | A     | 624 | LEU  | CA-C  | -7.94 | 1.42        | 1.52     |
| 2   | B     | 408 | VAL  | CA-C  | -7.94 | 1.41        | 1.52     |
| 2   | B     | 416 | LYS  | CA-C  | -7.92 | 1.42        | 1.52     |
| 3   | M     | 398 | ILE  | CA-C  | 7.91  | 1.62        | 1.52     |
| 4   | S     | 125 | TRP  | CA-C  | -7.91 | 1.42        | 1.52     |
| 4   | S     | 27  | LYS  | CA-C  | -7.90 | 1.42        | 1.52     |
| 3   | M     | 441 | GLY  | CA-C  | -7.89 | 1.40        | 1.51     |
| 4   | S     | 157 | ASN  | CA-C  | -7.89 | 1.42        | 1.52     |
| 2   | B     | 363 | ILE  | CA-C  | -7.88 | 1.41        | 1.52     |
| 3   | M     | 137 | SER  | C-N   | -7.88 | 1.22        | 1.33     |
| 2   | B     | 574 | ASN  | N-CA  | -7.87 | 1.35        | 1.46     |
| 1   | A     | 399 | ASP  | N-CA  | -7.87 | 1.36        | 1.46     |
| 3   | M     | 90  | PHE  | CA-C  | -7.87 | 1.42        | 1.52     |
| 2   | B     | 108 | PHE  | C-N   | -7.85 | 1.23        | 1.34     |
| 2   | B     | 526 | CYS  | N-CA  | -7.84 | 1.35        | 1.46     |
| 2   | B     | 207 | VAL  | CA-C  | -7.83 | 1.42        | 1.52     |
| 3   | M     | 123 | LEU  | CA-C  | -7.83 | 1.42        | 1.52     |
| 1   | A     | 516 | ILE  | CA-C  | -7.82 | 1.42        | 1.52     |
| 4   | S     | 71  | GLU  | C-N   | -7.82 | 1.22        | 1.33     |
| 3   | M     | 407 | THR  | N-CA  | -7.82 | 1.36        | 1.45     |
| 3   | M     | 248 | SER  | CA-C  | -7.79 | 1.43        | 1.52     |
| 3   | M     | 68  | VAL  | C-N   | -7.79 | 1.23        | 1.33     |
| 1   | A     | 404 | GLN  | N-CA  | -7.78 | 1.36        | 1.46     |
| 1   | A     | 472 | LYS  | CA-C  | -7.78 | 1.42        | 1.52     |
| 1   | A     | 353 | ASP  | N-CA  | -7.78 | 1.36        | 1.46     |
| 1   | A     | 417 | PRO  | C-N   | -7.78 | 1.23        | 1.33     |
| 2   | B     | 421 | SER  | CA-C  | -7.78 | 1.42        | 1.52     |
| 1   | A     | 233 | PHE  | C-N   | -7.78 | 1.25        | 1.34     |
| 1   | A     | 562 | TRP  | CA-C  | -7.77 | 1.43        | 1.52     |
| 1   | A     | 450 | TYR  | CA-C  | -7.77 | 1.43        | 1.52     |
| 1   | A     | 421 | PRO  | CA-C  | -7.76 | 1.43        | 1.52     |
| 1   | A     | 434 | SER  | CA-C  | -7.76 | 1.42        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 547 | VAL  | N-CA  | -7.76 | 1.37        | 1.46     |
| 3   | M     | 56  | VAL  | C-N   | -7.76 | 1.22        | 1.33     |
| 4   | S     | 117 | ASN  | CA-C  | -7.75 | 1.43        | 1.52     |
| 2   | B     | 355 | ASN  | N-CA  | -7.74 | 1.36        | 1.46     |
| 2   | B     | 107 | ARG  | CA-C  | 7.72  | 1.62        | 1.52     |
| 3   | M     | 458 | LEU  | CA-C  | -7.72 | 1.42        | 1.52     |
| 3   | M     | 111 | ILE  | CA-C  | -7.72 | 1.43        | 1.52     |
| 4   | S     | 120 | ASP  | CA-C  | -7.71 | 1.42        | 1.52     |
| 3   | M     | 440 | ILE  | CA-C  | -7.69 | 1.42        | 1.52     |
| 3   | M     | 230 | LYS  | C-N   | 7.68  | 1.44        | 1.33     |
| 1   | A     | 148 | SER  | CA-C  | -7.67 | 1.42        | 1.52     |
| 1   | A     | 519 | LEU  | CA-C  | 7.67  | 1.63        | 1.52     |
| 4   | S     | 54  | PRO  | N-CA  | 7.67  | 1.62        | 1.46     |
| 1   | A     | 302 | ASN  | N-CA  | -7.67 | 1.36        | 1.46     |
| 3   | M     | 63  | TYR  | C-N   | -7.67 | 1.22        | 1.33     |
| 4   | S     | 24  | ASP  | CA-C  | -7.66 | 1.42        | 1.52     |
| 2   | B     | 220 | ALA  | N-CA  | -7.66 | 1.37        | 1.46     |
| 2   | B     | 443 | SER  | N-CA  | -7.64 | 1.36        | 1.46     |
| 2   | B     | 402 | LEU  | C-N   | -7.63 | 1.24        | 1.33     |
| 3   | M     | 374 | TYR  | N-CA  | -7.63 | 1.36        | 1.45     |
| 2   | B     | 563 | PHE  | CA-C  | -7.63 | 1.45        | 1.53     |
| 4   | S     | 54  | PRO  | CA-C  | 7.61  | 1.59        | 1.52     |
| 1   | A     | 435 | ILE  | N-CA  | -7.60 | 1.37        | 1.46     |
| 3   | M     | 6   | TYR  | CA-C  | 7.60  | 1.62        | 1.52     |
| 2   | B     | 299 | LEU  | CA-C  | -7.59 | 1.43        | 1.52     |
| 3   | M     | 55  | MET  | CA-C  | 7.58  | 1.61        | 1.53     |
| 1   | A     | 308 | ASP  | N-CA  | -7.58 | 1.35        | 1.46     |
| 4   | S     | 58  | LEU  | N-CA  | -7.57 | 1.36        | 1.45     |
| 4   | S     | 90  | ASP  | CA-C  | -7.56 | 1.42        | 1.53     |
| 4   | S     | 105 | PHE  | N-CA  | -7.56 | 1.36        | 1.46     |
| 2   | B     | 275 | ARG  | CA-C  | -7.56 | 1.42        | 1.53     |
| 2   | B     | 488 | ARG  | CA-C  | -7.56 | 1.42        | 1.52     |
| 4   | S     | 7   | ILE  | C-N   | 7.56  | 1.44        | 1.33     |
| 3   | M     | 297 | PHE  | N-CA  | -7.56 | 1.36        | 1.46     |
| 3   | M     | 424 | PHE  | C-N   | -7.55 | 1.22        | 1.33     |
| 1   | A     | 338 | PHE  | CA-C  | -7.55 | 1.43        | 1.52     |
| 2   | B     | 447 | GLU  | N-CA  | -7.54 | 1.37        | 1.46     |
| 2   | B     | 419 | VAL  | N-CA  | -7.53 | 1.37        | 1.46     |
| 1   | A     | 103 | LYS  | C-N   | -7.51 | 1.23        | 1.33     |
| 2   | B     | 592 | TYR  | CA-C  | -7.50 | 1.43        | 1.52     |
| 2   | B     | 411 | ILE  | CA-C  | -7.50 | 1.43        | 1.52     |
| 1   | A     | 388 | VAL  | N-CA  | -7.49 | 1.37        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 331 | ARG  | CA-C  | -7.48 | 1.43        | 1.52     |
| 2   | B     | 83  | PHE  | N-CA  | -7.48 | 1.36        | 1.46     |
| 2   | B     | 381 | PHE  | C-N   | -7.47 | 1.23        | 1.33     |
| 2   | B     | 554 | LYS  | CA-C  | -7.47 | 1.43        | 1.52     |
| 1   | A     | 505 | ASN  | C-N   | -7.47 | 1.23        | 1.33     |
| 1   | A     | 548 | GLN  | CA-C  | -7.47 | 1.43        | 1.52     |
| 1   | A     | 451 | ASN  | CA-C  | -7.47 | 1.42        | 1.52     |
| 3   | M     | 128 | CYS  | C-O   | 7.46  | 1.33        | 1.24     |
| 2   | B     | 271 | GLU  | CA-C  | -7.46 | 1.43        | 1.52     |
| 2   | B     | 276 | SER  | N-CA  | -7.46 | 1.35        | 1.45     |
| 1   | A     | 158 | LEU  | CA-C  | -7.45 | 1.43        | 1.52     |
| 3   | M     | 269 | ILE  | N-CA  | -7.45 | 1.39        | 1.46     |
| 4   | S     | 3   | HIS  | C-N   | 7.45  | 1.42        | 1.33     |
| 3   | M     | 438 | SER  | N-CA  | -7.44 | 1.36        | 1.46     |
| 3   | M     | 279 | ASN  | CA-C  | 7.43  | 1.62        | 1.52     |
| 1   | A     | 379 | VAL  | N-CA  | -7.42 | 1.37        | 1.46     |
| 1   | A     | 395 | PHE  | CA-C  | -7.41 | 1.42        | 1.52     |
| 2   | B     | 75  | ASP  | C-N   | -7.41 | 1.22        | 1.33     |
| 2   | B     | 289 | PRO  | C-N   | -7.40 | 1.22        | 1.33     |
| 1   | A     | 409 | VAL  | CA-C  | -7.40 | 1.44        | 1.52     |
| 3   | M     | 51  | LEU  | N-CA  | 7.40  | 1.55        | 1.46     |
| 2   | B     | 407 | ASN  | N-CA  | -7.39 | 1.36        | 1.46     |
| 2   | B     | 426 | GLU  | N-CA  | -7.39 | 1.37        | 1.46     |
| 2   | B     | 317 | VAL  | CA-C  | -7.39 | 1.41        | 1.52     |
| 1   | A     | 430 | ASN  | CA-C  | -7.38 | 1.42        | 1.52     |
| 3   | M     | 456 | SER  | C-N   | 7.38  | 1.43        | 1.33     |
| 4   | S     | 145 | ASN  | N-CA  | -7.37 | 1.37        | 1.46     |
| 2   | B     | 490 | ILE  | CA-C  | -7.36 | 1.43        | 1.52     |
| 1   | A     | 511 | VAL  | CA-C  | -7.35 | 1.43        | 1.52     |
| 3   | M     | 250 | LEU  | C-N   | -7.34 | 1.22        | 1.33     |
| 3   | M     | 476 | THR  | C-N   | -7.33 | 1.23        | 1.33     |
| 2   | B     | 295 | ASN  | CA-C  | 7.33  | 1.60        | 1.53     |
| 1   | A     | 392 | MET  | CA-C  | -7.32 | 1.43        | 1.52     |
| 1   | A     | 166 | LEU  | CA-C  | -7.32 | 1.43        | 1.52     |
| 3   | M     | 389 | SER  | CA-C  | -7.32 | 1.43        | 1.53     |
| 1   | A     | 243 | ILE  | N-CA  | -7.30 | 1.32        | 1.46     |
| 1   | A     | 221 | VAL  | C-N   | -7.30 | 1.25        | 1.34     |
| 1   | A     | 598 | GLU  | CA-C  | -7.29 | 1.42        | 1.52     |
| 1   | A     | 468 | SER  | N-CA  | -7.28 | 1.36        | 1.46     |
| 1   | A     | 532 | LEU  | C-N   | 7.28  | 1.43        | 1.33     |
| 1   | A     | 85  | ALA  | CA-C  | 7.28  | 1.62        | 1.52     |
| 2   | B     | 209 | SER  | CA-C  | -7.28 | 1.42        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 468 | LYS  | CA-C  | -7.27 | 1.44        | 1.52     |
| 2   | B     | 584 | SER  | C-N   | -7.26 | 1.22        | 1.33     |
| 3   | M     | 303 | SER  | N-CA  | -7.26 | 1.37        | 1.46     |
| 4   | S     | 100 | ASP  | CA-C  | -7.26 | 1.42        | 1.52     |
| 2   | B     | 255 | TYR  | CA-C  | -7.25 | 1.43        | 1.52     |
| 4   | S     | 117 | ASN  | N-CA  | -7.25 | 1.36        | 1.45     |
| 1   | A     | 529 | GLY  | N-CA  | -7.25 | 1.35        | 1.45     |
| 2   | B     | 584 | SER  | N-CA  | -7.24 | 1.37        | 1.46     |
| 2   | B     | 192 | LEU  | CA-C  | -7.24 | 1.42        | 1.52     |
| 3   | M     | 373 | ALA  | C-N   | -7.24 | 1.23        | 1.33     |
| 4   | S     | 113 | PHE  | C-N   | -7.24 | 1.24        | 1.33     |
| 1   | A     | 271 | ARG  | CA-C  | -7.23 | 1.43        | 1.52     |
| 2   | B     | 346 | THR  | CA-C  | -7.23 | 1.43        | 1.52     |
| 3   | M     | 455 | VAL  | CA-C  | -7.23 | 1.43        | 1.52     |
| 1   | A     | 589 | SER  | N-CA  | -7.22 | 1.36        | 1.46     |
| 2   | B     | 286 | ILE  | CA-C  | -7.22 | 1.41        | 1.52     |
| 3   | M     | 72  | LEU  | C-N   | -7.22 | 1.23        | 1.33     |
| 1   | A     | 85  | ALA  | CA-CB | -7.21 | 1.41        | 1.53     |
| 2   | B     | 109 | ALA  | CA-CB | -7.21 | 1.41        | 1.53     |
| 3   | M     | 71  | LYS  | N-CA  | -7.20 | 1.36        | 1.46     |
| 2   | B     | 460 | SER  | C-N   | -7.19 | 1.24        | 1.33     |
| 3   | M     | 51  | LEU  | CA-C  | 7.18  | 1.62        | 1.52     |
| 4   | S     | 17  | VAL  | C-N   | -7.18 | 1.23        | 1.33     |
| 3   | M     | 238 | GLY  | CA-C  | -7.18 | 1.43        | 1.51     |
| 4   | S     | 5   | VAL  | C-N   | -7.17 | 1.23        | 1.33     |
| 2   | B     | 188 | TYR  | CA-C  | -7.16 | 1.43        | 1.52     |
| 2   | B     | 587 | ARG  | CA-C  | -7.16 | 1.43        | 1.52     |
| 1   | A     | 533 | ILE  | CA-C  | -7.15 | 1.44        | 1.52     |
| 3   | M     | 5   | PHE  | N-CA  | -7.15 | 1.37        | 1.46     |
| 1   | A     | 298 | ILE  | CA-C  | 7.15  | 1.61        | 1.52     |
| 1   | A     | 405 | THR  | C-N   | -7.14 | 1.23        | 1.33     |
| 2   | B     | 191 | GLU  | CA-C  | -7.13 | 1.43        | 1.52     |
| 2   | B     | 151 | ALA  | CA-C  | -7.13 | 1.43        | 1.52     |
| 1   | A     | 252 | ILE  | CA-C  | -7.12 | 1.43        | 1.52     |
| 2   | B     | 262 | LYS  | CA-C  | -7.12 | 1.43        | 1.52     |
| 2   | B     | 84  | ALA  | CA-C  | -7.12 | 1.43        | 1.52     |
| 3   | M     | 253 | ASN  | N-CA  | -7.12 | 1.36        | 1.46     |
| 2   | B     | 46  | GLN  | CA-C  | -7.11 | 1.43        | 1.52     |
| 2   | B     | 435 | SER  | CA-C  | -7.11 | 1.44        | 1.52     |
| 3   | M     | 20  | LEU  | N-CA  | -7.11 | 1.37        | 1.46     |
| 3   | M     | 24  | ALA  | N-CA  | -7.10 | 1.35        | 1.46     |
| 4   | S     | 113 | PHE  | N-CA  | -7.10 | 1.36        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 568 | GLU  | N-CA  | -7.09 | 1.37        | 1.46     |
| 1   | A     | 476 | GLN  | CA-C  | -7.09 | 1.43        | 1.52     |
| 1   | A     | 280 | GLU  | C-N   | 7.08  | 1.43        | 1.34     |
| 3   | M     | 347 | PHE  | CA-C  | 7.08  | 1.62        | 1.52     |
| 2   | B     | 158 | VAL  | CA-C  | -7.06 | 1.43        | 1.52     |
| 4   | S     | 66  | ASP  | C-N   | -7.05 | 1.23        | 1.33     |
| 3   | M     | 94  | GLU  | CA-C  | -7.05 | 1.44        | 1.52     |
| 3   | M     | 478 | ASN  | N-CA  | -7.04 | 1.37        | 1.45     |
| 1   | A     | 114 | PHE  | CA-C  | -7.04 | 1.42        | 1.52     |
| 4   | S     | 69  | ASN  | C-N   | -7.04 | 1.23        | 1.33     |
| 4   | S     | 148 | ARG  | CA-C  | -7.04 | 1.43        | 1.52     |
| 1   | A     | 201 | ASP  | CA-C  | -7.03 | 1.43        | 1.52     |
| 2   | B     | 331 | PRO  | N-CA  | -7.03 | 1.38        | 1.47     |
| 3   | M     | 378 | ILE  | CA-C  | 7.03  | 1.61        | 1.52     |
| 1   | A     | 617 | ASP  | CA-C  | -7.02 | 1.43        | 1.52     |
| 3   | M     | 446 | GLY  | CA-C  | 7.01  | 1.61        | 1.51     |
| 1   | A     | 202 | LYS  | CA-C  | -7.01 | 1.43        | 1.52     |
| 2   | B     | 503 | LEU  | CA-C  | -7.01 | 1.43        | 1.52     |
| 2   | B     | 583 | PHE  | C-N   | -7.00 | 1.24        | 1.33     |
| 2   | B     | 523 | PHE  | N-CA  | -6.98 | 1.37        | 1.46     |
| 1   | A     | 181 | ALA  | CA-C  | -6.97 | 1.43        | 1.52     |
| 1   | A     | 495 | ILE  | CA-C  | -6.97 | 1.43        | 1.52     |
| 1   | A     | 586 | GLU  | N-CA  | -6.96 | 1.37        | 1.46     |
| 3   | M     | 47  | SER  | N-CA  | 6.96  | 1.54        | 1.45     |
| 2   | B     | 333 | GLN  | N-CA  | -6.93 | 1.37        | 1.46     |
| 2   | B     | 461 | HIS  | CA-C  | -6.93 | 1.43        | 1.52     |
| 2   | B     | 382 | TYR  | C-N   | -6.93 | 1.25        | 1.33     |
| 4   | S     | 132 | LEU  | CA-C  | -6.92 | 1.43        | 1.52     |
| 2   | B     | 475 | ILE  | CA-C  | -6.91 | 1.43        | 1.52     |
| 1   | A     | 204 | VAL  | N-CA  | -6.91 | 1.38        | 1.46     |
| 1   | A     | 634 | ASN  | CA-C  | -6.90 | 1.43        | 1.52     |
| 1   | A     | 403 | LEU  | N-CA  | -6.90 | 1.37        | 1.46     |
| 1   | A     | 341 | ILE  | N-CA  | -6.90 | 1.38        | 1.46     |
| 3   | M     | 427 | LYS  | N-CA  | -6.90 | 1.38        | 1.46     |
| 1   | A     | 264 | SER  | CA-C  | -6.89 | 1.43        | 1.52     |
| 3   | M     | 418 | GLU  | N-CA  | -6.89 | 1.37        | 1.46     |
| 4   | S     | 33  | GLU  | CA-C  | -6.88 | 1.43        | 1.52     |
| 1   | A     | 77  | LEU  | CA-C  | 6.88  | 1.61        | 1.52     |
| 3   | M     | 44  | ASP  | N-CA  | -6.88 | 1.37        | 1.46     |
| 1   | A     | 604 | LEU  | CA-C  | -6.88 | 1.43        | 1.52     |
| 3   | M     | 378 | ILE  | N-CA  | -6.88 | 1.38        | 1.46     |
| 2   | B     | 259 | TYR  | C-N   | -6.88 | 1.19        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 243 | ILE  | C-N   | 6.87  | 1.43        | 1.34     |
| 2   | B     | 99  | ARG  | CA-C  | -6.87 | 1.44        | 1.52     |
| 4   | S     | 88  | ILE  | CA-C  | -6.87 | 1.44        | 1.52     |
| 1   | A     | 446 | ASP  | N-CA  | -6.87 | 1.37        | 1.46     |
| 2   | B     | 323 | ASN  | CA-C  | -6.86 | 1.43        | 1.52     |
| 4   | S     | 74  | GLN  | C-N   | -6.86 | 1.25        | 1.33     |
| 2   | B     | 439 | CYS  | N-CA  | -6.86 | 1.38        | 1.46     |
| 3   | M     | 427 | LYS  | CA-C  | 6.86  | 1.60        | 1.52     |
| 2   | B     | 512 | VAL  | C-N   | 6.85  | 1.42        | 1.33     |
| 1   | A     | 74  | LEU  | C-N   | 6.84  | 1.42        | 1.33     |
| 4   | S     | 43  | ASN  | N-CA  | -6.83 | 1.37        | 1.46     |
| 3   | M     | 396 | GLN  | C-N   | -6.83 | 1.24        | 1.33     |
| 4   | S     | 16  | LEU  | C-N   | -6.82 | 1.25        | 1.33     |
| 1   | A     | 139 | ASP  | CA-C  | -6.82 | 1.44        | 1.52     |
| 4   | S     | 164 | ASP  | N-CA  | 6.82  | 1.54        | 1.46     |
| 1   | A     | 91  | ILE  | CA-C  | -6.82 | 1.44        | 1.52     |
| 1   | A     | 613 | ALA  | CA-C  | -6.81 | 1.44        | 1.52     |
| 2   | B     | 48  | VAL  | CA-C  | -6.81 | 1.44        | 1.52     |
| 1   | A     | 309 | PHE  | CA-C  | -6.80 | 1.44        | 1.52     |
| 3   | M     | 388 | ASN  | CA-C  | 6.80  | 1.61        | 1.52     |
| 3   | M     | 278 | ILE  | N-CA  | 6.79  | 1.54        | 1.46     |
| 1   | A     | 225 | LEU  | N-CA  | -6.79 | 1.37        | 1.46     |
| 3   | M     | 212 | ASN  | N-CA  | -6.79 | 1.33        | 1.46     |
| 1   | A     | 454 | ILE  | CA-C  | -6.79 | 1.44        | 1.52     |
| 1   | A     | 394 | GLN  | C-O   | -6.78 | 1.16        | 1.24     |
| 2   | B     | 292 | GLU  | CA-C  | -6.78 | 1.43        | 1.52     |
| 4   | S     | 25  | LEU  | C-N   | -6.77 | 1.25        | 1.33     |
| 2   | B     | 177 | ILE  | CA-C  | -6.77 | 1.44        | 1.52     |
| 2   | B     | 335 | LYS  | N-CA  | -6.77 | 1.38        | 1.46     |
| 4   | S     | 63  | ASN  | C-O   | -6.76 | 1.16        | 1.24     |
| 3   | M     | 302 | TYR  | CA-C  | -6.76 | 1.44        | 1.52     |
| 1   | A     | 387 | ILE  | N-CA  | -6.75 | 1.38        | 1.46     |
| 1   | A     | 555 | LEU  | CA-C  | -6.75 | 1.43        | 1.52     |
| 2   | B     | 555 | LEU  | CA-C  | -6.75 | 1.43        | 1.52     |
| 3   | M     | 83  | SER  | C-N   | -6.75 | 1.24        | 1.33     |
| 1   | A     | 286 | VAL  | N-CA  | -6.75 | 1.37        | 1.46     |
| 1   | A     | 323 | CYS  | C-N   | 6.75  | 1.42        | 1.33     |
| 4   | S     | 1   | MET  | C-N   | -6.75 | 1.25        | 1.33     |
| 1   | A     | 230 | PRO  | N-CD  | -6.74 | 1.38        | 1.47     |
| 2   | B     | 378 | THR  | N-CA  | -6.74 | 1.38        | 1.46     |
| 3   | M     | 40  | GLN  | C-N   | 6.74  | 1.43        | 1.33     |
| 4   | S     | 33  | GLU  | N-CA  | -6.74 | 1.37        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | S     | 106 | VAL  | CA-C  | -6.73 | 1.44        | 1.52     |
| 2   | B     | 67  | ILE  | CA-C  | -6.72 | 1.44        | 1.52     |
| 2   | B     | 139 | LEU  | CA-C  | -6.72 | 1.43        | 1.52     |
| 3   | M     | 129 | VAL  | N-CA  | -6.72 | 1.37        | 1.46     |
| 1   | A     | 509 | PRO  | N-CD  | 6.72  | 1.57        | 1.47     |
| 1   | A     | 517 | TRP  | CA-C  | -6.72 | 1.44        | 1.52     |
| 2   | B     | 497 | LEU  | N-CA  | -6.72 | 1.37        | 1.46     |
| 3   | M     | 362 | PHE  | CA-C  | -6.71 | 1.44        | 1.53     |
| 3   | M     | 451 | ALA  | N-CA  | -6.71 | 1.37        | 1.45     |
| 2   | B     | 267 | ASP  | C-N   | -6.70 | 1.24        | 1.33     |
| 1   | A     | 628 | VAL  | CA-C  | -6.70 | 1.44        | 1.52     |
| 4   | S     | 34  | GLN  | CA-C  | -6.69 | 1.43        | 1.52     |
| 2   | B     | 291 | TYR  | N-CA  | -6.69 | 1.37        | 1.46     |
| 2   | B     | 259 | TYR  | CA-C  | -6.68 | 1.37        | 1.52     |
| 1   | A     | 440 | ASN  | CA-C  | 6.67  | 1.61        | 1.52     |
| 2   | B     | 185 | LYS  | C-N   | -6.66 | 1.24        | 1.33     |
| 1   | A     | 452 | ALA  | CA-C  | -6.66 | 1.44        | 1.52     |
| 2   | B     | 384 | PHE  | N-CA  | -6.66 | 1.35        | 1.46     |
| 4   | S     | 122 | ILE  | N-CA  | -6.65 | 1.38        | 1.46     |
| 4   | S     | 154 | ASP  | CA-C  | -6.65 | 1.43        | 1.52     |
| 2   | B     | 537 | PHE  | CA-C  | -6.64 | 1.43        | 1.52     |
| 2   | B     | 454 | LEU  | CA-C  | -6.63 | 1.44        | 1.52     |
| 3   | M     | 266 | ASP  | C-N   | 6.62  | 1.41        | 1.33     |
| 3   | M     | 441 | GLY  | N-CA  | -6.61 | 1.35        | 1.45     |
| 4   | S     | 139 | GLY  | CA-C  | -6.60 | 1.42        | 1.51     |
| 1   | A     | 531 | ASP  | N-CA  | -6.60 | 1.37        | 1.46     |
| 1   | A     | 601 | VAL  | C-N   | -6.60 | 1.25        | 1.33     |
| 3   | M     | 92  | PHE  | C-N   | 6.59  | 1.42        | 1.33     |
| 4   | S     | 127 | THR  | CA-C  | -6.59 | 1.44        | 1.52     |
| 1   | A     | 407 | SER  | CA-C  | -6.58 | 1.44        | 1.52     |
| 1   | A     | 304 | LEU  | C-O   | 6.58  | 1.31        | 1.24     |
| 3   | M     | 419 | ASN  | C-N   | -6.58 | 1.23        | 1.33     |
| 4   | S     | 55  | PRO  | N-CD  | 6.58  | 1.56        | 1.47     |
| 2   | B     | 128 | SER  | CA-C  | 6.57  | 1.61        | 1.52     |
| 3   | M     | 138 | ASP  | N-CA  | -6.56 | 1.33        | 1.46     |
| 3   | M     | 477 | GLY  | CA-C  | -6.56 | 1.44        | 1.51     |
| 4   | S     | 73  | ILE  | N-CA  | 6.56  | 1.54        | 1.46     |
| 1   | A     | 159 | ALA  | CA-C  | -6.56 | 1.43        | 1.52     |
| 1   | A     | 390 | THR  | CA-C  | -6.56 | 1.44        | 1.52     |
| 3   | M     | 128 | CYS  | N-CA  | -6.55 | 1.38        | 1.46     |
| 3   | M     | 287 | ASN  | C-N   | 6.55  | 1.42        | 1.33     |
| 2   | B     | 243 | TRP  | CA-C  | -6.55 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 451 | ALA  | CA-CB | 6.55  | 1.65        | 1.53     |
| 1   | A     | 445 | ASN  | N-CA  | -6.55 | 1.37        | 1.46     |
| 2   | B     | 544 | THR  | CA-C  | -6.54 | 1.44        | 1.52     |
| 4   | S     | 159 | ALA  | CA-C  | -6.54 | 1.44        | 1.52     |
| 2   | B     | 424 | PHE  | N-CA  | -6.54 | 1.36        | 1.46     |
| 2   | B     | 344 | VAL  | CA-C  | -6.53 | 1.44        | 1.52     |
| 2   | B     | 326 | TYR  | N-CA  | -6.53 | 1.37        | 1.46     |
| 1   | A     | 265 | GLN  | CA-C  | -6.52 | 1.44        | 1.52     |
| 2   | B     | 374 | PHE  | N-CA  | -6.52 | 1.37        | 1.46     |
| 4   | S     | 137 | GLN  | N-CA  | -6.52 | 1.37        | 1.46     |
| 2   | B     | 569 | THR  | CA-C  | -6.51 | 1.44        | 1.52     |
| 1   | A     | 330 | LEU  | CA-C  | -6.51 | 1.44        | 1.52     |
| 4   | S     | 134 | GLU  | CA-C  | -6.50 | 1.43        | 1.52     |
| 1   | A     | 477 | PHE  | CA-C  | -6.50 | 1.44        | 1.52     |
| 2   | B     | 584 | SER  | CA-C  | -6.50 | 1.44        | 1.52     |
| 2   | B     | 215 | TYR  | CA-C  | -6.50 | 1.44        | 1.52     |
| 3   | M     | 417 | TYR  | CA-C  | -6.50 | 1.44        | 1.53     |
| 2   | B     | 158 | VAL  | N-CA  | -6.49 | 1.39        | 1.46     |
| 3   | M     | 128 | CYS  | C-N   | 6.48  | 1.41        | 1.33     |
| 1   | A     | 176 | TYR  | CA-C  | -6.48 | 1.44        | 1.52     |
| 1   | A     | 515 | CYS  | CA-C  | -6.48 | 1.43        | 1.52     |
| 1   | A     | 533 | ILE  | C-N   | 6.48  | 1.42        | 1.33     |
| 1   | A     | 278 | ILE  | N-CA  | -6.48 | 1.33        | 1.46     |
| 2   | B     | 594 | ALA  | CA-C  | -6.48 | 1.44        | 1.52     |
| 2   | B     | 383 | VAL  | N-CA  | -6.48 | 1.38        | 1.46     |
| 1   | A     | 506 | LYS  | N-CA  | -6.47 | 1.38        | 1.46     |
| 1   | A     | 433 | ILE  | C-N   | 6.47  | 1.42        | 1.33     |
| 1   | A     | 179 | LYS  | CA-C  | -6.47 | 1.44        | 1.52     |
| 1   | A     | 450 | TYR  | C-N   | 6.47  | 1.42        | 1.34     |
| 2   | B     | 439 | CYS  | CA-C  | -6.46 | 1.44        | 1.52     |
| 3   | M     | 74  | TYR  | C-N   | -6.46 | 1.24        | 1.33     |
| 3   | M     | 289 | THR  | C-N   | 6.46  | 1.42        | 1.33     |
| 1   | A     | 226 | SER  | CA-C  | -6.45 | 1.43        | 1.52     |
| 2   | B     | 495 | ASP  | CA-C  | -6.45 | 1.44        | 1.52     |
| 2   | B     | 312 | SER  | C-N   | -6.45 | 1.24        | 1.33     |
| 4   | S     | 77  | TYR  | N-CA  | -6.44 | 1.38        | 1.46     |
| 4   | S     | 125 | TRP  | N-CA  | -6.44 | 1.38        | 1.46     |
| 2   | B     | 502 | SER  | CA-C  | -6.43 | 1.43        | 1.52     |
| 1   | A     | 610 | SER  | CA-C  | -6.43 | 1.43        | 1.52     |
| 2   | B     | 589 | SER  | CA-C  | -6.42 | 1.44        | 1.52     |
| 3   | M     | 273 | HIS  | C-N   | -6.42 | 1.25        | 1.34     |
| 3   | M     | 405 | THR  | C-N   | -6.42 | 1.24        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 492 | ILE  | CA-C  | -6.41 | 1.45        | 1.52     |
| 2   | B     | 489 | ILE  | CA-C  | -6.41 | 1.43        | 1.52     |
| 1   | A     | 458 | ALA  | CA-C  | -6.40 | 1.44        | 1.52     |
| 3   | M     | 46  | SER  | N-CA  | -6.40 | 1.37        | 1.46     |
| 3   | M     | 363 | ASN  | N-CA  | -6.40 | 1.38        | 1.46     |
| 2   | B     | 602 | ASP  | C-N   | -6.39 | 1.24        | 1.33     |
| 2   | B     | 134 | LEU  | CA-C  | -6.39 | 1.44        | 1.52     |
| 1   | A     | 292 | TYR  | N-CA  | -6.39 | 1.38        | 1.46     |
| 4   | S     | 31  | LEU  | CA-C  | -6.39 | 1.44        | 1.52     |
| 4   | S     | 57  | LEU  | C-N   | -6.38 | 1.24        | 1.33     |
| 1   | A     | 397 | ASP  | CA-C  | 6.38  | 1.60        | 1.52     |
| 4   | S     | 159 | ALA  | CA-CB | 6.38  | 1.63        | 1.53     |
| 2   | B     | 359 | LEU  | CA-C  | -6.37 | 1.44        | 1.52     |
| 2   | B     | 263 | PRO  | N-CA  | -6.37 | 1.40        | 1.47     |
| 3   | M     | 444 | ALA  | CA-CB | 6.36  | 1.63        | 1.53     |
| 1   | A     | 473 | ILE  | CA-C  | -6.36 | 1.44        | 1.52     |
| 4   | S     | 118 | GLU  | C-N   | 6.35  | 1.43        | 1.33     |
| 2   | B     | 513 | TRP  | CA-C  | -6.35 | 1.44        | 1.52     |
| 2   | B     | 345 | ARG  | CA-C  | -6.35 | 1.44        | 1.52     |
| 4   | S     | 118 | GLU  | CA-C  | -6.35 | 1.44        | 1.52     |
| 3   | M     | 252 | ASP  | C-N   | -6.34 | 1.20        | 1.33     |
| 2   | B     | 437 | SER  | CA-C  | -6.34 | 1.44        | 1.52     |
| 2   | B     | 493 | LEU  | CA-C  | -6.33 | 1.44        | 1.52     |
| 2   | B     | 155 | LEU  | CA-C  | -6.33 | 1.44        | 1.52     |
| 2   | B     | 306 | LEU  | N-CA  | -6.32 | 1.38        | 1.46     |
| 3   | M     | 5   | PHE  | C-N   | -6.32 | 1.24        | 1.33     |
| 3   | M     | 86  | PRO  | N-CA  | -6.32 | 1.39        | 1.47     |
| 1   | A     | 507 | GLN  | CA-C  | -6.32 | 1.44        | 1.52     |
| 1   | A     | 383 | ASN  | CA-C  | -6.32 | 1.44        | 1.52     |
| 1   | A     | 77  | LEU  | C-O   | 6.31  | 1.31        | 1.24     |
| 2   | B     | 559 | ASP  | N-CA  | -6.31 | 1.37        | 1.46     |
| 1   | A     | 86  | TRP  | CA-C  | -6.31 | 1.43        | 1.52     |
| 1   | A     | 439 | ASP  | CA-C  | -6.31 | 1.46        | 1.53     |
| 1   | A     | 528 | ASN  | C-N   | -6.30 | 1.26        | 1.33     |
| 3   | M     | 296 | LYS  | C-N   | -6.30 | 1.24        | 1.33     |
| 3   | M     | 355 | ASP  | C-N   | -6.30 | 1.24        | 1.33     |
| 2   | B     | 563 | PHE  | C-N   | 6.30  | 1.42        | 1.33     |
| 1   | A     | 600 | SER  | CA-C  | -6.29 | 1.44        | 1.52     |
| 2   | B     | 189 | HIS  | N-CA  | -6.29 | 1.38        | 1.46     |
| 4   | S     | 100 | ASP  | C-O   | 6.29  | 1.32        | 1.24     |
| 1   | A     | 180 | LYS  | N-CA  | -6.29 | 1.38        | 1.46     |
| 2   | B     | 531 | ARG  | N-CA  | -6.28 | 1.38        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 551 | LEU  | CA-C  | -6.28 | 1.44        | 1.52     |
| 3   | M     | 23  | THR  | CA-C  | -6.27 | 1.45        | 1.52     |
| 3   | M     | 345 | GLU  | N-CA  | -6.27 | 1.38        | 1.46     |
| 4   | S     | 46  | PHE  | N-CA  | -6.27 | 1.38        | 1.46     |
| 2   | B     | 184 | GLY  | N-CA  | 6.27  | 1.54        | 1.45     |
| 1   | A     | 488 | ARG  | C-N   | 6.27  | 1.42        | 1.34     |
| 2   | B     | 461 | HIS  | N-CA  | -6.26 | 1.38        | 1.46     |
| 2   | B     | 422 | ALA  | N-CA  | -6.26 | 1.37        | 1.45     |
| 4   | S     | 95  | GLU  | CA-C  | -6.25 | 1.44        | 1.52     |
| 1   | A     | 309 | PHE  | N-CA  | -6.25 | 1.39        | 1.46     |
| 2   | B     | 532 | ARG  | CA-C  | -6.25 | 1.44        | 1.52     |
| 1   | A     | 609 | LEU  | CA-C  | -6.25 | 1.45        | 1.52     |
| 3   | M     | 75  | TRP  | C-O   | -6.23 | 1.16        | 1.24     |
| 1   | A     | 125 | THR  | CA-C  | -6.22 | 1.45        | 1.52     |
| 3   | M     | 362 | PHE  | C-N   | -6.22 | 1.25        | 1.33     |
| 3   | M     | 407 | THR  | CA-C  | -6.22 | 1.45        | 1.52     |
| 2   | B     | 163 | THR  | N-CA  | -6.21 | 1.37        | 1.46     |
| 3   | M     | 16  | PHE  | C-N   | -6.20 | 1.25        | 1.33     |
| 2   | B     | 607 | ILE  | CA-C  | -6.20 | 1.45        | 1.52     |
| 1   | A     | 256 | LEU  | CA-C  | -6.19 | 1.44        | 1.52     |
| 3   | M     | 415 | ILE  | C-N   | -6.18 | 1.25        | 1.33     |
| 3   | M     | 108 | LYS  | C-N   | -6.18 | 1.23        | 1.33     |
| 3   | M     | 387 | GLU  | N-CA  | -6.18 | 1.38        | 1.46     |
| 2   | B     | 447 | GLU  | CA-C  | -6.17 | 1.44        | 1.52     |
| 2   | B     | 102 | HIS  | C-N   | -6.17 | 1.25        | 1.33     |
| 1   | A     | 552 | ILE  | CA-C  | -6.17 | 1.45        | 1.52     |
| 1   | A     | 602 | GLU  | CA-C  | -6.17 | 1.44        | 1.52     |
| 2   | B     | 341 | GLU  | CA-C  | -6.16 | 1.44        | 1.52     |
| 2   | B     | 522 | GLU  | C-N   | -6.16 | 1.25        | 1.33     |
| 2   | B     | 350 | THR  | N-CA  | -6.15 | 1.38        | 1.46     |
| 4   | S     | 72  | ASP  | CA-C  | 6.15  | 1.61        | 1.52     |
| 2   | B     | 336 | ASN  | N-CA  | -6.14 | 1.38        | 1.46     |
| 3   | M     | 13  | LYS  | N-CA  | -6.14 | 1.38        | 1.46     |
| 4   | S     | 151 | ALA  | CA-C  | -6.14 | 1.44        | 1.52     |
| 2   | B     | 273 | SER  | N-CA  | -6.13 | 1.36        | 1.46     |
| 3   | M     | 67  | SER  | N-CA  | -6.13 | 1.38        | 1.45     |
| 2   | B     | 301 | LEU  | CA-C  | -6.13 | 1.44        | 1.52     |
| 2   | B     | 459 | GLU  | CA-C  | 6.12  | 1.60        | 1.52     |
| 1   | A     | 115 | TYR  | N-CA  | -6.12 | 1.38        | 1.46     |
| 2   | B     | 474 | VAL  | CA-C  | -6.12 | 1.45        | 1.52     |
| 4   | S     | 165 | SER  | C-N   | 6.11  | 1.42        | 1.33     |
| 1   | A     | 607 | LEU  | N-CA  | -6.11 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 370 | ASP  | CA-C  | -6.10 | 1.46        | 1.53     |
| 2   | B     | 23  | ALA  | N-CA  | 6.09  | 1.54        | 1.46     |
| 4   | S     | 114 | THR  | N-CA  | -6.09 | 1.38        | 1.46     |
| 2   | B     | 299 | LEU  | C-N   | 6.08  | 1.41        | 1.33     |
| 3   | M     | 317 | MET  | CA-C  | -6.08 | 1.44        | 1.52     |
| 2   | B     | 334 | MET  | CA-C  | -6.07 | 1.44        | 1.52     |
| 3   | M     | 99  | ILE  | C-N   | 6.07  | 1.43        | 1.33     |
| 3   | M     | 462 | LYS  | C-N   | -6.07 | 1.25        | 1.33     |
| 4   | S     | 39  | ILE  | N-CA  | -6.07 | 1.38        | 1.46     |
| 1   | A     | 602 | GLU  | N-CA  | -6.06 | 1.39        | 1.46     |
| 2   | B     | 531 | ARG  | CA-C  | -6.06 | 1.45        | 1.52     |
| 2   | B     | 170 | ARG  | CA-C  | 6.05  | 1.61        | 1.52     |
| 3   | M     | 290 | PHE  | C-N   | -6.05 | 1.26        | 1.33     |
| 2   | B     | 361 | GLN  | CA-C  | -6.04 | 1.45        | 1.52     |
| 4   | S     | 93  | GLU  | C-N   | -6.04 | 1.25        | 1.33     |
| 3   | M     | 313 | SER  | CA-C  | 6.04  | 1.60        | 1.52     |
| 2   | B     | 305 | SER  | CA-C  | -6.04 | 1.45        | 1.52     |
| 4   | S     | 84  | TYR  | N-CA  | -6.03 | 1.38        | 1.46     |
| 2   | B     | 302 | PHE  | CA-C  | -6.02 | 1.45        | 1.52     |
| 1   | A     | 490 | VAL  | CA-C  | -6.01 | 1.45        | 1.52     |
| 4   | S     | 129 | GLU  | CA-C  | -6.01 | 1.45        | 1.52     |
| 4   | S     | 150 | VAL  | CA-C  | -6.01 | 1.45        | 1.52     |
| 2   | B     | 408 | VAL  | N-CA  | -6.01 | 1.38        | 1.46     |
| 1   | A     | 436 | CYS  | CA-C  | 6.01  | 1.60        | 1.52     |
| 2   | B     | 285 | GLU  | C-N   | -6.01 | 1.26        | 1.33     |
| 3   | M     | 25  | PRO  | N-CA  | -6.01 | 1.38        | 1.47     |
| 2   | B     | 109 | ALA  | CA-C  | -6.01 | 1.44        | 1.52     |
| 2   | B     | 157 | THR  | CA-C  | -6.01 | 1.45        | 1.52     |
| 3   | M     | 480 | GLN  | C-N   | -6.00 | 1.25        | 1.33     |
| 2   | B     | 458 | MET  | N-CA  | -6.00 | 1.39        | 1.46     |
| 1   | A     | 612 | GLU  | N-CA  | -5.99 | 1.39        | 1.46     |
| 3   | M     | 418 | GLU  | CA-C  | 5.99  | 1.60        | 1.52     |
| 1   | A     | 495 | ILE  | N-CA  | -5.99 | 1.39        | 1.46     |
| 1   | A     | 613 | ALA  | N-CA  | -5.98 | 1.39        | 1.46     |
| 1   | A     | 416 | ILE  | C-N   | 5.98  | 1.41        | 1.33     |
| 2   | B     | 530 | LEU  | CA-C  | -5.98 | 1.44        | 1.52     |
| 3   | M     | 447 | ILE  | N-CA  | 5.98  | 1.53        | 1.46     |
| 1   | A     | 134 | TYR  | CA-C  | -5.98 | 1.45        | 1.52     |
| 1   | A     | 582 | ILE  | CA-C  | -5.98 | 1.45        | 1.52     |
| 2   | B     | 469 | ASP  | CA-C  | -5.98 | 1.45        | 1.52     |
| 3   | M     | 124 | ILE  | CA-C  | -5.98 | 1.45        | 1.52     |
| 4   | S     | 143 | GLU  | N-CA  | -5.98 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 475 | GLU  | CA-C  | -5.98 | 1.44        | 1.52     |
| 3   | M     | 424 | PHE  | N-CA  | -5.98 | 1.38        | 1.46     |
| 2   | B     | 353 | GLN  | N-CA  | -5.97 | 1.39        | 1.46     |
| 1   | A     | 605 | GLU  | C-N   | 5.97  | 1.41        | 1.33     |
| 3   | M     | 118 | TYR  | CA-C  | -5.97 | 1.44        | 1.52     |
| 2   | B     | 521 | ILE  | N-CA  | -5.97 | 1.38        | 1.46     |
| 1   | A     | 216 | SER  | C-O   | 5.96  | 1.31        | 1.24     |
| 1   | A     | 621 | LEU  | C-N   | -5.96 | 1.26        | 1.34     |
| 3   | M     | 371 | GLU  | N-CA  | -5.96 | 1.39        | 1.46     |
| 3   | M     | 457 | GLY  | CA-C  | -5.96 | 1.43        | 1.51     |
| 2   | B     | 213 | LEU  | N-CA  | -5.96 | 1.38        | 1.46     |
| 3   | M     | 97  | ASP  | C-N   | 5.95  | 1.42        | 1.33     |
| 2   | B     | 450 | VAL  | N-CA  | -5.95 | 1.39        | 1.46     |
| 2   | B     | 486 | HIS  | N-CA  | -5.95 | 1.39        | 1.46     |
| 3   | M     | 124 | ILE  | N-CA  | -5.94 | 1.39        | 1.46     |
| 2   | B     | 263 | PRO  | C-N   | -5.94 | 1.25        | 1.33     |
| 3   | M     | 276 | VAL  | CA-C  | 5.94  | 1.59        | 1.52     |
| 2   | B     | 74  | ASP  | C-N   | -5.94 | 1.25        | 1.33     |
| 3   | M     | 79  | SER  | N-CA  | -5.93 | 1.38        | 1.45     |
| 1   | A     | 375 | VAL  | C-O   | 5.92  | 1.31        | 1.24     |
| 4   | S     | 44  | SER  | N-CA  | 5.92  | 1.53        | 1.46     |
| 4   | S     | 101 | LEU  | CA-C  | -5.92 | 1.44        | 1.52     |
| 2   | B     | 410 | GLU  | CA-C  | -5.92 | 1.44        | 1.52     |
| 2   | B     | 100 | LEU  | N-CA  | -5.91 | 1.39        | 1.46     |
| 3   | M     | 385 | ARG  | CA-C  | 5.91  | 1.59        | 1.52     |
| 1   | A     | 523 | SER  | N-CA  | -5.90 | 1.38        | 1.46     |
| 1   | A     | 270 | LEU  | C-N   | 5.90  | 1.41        | 1.33     |
| 1   | A     | 107 | TYR  | CA-C  | -5.90 | 1.45        | 1.52     |
| 3   | M     | 318 | ASN  | N-CA  | -5.90 | 1.38        | 1.46     |
| 1   | A     | 612 | GLU  | CA-C  | -5.89 | 1.45        | 1.52     |
| 2   | B     | 412 | PHE  | CA-C  | -5.89 | 1.44        | 1.52     |
| 2   | B     | 585 | GLY  | N-CA  | -5.89 | 1.36        | 1.45     |
| 2   | B     | 76  | SER  | N-CA  | -5.89 | 1.38        | 1.46     |
| 3   | M     | 107 | ASP  | C-N   | 5.89  | 1.42        | 1.33     |
| 4   | S     | 35  | VAL  | CA-C  | -5.88 | 1.43        | 1.52     |
| 1   | A     | 173 | THR  | CA-C  | 5.88  | 1.61        | 1.53     |
| 2   | B     | 543 | GLU  | CA-C  | -5.88 | 1.45        | 1.52     |
| 1   | A     | 300 | LYS  | CA-C  | -5.87 | 1.45        | 1.52     |
| 3   | M     | 368 | ASP  | CA-C  | -5.87 | 1.45        | 1.52     |
| 2   | B     | 294 | VAL  | N-CA  | -5.87 | 1.38        | 1.46     |
| 1   | A     | 151 | SER  | N-CA  | -5.87 | 1.38        | 1.46     |
| 2   | B     | 74  | ASP  | CA-C  | -5.87 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 595 | VAL  | CA-C  | -5.86 | 1.45        | 1.52     |
| 1   | A     | 359 | LEU  | CA-C  | -5.86 | 1.44        | 1.52     |
| 2   | B     | 119 | SER  | CA-C  | -5.86 | 1.44        | 1.52     |
| 1   | A     | 141 | VAL  | CA-C  | -5.86 | 1.45        | 1.52     |
| 3   | M     | 382 | THR  | C-N   | 5.85  | 1.41        | 1.33     |
| 1   | A     | 380 | ASP  | CA-C  | -5.85 | 1.45        | 1.52     |
| 3   | M     | 120 | ARG  | N-CA  | -5.85 | 1.38        | 1.46     |
| 4   | S     | 27  | LYS  | N-CA  | -5.85 | 1.38        | 1.46     |
| 1   | A     | 389 | GLN  | CA-C  | -5.85 | 1.45        | 1.52     |
| 2   | B     | 319 | LEU  | CA-C  | -5.85 | 1.45        | 1.52     |
| 1   | A     | 628 | VAL  | N-CA  | -5.84 | 1.39        | 1.46     |
| 2   | B     | 422 | ALA  | C-N   | -5.84 | 1.26        | 1.33     |
| 3   | M     | 125 | PHE  | N-CA  | -5.84 | 1.39        | 1.46     |
| 3   | M     | 405 | THR  | N-CA  | -5.84 | 1.38        | 1.46     |
| 2   | B     | 494 | ALA  | N-CA  | -5.83 | 1.39        | 1.46     |
| 3   | M     | 277 | GLU  | C-O   | 5.83  | 1.31        | 1.24     |
| 3   | M     | 100 | LEU  | N-CA  | -5.83 | 1.38        | 1.46     |
| 1   | A     | 494 | ASN  | CA-C  | -5.82 | 1.44        | 1.52     |
| 2   | B     | 63  | MET  | N-CA  | -5.82 | 1.39        | 1.46     |
| 2   | B     | 77  | ILE  | N-CA  | -5.82 | 1.39        | 1.46     |
| 4   | S     | 98  | ILE  | CA-C  | -5.82 | 1.43        | 1.52     |
| 1   | A     | 236 | LEU  | CA-C  | -5.82 | 1.44        | 1.52     |
| 3   | M     | 122 | SER  | C-N   | 5.82  | 1.42        | 1.34     |
| 3   | M     | 455 | VAL  | C-N   | 5.82  | 1.40        | 1.33     |
| 3   | M     | 331 | LEU  | C-N   | -5.81 | 1.27        | 1.33     |
| 1   | A     | 566 | PHE  | C-N   | -5.80 | 1.25        | 1.33     |
| 4   | S     | 109 | LEU  | C-O   | -5.80 | 1.17        | 1.24     |
| 4   | S     | 142 | ILE  | N-CA  | 5.80  | 1.52        | 1.46     |
| 1   | A     | 76  | TYR  | CA-C  | -5.80 | 1.45        | 1.52     |
| 1   | A     | 239 | LEU  | CA-C  | -5.79 | 1.45        | 1.52     |
| 1   | A     | 110 | ALA  | CA-CB | 5.79  | 1.62        | 1.53     |
| 1   | A     | 581 | LEU  | CA-C  | -5.79 | 1.44        | 1.52     |
| 3   | M     | 77  | LEU  | C-N   | -5.79 | 1.25        | 1.33     |
| 1   | A     | 606 | PHE  | CA-C  | -5.79 | 1.45        | 1.52     |
| 1   | A     | 229 | ASN  | CA-C  | -5.79 | 1.46        | 1.53     |
| 2   | B     | 409 | LYS  | CA-C  | -5.79 | 1.44        | 1.52     |
| 2   | B     | 34  | SER  | CA-C  | -5.78 | 1.45        | 1.52     |
| 2   | B     | 138 | ALA  | CA-C  | -5.78 | 1.45        | 1.52     |
| 2   | B     | 496 | LEU  | CA-C  | -5.78 | 1.45        | 1.52     |
| 1   | A     | 404 | GLN  | CA-C  | 5.78  | 1.60        | 1.53     |
| 2   | B     | 512 | VAL  | CA-C  | -5.78 | 1.45        | 1.52     |
| 1   | A     | 491 | THR  | CA-C  | -5.77 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 237 | THR  | C-N   | -5.77 | 1.25        | 1.33     |
| 3   | M     | 50  | TYR  | CA-C  | 5.76  | 1.60        | 1.52     |
| 3   | M     | 126 | ASN  | N-CA  | -5.76 | 1.39        | 1.46     |
| 2   | B     | 571 | SER  | N-CA  | -5.76 | 1.38        | 1.45     |
| 4   | S     | 5   | VAL  | N-CA  | -5.75 | 1.39        | 1.46     |
| 2   | B     | 82  | TYR  | CA-C  | -5.75 | 1.44        | 1.52     |
| 3   | M     | 303 | SER  | CA-C  | -5.75 | 1.45        | 1.52     |
| 2   | B     | 123 | LEU  | CA-C  | -5.75 | 1.44        | 1.52     |
| 1   | A     | 461 | CYS  | C-N   | -5.75 | 1.26        | 1.33     |
| 1   | A     | 150 | LEU  | N-CA  | -5.75 | 1.39        | 1.46     |
| 2   | B     | 261 | PRO  | N-CA  | -5.75 | 1.40        | 1.47     |
| 1   | A     | 452 | ALA  | N-CA  | -5.74 | 1.39        | 1.46     |
| 4   | S     | 124 | ASN  | CA-C  | -5.74 | 1.45        | 1.53     |
| 2   | B     | 352 | ASN  | CA-C  | -5.74 | 1.45        | 1.52     |
| 1   | A     | 448 | GLU  | C-N   | -5.73 | 1.25        | 1.33     |
| 2   | B     | 597 | TYR  | CA-C  | -5.73 | 1.45        | 1.52     |
| 2   | B     | 324 | ALA  | CA-C  | -5.73 | 1.45        | 1.52     |
| 1   | A     | 172 | SER  | CA-C  | -5.72 | 1.45        | 1.52     |
| 1   | A     | 425 | LYS  | CA-C  | -5.72 | 1.45        | 1.52     |
| 3   | M     | 83  | SER  | C-O   | -5.72 | 1.19        | 1.24     |
| 2   | B     | 364 | HIS  | CA-C  | -5.72 | 1.45        | 1.52     |
| 2   | B     | 444 | THR  | N-CA  | -5.72 | 1.39        | 1.46     |
| 2   | B     | 520 | SER  | CA-C  | -5.71 | 1.44        | 1.52     |
| 2   | B     | 251 | LEU  | CA-C  | -5.71 | 1.45        | 1.52     |
| 2   | B     | 605 | PHE  | CA-C  | -5.70 | 1.45        | 1.52     |
| 3   | M     | 291 | ILE  | CA-C  | 5.70  | 1.58        | 1.52     |
| 4   | S     | 128 | LEU  | CA-C  | -5.70 | 1.45        | 1.52     |
| 1   | A     | 550 | VAL  | CA-C  | -5.70 | 1.45        | 1.52     |
| 2   | B     | 55  | ASN  | CA-C  | -5.70 | 1.46        | 1.52     |
| 1   | A     | 518 | CYS  | CA-C  | -5.70 | 1.45        | 1.52     |
| 2   | B     | 166 | SER  | CA-C  | -5.70 | 1.45        | 1.52     |
| 4   | S     | 7   | ILE  | CA-C  | -5.69 | 1.45        | 1.52     |
| 2   | B     | 83  | PHE  | CA-C  | -5.69 | 1.45        | 1.52     |
| 2   | B     | 579 | PRO  | N-CD  | -5.69 | 1.39        | 1.47     |
| 4   | S     | 119 | LEU  | C-N   | 5.69  | 1.42        | 1.33     |
| 1   | A     | 440 | ASN  | C-N   | -5.68 | 1.26        | 1.33     |
| 1   | A     | 547 | VAL  | C-N   | 5.68  | 1.41        | 1.33     |
| 3   | M     | 51  | LEU  | C-N   | -5.67 | 1.25        | 1.33     |
| 3   | M     | 382 | THR  | CA-C  | 5.66  | 1.60        | 1.52     |
| 2   | B     | 444 | THR  | C-N   | -5.66 | 1.26        | 1.34     |
| 3   | M     | 256 | VAL  | C-N   | 5.66  | 1.41        | 1.33     |
| 3   | M     | 25  | PRO  | CA-C  | -5.66 | 1.41        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 386 | PHE  | C-N   | -5.66 | 1.25        | 1.33     |
| 1   | A     | 412 | LYS  | CA-C  | -5.66 | 1.45        | 1.52     |
| 1   | A     | 332 | TYR  | C-N   | 5.65  | 1.41        | 1.33     |
| 1   | A     | 501 | ASN  | C-N   | -5.65 | 1.26        | 1.33     |
| 1   | A     | 290 | VAL  | N-CA  | -5.64 | 1.39        | 1.46     |
| 1   | A     | 295 | VAL  | N-CA  | -5.64 | 1.39        | 1.46     |
| 1   | A     | 619 | GLU  | CA-C  | -5.64 | 1.45        | 1.52     |
| 2   | B     | 322 | CYS  | CA-C  | -5.63 | 1.45        | 1.52     |
| 1   | A     | 518 | CYS  | N-CA  | -5.63 | 1.39        | 1.46     |
| 2   | B     | 97  | VAL  | CA-C  | -5.63 | 1.46        | 1.52     |
| 2   | B     | 504 | ALA  | CA-C  | -5.63 | 1.45        | 1.52     |
| 4   | S     | 103 | GLN  | C-N   | 5.63  | 1.42        | 1.33     |
| 4   | S     | 40  | SER  | N-CA  | -5.63 | 1.39        | 1.46     |
| 1   | A     | 117 | ASP  | CA-C  | -5.62 | 1.45        | 1.52     |
| 2   | B     | 619 | ASP  | CA-C  | -5.62 | 1.45        | 1.52     |
| 1   | A     | 274 | LEU  | N-CA  | -5.62 | 1.39        | 1.46     |
| 2   | B     | 237 | ILE  | C-N   | -5.62 | 1.26        | 1.33     |
| 4   | S     | 71  | GLU  | CA-C  | 5.61  | 1.60        | 1.52     |
| 4   | S     | 85  | PHE  | C-N   | -5.61 | 1.26        | 1.33     |
| 2   | B     | 333 | GLN  | C-O   | -5.61 | 1.17        | 1.23     |
| 1   | A     | 473 | ILE  | N-CA  | -5.61 | 1.39        | 1.46     |
| 2   | B     | 253 | ILE  | CA-C  | -5.61 | 1.45        | 1.52     |
| 4   | S     | 156 | LEU  | CA-C  | -5.61 | 1.45        | 1.52     |
| 2   | B     | 404 | ASN  | C-N   | -5.61 | 1.26        | 1.34     |
| 2   | B     | 518 | ILE  | N-CA  | -5.61 | 1.40        | 1.46     |
| 3   | M     | 477 | GLY  | N-CA  | -5.60 | 1.39        | 1.45     |
| 2   | B     | 535 | GLN  | N-CA  | -5.60 | 1.39        | 1.46     |
| 3   | M     | 252 | ASP  | CA-C  | -5.60 | 1.45        | 1.52     |
| 2   | B     | 449 | HIS  | CA-C  | -5.60 | 1.45        | 1.52     |
| 1   | A     | 155 | THR  | C-N   | 5.60  | 1.41        | 1.33     |
| 4   | S     | 20  | TYR  | C-N   | -5.59 | 1.26        | 1.33     |
| 1   | A     | 287 | ALA  | C-N   | 5.58  | 1.41        | 1.33     |
| 4   | S     | 36  | TYR  | N-CA  | -5.58 | 1.39        | 1.46     |
| 1   | A     | 196 | LEU  | CA-C  | -5.58 | 1.45        | 1.52     |
| 2   | B     | 503 | LEU  | N-CA  | -5.58 | 1.39        | 1.46     |
| 3   | M     | 260 | LEU  | CA-C  | -5.58 | 1.46        | 1.52     |
| 1   | A     | 282 | MET  | N-CA  | -5.58 | 1.39        | 1.46     |
| 4   | S     | 163 | THR  | C-N   | 5.58  | 1.41        | 1.33     |
| 4   | S     | 53  | THR  | CA-C  | -5.58 | 1.47        | 1.52     |
| 4   | S     | 45  | ASP  | CA-C  | 5.57  | 1.60        | 1.52     |
| 4   | S     | 108 | SER  | C-N   | 5.57  | 1.41        | 1.33     |
| 1   | A     | 180 | LYS  | CA-C  | -5.57 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 466 | LEU  | CA-C  | 5.57  | 1.59        | 1.52     |
| 4   | S     | 86  | THR  | CA-C  | 5.57  | 1.59        | 1.52     |
| 1   | A     | 506 | LYS  | C-N   | -5.57 | 1.25        | 1.33     |
| 2   | B     | 430 | ILE  | C-N   | 5.57  | 1.41        | 1.33     |
| 4   | S     | 137 | GLN  | CA-C  | -5.57 | 1.45        | 1.52     |
| 1   | A     | 390 | THR  | N-CA  | -5.56 | 1.39        | 1.46     |
| 2   | B     | 210 | CYS  | C-N   | -5.56 | 1.26        | 1.33     |
| 2   | B     | 278 | PRO  | C-N   | -5.56 | 1.23        | 1.32     |
| 2   | B     | 549 | LEU  | CA-C  | -5.56 | 1.46        | 1.52     |
| 4   | S     | 152 | SER  | CA-C  | -5.56 | 1.45        | 1.52     |
| 3   | M     | 43  | GLU  | N-CA  | -5.55 | 1.39        | 1.46     |
| 1   | A     | 469 | LEU  | CA-C  | -5.55 | 1.45        | 1.52     |
| 3   | M     | 380 | ARG  | C-N   | -5.55 | 1.25        | 1.33     |
| 1   | A     | 603 | VAL  | CA-C  | -5.54 | 1.45        | 1.52     |
| 2   | B     | 252 | LEU  | CA-C  | -5.54 | 1.44        | 1.52     |
| 1   | A     | 559 | PHE  | CA-C  | -5.54 | 1.45        | 1.52     |
| 4   | S     | 153 | VAL  | CA-C  | -5.54 | 1.45        | 1.52     |
| 2   | B     | 430 | ILE  | CA-C  | -5.54 | 1.46        | 1.52     |
| 2   | B     | 63  | MET  | CA-C  | -5.53 | 1.45        | 1.52     |
| 2   | B     | 324 | ALA  | N-CA  | -5.53 | 1.39        | 1.46     |
| 2   | B     | 598 | LEU  | N-CA  | -5.53 | 1.39        | 1.46     |
| 1   | A     | 94  | VAL  | C-N   | -5.53 | 1.26        | 1.34     |
| 1   | A     | 253 | ILE  | CA-C  | -5.53 | 1.46        | 1.52     |
| 2   | B     | 244 | SER  | CA-C  | -5.52 | 1.45        | 1.52     |
| 2   | B     | 570 | GLY  | CA-C  | -5.52 | 1.44        | 1.51     |
| 2   | B     | 596 | LEU  | CA-C  | -5.52 | 1.45        | 1.52     |
| 3   | M     | 308 | SER  | C-N   | 5.52  | 1.41        | 1.33     |
| 2   | B     | 297 | PRO  | N-CA  | -5.51 | 1.40        | 1.47     |
| 3   | M     | 240 | ILE  | N-CA  | -5.51 | 1.39        | 1.46     |
| 4   | S     | 91  | ASP  | CA-C  | -5.51 | 1.44        | 1.52     |
| 4   | S     | 155 | GLU  | CA-C  | -5.51 | 1.45        | 1.52     |
| 2   | B     | 596 | LEU  | N-CA  | -5.51 | 1.39        | 1.46     |
| 1   | A     | 583 | GLU  | CA-C  | -5.50 | 1.45        | 1.52     |
| 1   | A     | 320 | HIS  | N-CA  | -5.50 | 1.39        | 1.46     |
| 1   | A     | 72  | LEU  | N-CA  | -5.50 | 1.39        | 1.46     |
| 1   | A     | 624 | LEU  | N-CA  | -5.50 | 1.39        | 1.46     |
| 2   | B     | 382 | TYR  | CA-C  | -5.50 | 1.45        | 1.52     |
| 1   | A     | 288 | THR  | N-CA  | 5.49  | 1.56        | 1.46     |
| 2   | B     | 278 | PRO  | CA-C  | -5.49 | 1.46        | 1.52     |
| 2   | B     | 325 | LEU  | C-N   | -5.49 | 1.25        | 1.33     |
| 2   | B     | 553 | ALA  | CA-C  | -5.49 | 1.46        | 1.52     |
| 3   | M     | 86  | PRO  | C-N   | 5.49  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 147 | LEU  | N-CA  | -5.49 | 1.39        | 1.46     |
| 3   | M     | 92  | PHE  | CA-C  | -5.48 | 1.45        | 1.52     |
| 2   | B     | 329 | ALA  | C-N   | -5.48 | 1.25        | 1.33     |
| 1   | A     | 325 | SER  | C-O   | 5.48  | 1.30        | 1.23     |
| 1   | A     | 96  | SER  | CA-C  | 5.48  | 1.60        | 1.52     |
| 2   | B     | 73  | ASP  | N-CA  | -5.48 | 1.38        | 1.46     |
| 3   | M     | 96  | ILE  | CA-C  | -5.47 | 1.44        | 1.52     |
| 3   | M     | 426 | LYS  | CA-C  | -5.47 | 1.47        | 1.53     |
| 1   | A     | 605 | GLU  | CA-C  | -5.47 | 1.45        | 1.52     |
| 2   | B     | 174 | ALA  | CA-CB | 5.47  | 1.61        | 1.53     |
| 3   | M     | 294 | ASP  | CA-C  | 5.47  | 1.60        | 1.53     |
| 1   | A     | 502 | ASP  | CA-C  | -5.47 | 1.45        | 1.52     |
| 1   | A     | 311 | THR  | N-CA  | -5.47 | 1.39        | 1.46     |
| 4   | S     | 50  | PHE  | C-N   | -5.46 | 1.25        | 1.33     |
| 2   | B     | 496 | LEU  | N-CA  | -5.46 | 1.39        | 1.46     |
| 1   | A     | 182 | ILE  | CA-C  | -5.45 | 1.46        | 1.52     |
| 1   | A     | 608 | ARG  | CA-C  | -5.45 | 1.45        | 1.52     |
| 2   | B     | 335 | LYS  | CA-C  | -5.45 | 1.45        | 1.52     |
| 3   | M     | 339 | GLU  | C-N   | -5.45 | 1.26        | 1.33     |
| 4   | S     | 102 | ILE  | CA-C  | -5.45 | 1.45        | 1.52     |
| 2   | B     | 346 | THR  | N-CA  | -5.45 | 1.39        | 1.46     |
| 3   | M     | 407 | THR  | C-N   | -5.45 | 1.28        | 1.33     |
| 1   | A     | 535 | ILE  | N-CA  | -5.45 | 1.35        | 1.46     |
| 3   | M     | 254 | PRO  | N-CA  | -5.45 | 1.40        | 1.47     |
| 4   | S     | 38  | LEU  | N-CA  | -5.45 | 1.39        | 1.46     |
| 1   | A     | 156 | PRO  | C-N   | -5.44 | 1.26        | 1.33     |
| 3   | M     | 445 | SER  | C-N   | 5.44  | 1.41        | 1.33     |
| 2   | B     | 211 | ALA  | N-CA  | 5.44  | 1.53        | 1.46     |
| 2   | B     | 432 | ALA  | CA-C  | -5.44 | 1.45        | 1.52     |
| 2   | B     | 463 | LEU  | C-N   | 5.44  | 1.40        | 1.33     |
| 4   | S     | 41  | GLN  | N-CA  | -5.44 | 1.39        | 1.46     |
| 1   | A     | 402 | ILE  | C-N   | -5.43 | 1.26        | 1.34     |
| 1   | A     | 200 | PHE  | N-CA  | -5.43 | 1.39        | 1.46     |
| 2   | B     | 498 | THR  | N-CA  | -5.43 | 1.39        | 1.46     |
| 2   | B     | 255 | TYR  | N-CA  | -5.43 | 1.39        | 1.46     |
| 3   | M     | 54  | SER  | N-CA  | 5.43  | 1.54        | 1.45     |
| 1   | A     | 257 | LEU  | N-CA  | -5.43 | 1.39        | 1.46     |
| 3   | M     | 22  | ALA  | C-N   | 5.42  | 1.41        | 1.33     |
| 1   | A     | 488 | ARG  | CA-C  | -5.42 | 1.45        | 1.52     |
| 3   | M     | 481 | VAL  | CA-C  | -5.42 | 1.45        | 1.52     |
| 1   | A     | 311 | THR  | CA-C  | -5.42 | 1.45        | 1.52     |
| 1   | A     | 636 | TYR  | CA-C  | -5.41 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 539 | ASN  | C-N   | -5.41 | 1.27        | 1.33     |
| 3   | M     | 298 | ARG  | C-N   | -5.41 | 1.25        | 1.33     |
| 3   | M     | 373 | ALA  | N-CA  | -5.41 | 1.39        | 1.46     |
| 1   | A     | 595 | GLU  | N-CA  | -5.41 | 1.39        | 1.46     |
| 2   | B     | 552 | SER  | CA-C  | -5.40 | 1.45        | 1.52     |
| 2   | B     | 145 | MET  | N-CA  | -5.40 | 1.39        | 1.45     |
| 1   | A     | 87  | CYS  | CA-C  | -5.40 | 1.45        | 1.52     |
| 4   | S     | 65  | ASN  | C-N   | -5.40 | 1.25        | 1.33     |
| 2   | B     | 135 | ARG  | CA-C  | -5.40 | 1.44        | 1.52     |
| 1   | A     | 618 | THR  | N-CA  | -5.39 | 1.39        | 1.46     |
| 1   | A     | 113 | SER  | C-N   | -5.39 | 1.26        | 1.33     |
| 1   | A     | 406 | GLY  | N-CA  | -5.39 | 1.37        | 1.45     |
| 1   | A     | 576 | MET  | CA-C  | -5.39 | 1.45        | 1.52     |
| 1   | A     | 615 | GLU  | N-CA  | -5.39 | 1.39        | 1.46     |
| 2   | B     | 167 | ALA  | CA-C  | -5.39 | 1.45        | 1.52     |
| 2   | B     | 389 | ILE  | C-N   | -5.39 | 1.27        | 1.33     |
| 3   | M     | 77  | LEU  | N-CA  | -5.39 | 1.39        | 1.46     |
| 4   | S     | 132 | LEU  | N-CA  | -5.39 | 1.39        | 1.46     |
| 1   | A     | 582 | ILE  | N-CA  | -5.38 | 1.40        | 1.46     |
| 2   | B     | 106 | LEU  | C-N   | 5.38  | 1.40        | 1.33     |
| 2   | B     | 341 | GLU  | N-CA  | -5.38 | 1.39        | 1.46     |
| 2   | B     | 192 | LEU  | N-CA  | -5.37 | 1.39        | 1.46     |
| 2   | B     | 213 | LEU  | CA-C  | -5.37 | 1.45        | 1.52     |
| 3   | M     | 127 | CYS  | CA-C  | -5.37 | 1.45        | 1.52     |
| 1   | A     | 124 | ALA  | CA-C  | -5.37 | 1.45        | 1.52     |
| 2   | B     | 193 | LEU  | N-CA  | -5.37 | 1.40        | 1.47     |
| 2   | B     | 585 | GLY  | CA-C  | -5.36 | 1.44        | 1.51     |
| 1   | A     | 191 | GLN  | CA-C  | 5.36  | 1.59        | 1.52     |
| 2   | B     | 573 | GLU  | CA-C  | -5.35 | 1.45        | 1.52     |
| 1   | A     | 493 | ALA  | CA-C  | -5.35 | 1.45        | 1.52     |
| 4   | S     | 10  | LYS  | C-N   | -5.35 | 1.26        | 1.33     |
| 2   | B     | 81  | LEU  | N-CA  | -5.35 | 1.39        | 1.46     |
| 3   | M     | 98  | ARG  | CA-C  | -5.35 | 1.45        | 1.52     |
| 1   | A     | 270 | LEU  | N-CA  | -5.34 | 1.39        | 1.46     |
| 1   | A     | 330 | LEU  | C-N   | 5.34  | 1.40        | 1.33     |
| 1   | A     | 433 | ILE  | N-CA  | -5.34 | 1.40        | 1.46     |
| 3   | M     | 40  | GLN  | N-CA  | -5.34 | 1.39        | 1.46     |
| 2   | B     | 580 | TYR  | C-N   | 5.34  | 1.40        | 1.33     |
| 3   | M     | 43  | GLU  | CA-C  | -5.34 | 1.45        | 1.52     |
| 1   | A     | 471 | SER  | CA-C  | -5.33 | 1.46        | 1.52     |
| 4   | S     | 109 | LEU  | C-N   | -5.33 | 1.26        | 1.34     |
| 2   | B     | 395 | LYS  | CA-C  | -5.33 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 134 | PRO  | N-CA  | -5.33 | 1.40        | 1.47     |
| 2   | B     | 406 | SER  | CA-C  | -5.32 | 1.45        | 1.52     |
| 2   | B     | 455 | ILE  | N-CA  | -5.32 | 1.40        | 1.46     |
| 2   | B     | 306 | LEU  | CA-C  | -5.32 | 1.45        | 1.52     |
| 2   | B     | 342 | ALA  | CA-C  | -5.32 | 1.45        | 1.52     |
| 3   | M     | 78  | ALA  | CA-C  | -5.32 | 1.46        | 1.52     |
| 2   | B     | 415 | LEU  | N-CA  | -5.32 | 1.39        | 1.46     |
| 2   | B     | 272 | GLY  | CA-C  | -5.31 | 1.43        | 1.51     |
| 4   | S     | 13  | GLN  | N-CA  | -5.31 | 1.37        | 1.46     |
| 1   | A     | 155 | THR  | CA-C  | -5.30 | 1.45        | 1.52     |
| 3   | M     | 475 | GLN  | CA-C  | -5.30 | 1.45        | 1.52     |
| 3   | M     | 240 | ILE  | CA-C  | -5.30 | 1.46        | 1.52     |
| 2   | B     | 320 | SER  | CA-C  | -5.29 | 1.46        | 1.52     |
| 3   | M     | 456 | SER  | N-CA  | -5.29 | 1.37        | 1.46     |
| 2   | B     | 116 | THR  | CA-C  | -5.29 | 1.46        | 1.52     |
| 3   | M     | 310 | VAL  | CA-C  | 5.29  | 1.59        | 1.52     |
| 2   | B     | 111 | ASN  | N-CA  | 5.28  | 1.53        | 1.46     |
| 2   | B     | 191 | GLU  | N-CA  | -5.28 | 1.39        | 1.46     |
| 2   | B     | 48  | VAL  | N-CA  | -5.27 | 1.40        | 1.46     |
| 1   | A     | 447 | PHE  | N-CA  | -5.27 | 1.39        | 1.46     |
| 1   | A     | 67  | LYS  | CA-C  | -5.27 | 1.46        | 1.52     |
| 2   | B     | 111 | ASN  | CA-C  | 5.27  | 1.59        | 1.52     |
| 2   | B     | 195 | ILE  | CA-C  | -5.27 | 1.46        | 1.52     |
| 1   | A     | 593 | THR  | CA-C  | -5.27 | 1.46        | 1.52     |
| 3   | M     | 329 | ASN  | CA-C  | 5.26  | 1.60        | 1.53     |
| 2   | B     | 105 | LEU  | C-N   | -5.26 | 1.26        | 1.34     |
| 2   | B     | 277 | CYS  | C-N   | 5.26  | 1.39        | 1.33     |
| 2   | B     | 433 | VAL  | CA-C  | -5.25 | 1.45        | 1.52     |
| 3   | M     | 10  | THR  | N-CA  | -5.25 | 1.39        | 1.46     |
| 3   | M     | 48  | ASP  | CA-C  | -5.25 | 1.45        | 1.52     |
| 1   | A     | 174 | ARG  | N-CA  | 5.25  | 1.53        | 1.46     |
| 1   | A     | 193 | PRO  | N-CA  | -5.25 | 1.40        | 1.47     |
| 1   | A     | 152 | THR  | N-CA  | -5.25 | 1.39        | 1.46     |
| 3   | M     | 52  | ASP  | N-CA  | 5.23  | 1.53        | 1.46     |
| 1   | A     | 225 | LEU  | C-N   | 5.23  | 1.41        | 1.33     |
| 2   | B     | 38  | TYR  | N-CA  | -5.23 | 1.39        | 1.46     |
| 1   | A     | 462 | GLN  | C-N   | -5.23 | 1.26        | 1.34     |
| 2   | B     | 321 | CYS  | CA-C  | -5.23 | 1.45        | 1.52     |
| 1   | A     | 312 | ALA  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | A     | 64  | LEU  | C-N   | -5.22 | 1.26        | 1.34     |
| 1   | A     | 441 | TYR  | N-CA  | -5.22 | 1.40        | 1.46     |
| 1   | A     | 434 | SER  | C-N   | 5.22  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | S     | 17  | VAL  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | A     | 128 | LEU  | CA-C  | -5.21 | 1.45        | 1.52     |
| 1   | A     | 313 | MET  | N-CA  | -5.21 | 1.40        | 1.46     |
| 1   | A     | 428 | MET  | CA-C  | -5.21 | 1.46        | 1.52     |
| 3   | M     | 87  | LEU  | CA-C  | -5.21 | 1.46        | 1.52     |
| 3   | M     | 247 | ARG  | CA-C  | -5.21 | 1.46        | 1.52     |
| 2   | B     | 448 | SER  | CA-C  | -5.20 | 1.46        | 1.52     |
| 1   | A     | 242 | GLU  | C-N   | -5.20 | 1.26        | 1.33     |
| 4   | S     | 93  | GLU  | N-CA  | 5.20  | 1.51        | 1.45     |
| 1   | A     | 556 | VAL  | CA-C  | -5.20 | 1.45        | 1.52     |
| 2   | B     | 356 | LYS  | CA-C  | -5.19 | 1.46        | 1.52     |
| 2   | B     | 493 | LEU  | N-CA  | -5.19 | 1.39        | 1.46     |
| 3   | M     | 47  | SER  | CA-C  | -5.19 | 1.46        | 1.52     |
| 4   | S     | 87  | PHE  | C-N   | -5.19 | 1.26        | 1.33     |
| 2   | B     | 232 | ARG  | CA-C  | -5.19 | 1.45        | 1.52     |
| 2   | B     | 590 | GLN  | N-CA  | -5.19 | 1.39        | 1.46     |
| 3   | M     | 473 | LYS  | C-N   | -5.19 | 1.26        | 1.33     |
| 2   | B     | 72  | SER  | CA-C  | -5.18 | 1.45        | 1.52     |
| 2   | B     | 478 | LEU  | C-N   | -5.18 | 1.27        | 1.34     |
| 3   | M     | 104 | PHE  | C-O   | -5.18 | 1.17        | 1.24     |
| 1   | A     | 240 | LEU  | N-CA  | -5.18 | 1.39        | 1.46     |
| 2   | B     | 459 | GLU  | C-O   | 5.18  | 1.30        | 1.24     |
| 2   | B     | 451 | MET  | CA-C  | -5.17 | 1.46        | 1.52     |
| 1   | A     | 294 | SER  | CA-C  | -5.17 | 1.45        | 1.52     |
| 1   | A     | 462 | GLN  | N-CA  | -5.17 | 1.39        | 1.46     |
| 2   | B     | 154 | ILE  | N-CA  | -5.17 | 1.40        | 1.46     |
| 2   | B     | 310 | ILE  | N-CA  | -5.17 | 1.39        | 1.46     |
| 1   | A     | 426 | ILE  | CA-C  | -5.17 | 1.46        | 1.52     |
| 4   | S     | 142 | ILE  | CA-C  | -5.17 | 1.44        | 1.52     |
| 3   | M     | 7   | ILE  | C-O   | -5.17 | 1.18        | 1.24     |
| 4   | S     | 18  | LYS  | C-N   | -5.16 | 1.26        | 1.33     |
| 1   | A     | 571 | ARG  | C-N   | -5.16 | 1.27        | 1.34     |
| 2   | B     | 373 | LEU  | CA-C  | -5.16 | 1.45        | 1.52     |
| 3   | M     | 333 | LYS  | CA-C  | 5.16  | 1.59        | 1.52     |
| 4   | S     | 12  | CYS  | CA-C  | -5.16 | 1.45        | 1.53     |
| 2   | B     | 20  | ARG  | CA-C  | 5.15  | 1.59        | 1.52     |
| 2   | B     | 362 | ALA  | CA-C  | -5.15 | 1.45        | 1.52     |
| 3   | M     | 18  | TYR  | C-N   | -5.15 | 1.26        | 1.33     |
| 3   | M     | 451 | ALA  | C-N   | 5.15  | 1.39        | 1.33     |
| 1   | A     | 431 | VAL  | C-N   | 5.14  | 1.40        | 1.33     |
| 1   | A     | 552 | ILE  | N-CA  | -5.14 | 1.40        | 1.46     |
| 2   | B     | 531 | ARG  | C-N   | 5.14  | 1.41        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 306 | GLU  | N-CA  | 5.13  | 1.52        | 1.46     |
| 3   | M     | 404 | ALA  | C-N   | -5.13 | 1.26        | 1.33     |
| 4   | S     | 141 | VAL  | C-N   | -5.13 | 1.27        | 1.33     |
| 1   | A     | 575 | LYS  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | A     | 227 | LYS  | N-CA  | -5.12 | 1.40        | 1.46     |
| 2   | B     | 614 | ILE  | CA-C  | -5.12 | 1.46        | 1.52     |
| 2   | B     | 588 | ILE  | C-N   | 5.12  | 1.40        | 1.33     |
| 1   | A     | 122 | MET  | CA-C  | -5.12 | 1.46        | 1.52     |
| 3   | M     | 406 | GLY  | C-N   | 5.12  | 1.40        | 1.33     |
| 2   | B     | 620 | SER  | N-CA  | -5.11 | 1.39        | 1.46     |
| 4   | S     | 30  | LEU  | CA-C  | -5.11 | 1.46        | 1.52     |
| 3   | M     | 304 | VAL  | CA-C  | -5.11 | 1.46        | 1.52     |
| 1   | A     | 378 | ILE  | N-CA  | 5.11  | 1.50        | 1.46     |
| 1   | A     | 596 | VAL  | N-CA  | -5.10 | 1.40        | 1.46     |
| 2   | B     | 618 | PHE  | N-CA  | -5.10 | 1.40        | 1.46     |
| 3   | M     | 408 | VAL  | CA-C  | -5.10 | 1.47        | 1.52     |
| 1   | A     | 186 | PHE  | CA-C  | -5.10 | 1.46        | 1.52     |
| 1   | A     | 234 | ILE  | N-CA  | -5.10 | 1.39        | 1.46     |
| 2   | B     | 339 | PHE  | C-N   | 5.10  | 1.40        | 1.33     |
| 1   | A     | 121 | LEU  | CA-C  | -5.09 | 1.46        | 1.52     |
| 2   | B     | 465 | ALA  | CA-C  | -5.09 | 1.46        | 1.52     |
| 1   | A     | 330 | LEU  | N-CA  | -5.09 | 1.39        | 1.46     |
| 3   | M     | 367 | ALA  | CA-C  | 5.09  | 1.58        | 1.52     |
| 1   | A     | 509 | PRO  | N-CA  | -5.09 | 1.40        | 1.47     |
| 2   | B     | 407 | ASN  | CA-C  | -5.09 | 1.46        | 1.52     |
| 1   | A     | 219 | VAL  | CA-C  | -5.08 | 1.46        | 1.52     |
| 3   | M     | 367 | ALA  | C-N   | -5.08 | 1.24        | 1.33     |
| 4   | S     | 101 | LEU  | C-O   | 5.08  | 1.30        | 1.24     |
| 1   | A     | 489 | GLU  | CA-C  | -5.08 | 1.45        | 1.52     |
| 1   | A     | 633 | PHE  | CA-C  | -5.08 | 1.46        | 1.52     |
| 1   | A     | 276 | PRO  | CA-C  | 5.07  | 1.59        | 1.52     |
| 3   | M     | 41  | LEU  | C-O   | -5.07 | 1.17        | 1.24     |
| 1   | A     | 412 | LYS  | C-N   | -5.07 | 1.26        | 1.33     |
| 2   | B     | 211 | ALA  | C-O   | 5.07  | 1.30        | 1.24     |
| 1   | A     | 442 | SER  | CA-C  | 5.06  | 1.59        | 1.52     |
| 1   | A     | 522 | PHE  | N-CA  | -5.06 | 1.39        | 1.46     |
| 2   | B     | 33  | SER  | C-N   | 5.06  | 1.40        | 1.33     |
| 2   | B     | 240 | LEU  | C-N   | 5.06  | 1.40        | 1.33     |
| 1   | A     | 275 | LEU  | N-CA  | -5.05 | 1.39        | 1.46     |
| 2   | B     | 190 | GLU  | CA-C  | -5.05 | 1.46        | 1.52     |
| 1   | A     | 532 | LEU  | N-CA  | -5.05 | 1.40        | 1.46     |
| 2   | B     | 492 | LYS  | CA-C  | -5.05 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | M     | 242 | GLY  | CA-C  | -5.05 | 1.48        | 1.52     |
| 1   | A     | 420 | ILE  | C-N   | -5.04 | 1.27        | 1.33     |
| 4   | S     | 87  | PHE  | CA-C  | 5.04  | 1.58        | 1.52     |
| 4   | S     | 120 | ASP  | N-CA  | -5.04 | 1.39        | 1.46     |
| 1   | A     | 417 | PRO  | N-CA  | -5.04 | 1.41        | 1.47     |
| 1   | A     | 85  | ALA  | C-O   | 5.03  | 1.30        | 1.24     |
| 2   | B     | 233 | TYR  | CA-C  | -5.03 | 1.46        | 1.52     |
| 2   | B     | 493 | LEU  | C-N   | 5.03  | 1.40        | 1.33     |
| 1   | A     | 158 | LEU  | C-N   | 5.03  | 1.40        | 1.34     |
| 1   | A     | 514 | GLU  | CA-C  | -5.03 | 1.46        | 1.52     |
| 3   | M     | 412 | ARG  | C-N   | -5.03 | 1.28        | 1.33     |
| 3   | M     | 90  | PHE  | C-N   | 5.03  | 1.40        | 1.34     |
| 3   | M     | 480 | GLN  | CA-C  | -5.03 | 1.46        | 1.52     |
| 2   | B     | 129 | ASP  | C-N   | -5.02 | 1.27        | 1.33     |
| 2   | B     | 536 | ASN  | N-CA  | -5.02 | 1.40        | 1.46     |
| 1   | A     | 584 | PHE  | CA-C  | -5.02 | 1.46        | 1.52     |
| 3   | M     | 405 | THR  | CA-C  | -5.02 | 1.46        | 1.52     |
| 2   | B     | 467 | VAL  | CA-C  | -5.01 | 1.46        | 1.52     |
| 4   | S     | 52  | VAL  | C-N   | -5.01 | 1.26        | 1.33     |
| 1   | A     | 163 | ALA  | CA-CB | 5.01  | 1.61        | 1.53     |
| 3   | M     | 439 | TYR  | N-CA  | -5.01 | 1.39        | 1.45     |
| 4   | S     | 144 | THR  | CA-C  | -5.01 | 1.46        | 1.52     |
| 2   | B     | 311 | TYR  | N-CA  | -5.01 | 1.40        | 1.46     |
| 3   | M     | 271 | SER  | C-N   | 5.00  | 1.40        | 1.33     |

All (3409) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | S     | 69  | ASN  | N-CA-C | 46.05  | 173.71      | 114.31   |
| 2   | B     | 584 | SER  | N-CA-C | 36.98  | 151.67      | 111.36   |
| 3   | M     | 130 | GLU  | N-CA-C | -35.18 | 58.45       | 110.52   |
| 1   | A     | 444 | VAL  | N-CA-C | -33.13 | 66.84       | 109.58   |
| 4   | S     | 69  | ASN  | CA-C-O | -32.80 | 82.37       | 118.77   |
| 1   | A     | 275 | LEU  | CA-C-N | -31.99 | 87.33       | 119.64   |
| 1   | A     | 275 | LEU  | C-N-CA | -31.99 | 87.33       | 119.64   |
| 1   | A     | 242 | GLU  | CA-C-N | 31.64  | 178.65      | 121.70   |
| 1   | A     | 242 | GLU  | C-N-CA | 31.64  | 178.65      | 121.70   |
| 2   | B     | 275 | ARG  | N-CA-C | -31.00 | 70.54       | 110.53   |
| 1   | A     | 80  | TYR  | N-CA-C | -30.52 | 61.42       | 109.95   |
| 3   | M     | 103 | TYR  | N-CA-C | -30.38 | 65.49       | 110.46   |
| 1   | A     | 265 | GLN  | N-CA-C | -30.38 | 59.03       | 109.46   |
| 3   | M     | 292 | PRO  | CA-C-N | 29.98  | 157.31      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | M     | 292 | PRO  | C-N-CA | 29.98  | 157.31      | 119.84   |
| 4   | S     | 58  | LEU  | N-CA-C | -29.75 | 62.65       | 109.95   |
| 3   | M     | 82  | LYS  | CA-C-N | 28.27  | 164.32      | 123.04   |
| 3   | M     | 82  | LYS  | C-N-CA | 28.27  | 164.32      | 123.04   |
| 1   | A     | 439 | ASP  | N-CA-C | -27.60 | 67.15       | 108.00   |
| 4   | S     | 69  | ASN  | O-C-N  | 27.36  | 152.43      | 122.34   |
| 3   | M     | 354 | ASP  | N-CA-C | -26.46 | 66.28       | 109.40   |
| 2   | B     | 335 | LYS  | N-CA-C | -26.19 | 82.73       | 111.28   |
| 2   | B     | 580 | TYR  | CA-C-N | -25.82 | 84.05       | 120.71   |
| 2   | B     | 580 | TYR  | C-N-CA | -25.82 | 84.05       | 120.71   |
| 3   | M     | 351 | SER  | N-CA-C | 25.73  | 143.77      | 112.38   |
| 1   | A     | 532 | LEU  | CA-C-N | -25.31 | 88.17       | 120.56   |
| 1   | A     | 532 | LEU  | C-N-CA | -25.31 | 88.17       | 120.56   |
| 3   | M     | 294 | ASP  | N-CA-C | -25.09 | 73.38       | 110.52   |
| 3   | M     | 50  | TYR  | N-CA-C | 24.67  | 143.06      | 113.20   |
| 1   | A     | 621 | LEU  | CA-C-N | -24.61 | 93.11       | 119.19   |
| 1   | A     | 621 | LEU  | C-N-CA | -24.61 | 93.11       | 119.19   |
| 1   | A     | 629 | LEU  | CA-C-N | -24.14 | 95.18       | 119.56   |
| 1   | A     | 629 | LEU  | C-N-CA | -24.14 | 95.18       | 119.56   |
| 1   | A     | 154 | ILE  | N-CA-C | 23.98  | 134.84      | 112.29   |
| 1   | A     | 277 | LYS  | CA-C-N | 23.98  | 164.86      | 121.70   |
| 1   | A     | 277 | LYS  | C-N-CA | 23.98  | 164.86      | 121.70   |
| 3   | M     | 80  | THR  | N-CA-C | 23.79  | 147.18      | 114.12   |
| 3   | M     | 268 | GLY  | CA-C-N | -23.34 | 97.57       | 123.25   |
| 3   | M     | 268 | GLY  | C-N-CA | -23.34 | 97.57       | 123.25   |
| 2   | B     | 290 | SER  | CA-C-N | -23.32 | 85.29       | 121.66   |
| 2   | B     | 290 | SER  | C-N-CA | -23.32 | 85.29       | 121.66   |
| 2   | B     | 336 | ASN  | CA-C-N | 23.17  | 150.56      | 120.44   |
| 2   | B     | 336 | ASN  | C-N-CA | 23.17  | 150.56      | 120.44   |
| 3   | M     | 135 | ASN  | N-CA-C | -23.15 | 72.15       | 108.96   |
| 3   | M     | 52  | ASP  | N-CA-C | 23.06  | 141.28      | 112.23   |
| 1   | A     | 98  | ASN  | N-CA-C | -23.02 | 76.40       | 110.48   |
| 3   | M     | 462 | LYS  | N-CA-C | -22.70 | 80.57       | 110.53   |
| 2   | B     | 330 | SER  | N-CA-C | -22.34 | 79.25       | 110.08   |
| 2   | B     | 579 | PRO  | CA-C-N | -22.12 | 88.31       | 122.37   |
| 2   | B     | 579 | PRO  | C-N-CA | -22.12 | 88.31       | 122.37   |
| 2   | B     | 600 | LYS  | CA-C-N | -22.10 | 88.12       | 122.60   |
| 2   | B     | 600 | LYS  | C-N-CA | -22.10 | 88.12       | 122.60   |
| 3   | M     | 130 | GLU  | CA-C-N | 21.91  | 153.41      | 122.07   |
| 3   | M     | 130 | GLU  | C-N-CA | 21.91  | 153.41      | 122.07   |
| 3   | M     | 133 | GLU  | CA-C-N | -21.86 | 97.90       | 119.76   |
| 3   | M     | 133 | GLU  | C-N-CA | -21.86 | 97.90       | 119.76   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | M     | 59  | ASP  | CA-C-N | -21.75 | 89.95       | 121.05   |
| 3   | M     | 59  | ASP  | C-N-CA | -21.75 | 89.95       | 121.05   |
| 4   | S     | 46  | PHE  | CA-C-N | -21.72 | 90.55       | 120.95   |
| 4   | S     | 46  | PHE  | C-N-CA | -21.72 | 90.55       | 120.95   |
| 2   | B     | 581 | TYR  | CA-C-N | 21.59  | 152.79      | 123.00   |
| 2   | B     | 581 | TYR  | C-N-CA | 21.59  | 152.79      | 123.00   |
| 3   | M     | 354 | ASP  | CA-C-N | 21.58  | 162.76      | 121.54   |
| 3   | M     | 354 | ASP  | C-N-CA | 21.58  | 162.76      | 121.54   |
| 1   | A     | 98  | ASN  | CA-C-N | 21.24  | 159.93      | 121.70   |
| 1   | A     | 98  | ASN  | C-N-CA | 21.24  | 159.93      | 121.70   |
| 3   | M     | 403 | THR  | CA-C-N | 21.12  | 161.94      | 122.02   |
| 3   | M     | 403 | THR  | C-N-CA | 21.12  | 161.94      | 122.02   |
| 2   | B     | 263 | PRO  | CA-C-N | 20.99  | 158.09      | 122.82   |
| 2   | B     | 263 | PRO  | C-N-CA | 20.99  | 158.09      | 122.82   |
| 1   | A     | 416 | ILE  | CA-C-N | -20.75 | 98.89       | 119.85   |
| 1   | A     | 416 | ILE  | C-N-CA | -20.75 | 98.89       | 119.85   |
| 3   | M     | 54  | SER  | N-CA-C | 20.42  | 144.00      | 114.39   |
| 2   | B     | 286 | ILE  | N-CA-C | -20.41 | 80.32       | 109.51   |
| 1   | A     | 229 | ASN  | CA-C-N | -20.30 | 98.85       | 119.56   |
| 1   | A     | 229 | ASN  | C-N-CA | -20.30 | 98.85       | 119.56   |
| 1   | A     | 534 | LYS  | N-CA-C | -20.30 | 80.79       | 110.23   |
| 1   | A     | 415 | ARG  | CA-C-N | -20.25 | 105.72      | 123.33   |
| 1   | A     | 415 | ARG  | C-N-CA | -20.25 | 105.72      | 123.33   |
| 3   | M     | 103 | TYR  | O-C-N  | -19.96 | 99.69       | 122.84   |
| 4   | S     | 68  | VAL  | N-CA-C | 19.87  | 136.76      | 107.75   |
| 2   | B     | 262 | LYS  | CA-C-N | -19.86 | 95.81       | 120.23   |
| 2   | B     | 262 | LYS  | C-N-CA | -19.86 | 95.81       | 120.23   |
| 2   | B     | 292 | GLU  | CA-C-N | 19.82  | 147.62      | 120.46   |
| 2   | B     | 292 | GLU  | C-N-CA | 19.82  | 147.62      | 120.46   |
| 1   | A     | 464 | ILE  | CA-C-N | -19.77 | 89.91       | 120.94   |
| 1   | A     | 464 | ILE  | C-N-CA | -19.77 | 89.91       | 120.94   |
| 1   | A     | 534 | LYS  | CA-C-N | 19.63  | 157.03      | 121.70   |
| 1   | A     | 534 | LYS  | C-N-CA | 19.63  | 157.03      | 121.70   |
| 2   | B     | 576 | GLN  | N-CA-C | -19.62 | 84.63       | 110.53   |
| 3   | M     | 21  | GLY  | CA-C-N | 19.59  | 158.95      | 121.54   |
| 3   | M     | 21  | GLY  | C-N-CA | 19.59  | 158.95      | 121.54   |
| 1   | A     | 304 | LEU  | CA-C-N | -19.47 | 84.36       | 121.54   |
| 1   | A     | 304 | LEU  | C-N-CA | -19.47 | 84.36       | 121.54   |
| 2   | B     | 273 | SER  | CA-C-N | 19.44  | 144.14      | 119.84   |
| 2   | B     | 273 | SER  | C-N-CA | 19.44  | 144.14      | 119.84   |
| 4   | S     | 46  | PHE  | N-CA-C | -19.34 | 89.00       | 112.59   |
| 2   | B     | 78  | ASP  | CA-C-N | -19.32 | 88.60       | 120.86   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | B     | 78  | ASP  | C-N-CA  | -19.32 | 88.60       | 120.86   |
| 4   | S     | 21  | THR  | CA-C-N  | -19.32 | 99.13       | 119.99   |
| 4   | S     | 21  | THR  | C-N-CA  | -19.32 | 99.13       | 119.99   |
| 4   | S     | 69  | ASN  | CB-CA-C | -19.29 | 76.61       | 109.02   |
| 3   | M     | 280 | ASP  | N-CA-C  | 19.20  | 151.70      | 110.80   |
| 3   | M     | 82  | LYS  | N-CA-C  | -19.14 | 78.53       | 108.76   |
| 2   | B     | 571 | SER  | N-CA-C  | -18.99 | 83.73       | 110.50   |
| 3   | M     | 61  | GLU  | N-CA-C  | -18.79 | 78.10       | 108.73   |
| 3   | M     | 347 | PHE  | N-CA-C  | -18.78 | 88.02       | 114.12   |
| 2   | B     | 580 | TYR  | N-CA-C  | -18.77 | 86.47       | 112.94   |
| 3   | M     | 45  | SER  | CA-C-N  | -18.57 | 78.07       | 121.52   |
| 3   | M     | 45  | SER  | C-N-CA  | -18.57 | 78.07       | 121.52   |
| 1   | A     | 418 | ILE  | CA-C-N  | -18.46 | 88.74       | 121.97   |
| 1   | A     | 418 | ILE  | C-N-CA  | -18.46 | 88.74       | 121.97   |
| 1   | A     | 469 | LEU  | CA-C-N  | -18.38 | 96.88       | 120.22   |
| 1   | A     | 469 | LEU  | C-N-CA  | -18.38 | 96.88       | 120.22   |
| 3   | M     | 402 | SER  | CA-C-N  | -18.36 | 96.79       | 122.86   |
| 3   | M     | 402 | SER  | C-N-CA  | -18.36 | 96.79       | 122.86   |
| 1   | A     | 151 | SER  | CA-C-N  | -18.30 | 91.08       | 122.56   |
| 1   | A     | 151 | SER  | C-N-CA  | -18.30 | 91.08       | 122.56   |
| 3   | M     | 103 | TYR  | CA-C-N  | 18.26  | 156.42      | 121.54   |
| 3   | M     | 103 | TYR  | C-N-CA  | 18.26  | 156.42      | 121.54   |
| 1   | A     | 534 | LYS  | CA-C-O  | -18.22 | 101.14      | 121.19   |
| 1   | A     | 80  | TYR  | O-C-N   | -18.14 | 100.31      | 123.16   |
| 4   | S     | 167 | ILE  | N-CA-C  | 18.07  | 130.73      | 111.58   |
| 2   | B     | 570 | GLY  | N-CA-C  | -17.95 | 88.75       | 115.32   |
| 2   | B     | 577 | ASN  | CA-C-N  | -17.82 | 102.02      | 120.38   |
| 2   | B     | 577 | ASN  | C-N-CA  | -17.82 | 102.02      | 120.38   |
| 1   | A     | 300 | LYS  | N-CA-C  | 17.70  | 130.25      | 111.14   |
| 2   | B     | 404 | ASN  | CA-C-N  | -17.65 | 93.48       | 120.31   |
| 2   | B     | 404 | ASN  | C-N-CA  | -17.65 | 93.48       | 120.31   |
| 4   | S     | 25  | LEU  | CA-C-O  | 17.64  | 135.44      | 118.34   |
| 3   | M     | 404 | ALA  | N-CA-CB | -17.58 | 83.59       | 110.49   |
| 3   | M     | 23  | THR  | N-CA-C  | -17.53 | 80.82       | 109.40   |
| 1   | A     | 586 | GLU  | CA-C-N  | -17.46 | 95.50       | 120.29   |
| 1   | A     | 586 | GLU  | C-N-CA  | -17.46 | 95.50       | 120.29   |
| 2   | B     | 220 | ALA  | N-CA-C  | -17.29 | 90.36       | 111.11   |
| 2   | B     | 293 | VAL  | CA-C-N  | -17.21 | 102.05      | 122.35   |
| 2   | B     | 293 | VAL  | C-N-CA  | -17.21 | 102.05      | 122.35   |
| 1   | A     | 233 | PHE  | CA-C-N  | -17.14 | 92.23       | 120.86   |
| 1   | A     | 233 | PHE  | C-N-CA  | -17.14 | 92.23       | 120.86   |
| 1   | A     | 174 | ARG  | CA-C-N  | 17.11  | 137.01      | 119.56   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 174 | ARG  | C-N-CA  | 17.11  | 137.01      | 119.56   |
| 1   | A     | 442 | SER  | N-CA-C  | -17.08 | 92.06       | 111.71   |
| 1   | A     | 260 | PHE  | O-C-N   | -17.06 | 102.70      | 122.15   |
| 2   | B     | 310 | ILE  | CA-C-N  | -17.02 | 94.44       | 120.31   |
| 2   | B     | 310 | ILE  | C-N-CA  | -17.02 | 94.44       | 120.31   |
| 1   | A     | 242 | GLU  | N-CA-C  | -17.01 | 85.57       | 110.23   |
| 2   | B     | 569 | THR  | N-CA-C  | 16.92  | 134.89      | 108.67   |
| 1   | A     | 64  | LEU  | O-C-N   | -16.80 | 102.57      | 122.22   |
| 1   | A     | 307 | ASP  | N-CA-C  | -16.76 | 93.09       | 111.36   |
| 3   | M     | 284 | SER  | CA-C-N  | -16.68 | 102.55      | 119.56   |
| 3   | M     | 284 | SER  | C-N-CA  | -16.68 | 102.55      | 119.56   |
| 3   | M     | 46  | SER  | CA-C-N  | -16.63 | 94.37       | 122.64   |
| 3   | M     | 46  | SER  | C-N-CA  | -16.63 | 94.37       | 122.64   |
| 2   | B     | 461 | HIS  | CA-C-N  | -16.59 | 98.80       | 122.36   |
| 2   | B     | 461 | HIS  | C-N-CA  | -16.59 | 98.80       | 122.36   |
| 1   | A     | 204 | VAL  | O-C-N   | -16.58 | 105.78      | 121.87   |
| 1   | A     | 136 | GLY  | CA-C-N  | -16.54 | 93.10       | 120.72   |
| 1   | A     | 136 | GLY  | C-N-CA  | -16.54 | 93.10       | 120.72   |
| 2   | B     | 375 | LEU  | O-C-N   | -16.53 | 105.77      | 120.48   |
| 3   | M     | 404 | ALA  | CB-CA-C | 16.51  | 148.10      | 111.78   |
| 1   | A     | 443 | SER  | N-CA-C  | 16.48  | 133.14      | 113.20   |
| 1   | A     | 380 | ASP  | N-CA-C  | -16.46 | 84.38       | 109.24   |
| 1   | A     | 323 | CYS  | CA-C-N  | 16.12  | 150.72      | 121.70   |
| 1   | A     | 323 | CYS  | C-N-CA  | 16.12  | 150.72      | 121.70   |
| 4   | S     | 63  | ASN  | N-CA-C  | -16.04 | 82.27       | 108.41   |
| 1   | A     | 536 | MET  | CA-C-N  | -16.04 | 93.16       | 120.58   |
| 1   | A     | 536 | MET  | C-N-CA  | -16.04 | 93.16       | 120.58   |
| 3   | M     | 421 | GLY  | CA-C-N  | -16.03 | 103.20      | 119.87   |
| 3   | M     | 421 | GLY  | C-N-CA  | -16.03 | 103.20      | 119.87   |
| 2   | B     | 387 | ASP  | CA-C-N  | 16.00  | 135.57      | 120.21   |
| 2   | B     | 387 | ASP  | C-N-CA  | 16.00  | 135.57      | 120.21   |
| 1   | A     | 215 | VAL  | CA-C-O  | 15.99  | 137.80      | 120.85   |
| 3   | M     | 51  | LEU  | N-CA-C  | 15.99  | 144.85      | 110.80   |
| 2   | B     | 277 | CYS  | CA-C-N  | -15.96 | 104.67      | 120.31   |
| 2   | B     | 277 | CYS  | C-N-CA  | -15.96 | 104.67      | 120.31   |
| 3   | M     | 457 | GLY  | N-CA-C  | -15.92 | 92.40       | 115.64   |
| 1   | A     | 302 | ASN  | N-CA-C  | -15.88 | 76.97       | 110.80   |
| 4   | S     | 50  | PHE  | CA-C-N  | -15.82 | 99.97       | 123.07   |
| 4   | S     | 50  | PHE  | C-N-CA  | -15.82 | 99.97       | 123.07   |
| 2   | B     | 273 | SER  | N-CA-C  | 15.79  | 132.71      | 109.50   |
| 3   | M     | 458 | LEU  | O-C-N   | 15.77  | 140.85      | 123.03   |
| 4   | S     | 109 | LEU  | O-C-N   | -15.76 | 105.41      | 122.12   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | M     | 405 | THR  | N-CA-C | 15.72  | 144.29      | 110.80   |
| 1   | A     | 461 | CYS  | CA-C-O | 15.72  | 137.87      | 120.10   |
| 3   | M     | 252 | ASP  | N-CA-C | -15.72 | 85.72       | 107.88   |
| 1   | A     | 529 | GLY  | N-CA-C | -15.71 | 95.15       | 114.16   |
| 1   | A     | 394 | GLN  | CA-C-O | -15.70 | 103.91      | 120.55   |
| 3   | M     | 292 | PRO  | N-CA-C | -15.66 | 91.59       | 110.70   |
| 1   | A     | 281 | LEU  | CA-C-O | 15.50  | 137.80      | 119.97   |
| 2   | B     | 535 | GLN  | CA-C-N | -15.49 | 98.52       | 122.37   |
| 2   | B     | 535 | GLN  | C-N-CA | -15.49 | 98.52       | 122.37   |
| 1   | A     | 327 | ASP  | CA-C-N | 15.43  | 135.29      | 119.56   |
| 1   | A     | 327 | ASP  | C-N-CA | 15.43  | 135.29      | 119.56   |
| 1   | A     | 519 | LEU  | CA-C-N | -15.38 | 100.69      | 120.22   |
| 1   | A     | 519 | LEU  | C-N-CA | -15.38 | 100.69      | 120.22   |
| 1   | A     | 100 | LEU  | CA-C-N | -15.37 | 99.68       | 120.28   |
| 1   | A     | 100 | LEU  | C-N-CA | -15.37 | 99.68       | 120.28   |
| 3   | M     | 108 | LYS  | CA-C-N | -15.36 | 101.50      | 122.85   |
| 3   | M     | 108 | LYS  | C-N-CA | -15.36 | 101.50      | 122.85   |
| 1   | A     | 413 | SER  | N-CA-C | -15.32 | 88.02       | 110.23   |
| 1   | A     | 196 | LEU  | CA-C-N | -15.30 | 99.64       | 120.44   |
| 1   | A     | 196 | LEU  | C-N-CA | -15.30 | 99.64       | 120.44   |
| 1   | A     | 289 | SER  | O-C-N  | -15.27 | 103.50      | 122.27   |
| 2   | B     | 260 | LEU  | CA-C-N | -15.17 | 104.13      | 119.76   |
| 2   | B     | 260 | LEU  | C-N-CA | -15.17 | 104.13      | 119.76   |
| 3   | M     | 134 | PRO  | N-CA-C | -15.16 | 87.39       | 111.19   |
| 1   | A     | 88  | ASN  | CA-C-N | -15.15 | 99.97       | 120.28   |
| 1   | A     | 88  | ASN  | C-N-CA | -15.15 | 99.97       | 120.28   |
| 1   | A     | 103 | LYS  | CA-C-O | 15.15  | 137.21      | 120.10   |
| 1   | A     | 346 | THR  | CA-C-N | -15.14 | 97.30       | 120.31   |
| 1   | A     | 346 | THR  | C-N-CA | -15.14 | 97.30       | 120.31   |
| 2   | B     | 240 | LEU  | N-CA-C | 15.11  | 132.35      | 110.14   |
| 1   | A     | 569 | ASP  | N-CA-C | -15.10 | 85.68       | 108.79   |
| 2   | B     | 187 | ASP  | CA-C-N | -15.07 | 98.31       | 122.26   |
| 2   | B     | 187 | ASP  | C-N-CA | -15.07 | 98.31       | 122.26   |
| 4   | S     | 25  | LEU  | O-C-N  | -15.01 | 106.60      | 120.71   |
| 1   | A     | 381 | GLU  | CA-C-N | -15.00 | 98.68       | 120.28   |
| 1   | A     | 381 | GLU  | C-N-CA | -15.00 | 98.68       | 120.28   |
| 2   | B     | 109 | ALA  | CA-C-N | -14.96 | 100.23      | 120.28   |
| 2   | B     | 109 | ALA  | C-N-CA | -14.96 | 100.23      | 120.28   |
| 3   | M     | 91  | THR  | CA-C-O | -14.93 | 102.80      | 119.97   |
| 1   | A     | 287 | ALA  | CA-C-N | 14.89  | 148.50      | 121.70   |
| 1   | A     | 287 | ALA  | C-N-CA | 14.89  | 148.50      | 121.70   |
| 4   | S     | 164 | ASP  | CA-C-N | -14.87 | 95.89       | 120.72   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | S     | 164 | ASP  | C-N-CA | -14.87 | 95.89       | 120.72   |
| 4   | S     | 125 | TRP  | CA-C-O | -14.86 | 105.00      | 120.90   |
| 1   | A     | 465 | SER  | CA-C-N | 14.85  | 144.18      | 121.76   |
| 1   | A     | 465 | SER  | C-N-CA | 14.85  | 144.18      | 121.76   |
| 2   | B     | 108 | PHE  | CA-C-O | 14.84  | 136.78      | 120.90   |
| 1   | A     | 240 | LEU  | CA-C-N | -14.83 | 99.23       | 120.29   |
| 1   | A     | 240 | LEU  | C-N-CA | -14.83 | 99.23       | 120.29   |
| 1   | A     | 465 | SER  | N-CA-C | 14.81  | 131.39      | 110.50   |
| 1   | A     | 418 | ILE  | N-CA-C | 14.75  | 129.18      | 107.80   |
| 1   | A     | 536 | MET  | O-C-N  | -14.71 | 103.03      | 122.59   |
| 4   | S     | 46  | PHE  | CA-C-O | -14.71 | 102.60      | 119.95   |
| 1   | A     | 432 | ILE  | O-C-N  | 14.69  | 136.63      | 121.94   |
| 2   | B     | 82  | TYR  | CA-C-N | -14.69 | 95.47       | 120.58   |
| 2   | B     | 82  | TYR  | C-N-CA | -14.69 | 95.47       | 120.58   |
| 4   | S     | 109 | LEU  | CA-C-O | 14.69  | 136.12      | 120.55   |
| 1   | A     | 504 | ILE  | CA-C-O | 14.67  | 136.26      | 120.57   |
| 2   | B     | 418 | TYR  | CA-C-N | -14.66 | 102.38      | 120.70   |
| 2   | B     | 418 | TYR  | C-N-CA | -14.66 | 102.38      | 120.70   |
| 1   | A     | 432 | ILE  | CA-C-O | -14.65 | 106.03      | 121.27   |
| 1   | A     | 545 | HIS  | CA-C-N | -14.64 | 99.50       | 120.29   |
| 1   | A     | 545 | HIS  | C-N-CA | -14.64 | 99.50       | 120.29   |
| 3   | M     | 421 | GLY  | O-C-N  | -14.63 | 107.14      | 121.77   |
| 2   | B     | 559 | ASP  | CA-C-O | -14.56 | 101.66      | 119.28   |
| 1   | A     | 244 | LEU  | O-C-N  | -14.49 | 105.69      | 122.20   |
| 2   | B     | 288 | TYR  | CA-C-N | 14.47  | 137.93      | 119.84   |
| 2   | B     | 288 | TYR  | C-N-CA | 14.47  | 137.93      | 119.84   |
| 1   | A     | 264 | SER  | CA-C-N | -14.42 | 101.86      | 122.19   |
| 1   | A     | 264 | SER  | C-N-CA | -14.42 | 101.86      | 122.19   |
| 2   | B     | 22  | ALA  | N-CA-C | -14.41 | 95.66       | 111.36   |
| 1   | A     | 84  | MET  | CA-C-N | -14.40 | 95.95       | 120.58   |
| 1   | A     | 84  | MET  | C-N-CA | -14.40 | 95.95       | 120.58   |
| 2   | B     | 287 | GLU  | CA-C-N | 14.36  | 147.69      | 122.28   |
| 2   | B     | 287 | GLU  | C-N-CA | 14.36  | 147.69      | 122.28   |
| 2   | B     | 212 | VAL  | CA-C-O | 14.32  | 140.05      | 121.15   |
| 3   | M     | 406 | GLY  | CA-C-N | -14.32 | 99.82       | 122.87   |
| 3   | M     | 406 | GLY  | C-N-CA | -14.32 | 99.82       | 122.87   |
| 1   | A     | 566 | PHE  | N-CA-C | 14.30  | 130.03      | 112.87   |
| 3   | M     | 57  | GLY  | CA-C-N | 14.19  | 145.65      | 122.10   |
| 3   | M     | 57  | GLY  | C-N-CA | 14.19  | 145.65      | 122.10   |
| 1   | A     | 504 | ILE  | O-C-N  | -14.17 | 107.56      | 121.87   |
| 4   | S     | 43  | ASN  | O-C-N  | -14.16 | 105.39      | 122.81   |
| 4   | S     | 80  | TYR  | CA-C-O | 14.16  | 135.27      | 120.40   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | S     | 163 | THR  | CA-C-N | 14.13  | 148.52      | 121.54   |
| 4   | S     | 163 | THR  | C-N-CA | 14.13  | 148.52      | 121.54   |
| 2   | B     | 289 | PRO  | CA-C-N | -14.12 | 96.80       | 121.66   |
| 2   | B     | 289 | PRO  | C-N-CA | -14.12 | 96.80       | 121.66   |
| 2   | B     | 521 | ILE  | CA-C-N | -14.12 | 104.11      | 123.03   |
| 2   | B     | 521 | ILE  | C-N-CA | -14.12 | 104.11      | 123.03   |
| 1   | A     | 469 | LEU  | CA-C-O | 14.05  | 136.13      | 119.97   |
| 3   | M     | 74  | TYR  | CA-C-O | 14.03  | 137.02      | 121.16   |
| 3   | M     | 118 | TYR  | CA-C-O | -14.02 | 105.21      | 120.92   |
| 2   | B     | 337 | THR  | CA-C-O | -14.01 | 106.11      | 120.82   |
| 1   | A     | 448 | GLU  | N-CA-C | -14.00 | 89.93       | 110.23   |
| 1   | A     | 547 | VAL  | O-C-N  | 14.00  | 135.45      | 121.87   |
| 1   | A     | 391 | LEU  | CA-C-N | -13.99 | 100.42      | 120.29   |
| 1   | A     | 391 | LEU  | C-N-CA | -13.99 | 100.42      | 120.29   |
| 2   | B     | 577 | ASN  | N-CA-C | 13.95  | 136.11      | 108.21   |
| 3   | M     | 63  | TYR  | CA-C-N | -13.95 | 100.86      | 122.62   |
| 3   | M     | 63  | TYR  | C-N-CA | -13.95 | 100.86      | 122.62   |
| 1   | A     | 507 | GLN  | CA-C-N | -13.94 | 105.36      | 123.34   |
| 1   | A     | 507 | GLN  | C-N-CA | -13.94 | 105.36      | 123.34   |
| 2   | B     | 287 | GLU  | N-CA-C | -13.94 | 87.60       | 109.76   |
| 4   | S     | 99  | LEU  | CA-C-O | -13.88 | 105.71      | 120.42   |
| 1   | A     | 163 | ALA  | CA-C-N | -13.86 | 99.24       | 120.31   |
| 1   | A     | 163 | ALA  | C-N-CA | -13.86 | 99.24       | 120.31   |
| 1   | A     | 388 | VAL  | CA-C-O | -13.86 | 106.47      | 121.17   |
| 1   | A     | 88  | ASN  | CA-C-O | 13.82  | 135.87      | 119.97   |
| 1   | A     | 265 | GLN  | CA-C-O | -13.82 | 104.93      | 120.54   |
| 2   | B     | 158 | VAL  | CA-C-O | -13.74 | 106.76      | 121.05   |
| 3   | M     | 262 | THR  | CA-C-N | -13.70 | 101.93      | 122.21   |
| 3   | M     | 262 | THR  | C-N-CA | -13.70 | 101.93      | 122.21   |
| 1   | A     | 431 | VAL  | O-C-N  | 13.66  | 136.10      | 121.90   |
| 1   | A     | 492 | ILE  | CA-C-O | -13.65 | 106.69      | 121.17   |
| 3   | M     | 232 | HIS  | CA-C-O | 13.64  | 135.94      | 120.80   |
| 3   | M     | 80  | THR  | CA-C-N | 13.61  | 147.54      | 121.54   |
| 3   | M     | 80  | THR  | C-N-CA | 13.61  | 147.54      | 121.54   |
| 2   | B     | 366 | LEU  | O-C-N  | -13.59 | 107.71      | 122.12   |
| 1   | A     | 105 | VAL  | CA-C-N | 13.58  | 135.01      | 119.94   |
| 1   | A     | 105 | VAL  | C-N-CA | 13.58  | 135.01      | 119.94   |
| 1   | A     | 120 | ILE  | O-C-N  | 13.57  | 136.02      | 121.90   |
| 2   | B     | 102 | HIS  | O-C-N  | -13.56 | 107.75      | 122.12   |
| 1   | A     | 508 | LEU  | N-CA-C | 13.55  | 133.63      | 108.97   |
| 1   | A     | 325 | SER  | N-CA-C | -13.54 | 87.72       | 108.99   |
| 4   | S     | 5   | VAL  | O-C-N  | -13.55 | 108.63      | 123.26   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | M     | 373 | ALA  | CB-CA-C | 13.54  | 133.15      | 110.81   |
| 1   | A     | 569 | ASP  | CA-C-O  | -13.53 | 106.75      | 121.23   |
| 4   | S     | 139 | GLY  | CA-C-N  | -13.52 | 102.65      | 122.94   |
| 4   | S     | 139 | GLY  | C-N-CA  | -13.52 | 102.65      | 122.94   |
| 2   | B     | 478 | LEU  | CA-C-O  | 13.52  | 135.01      | 120.82   |
| 4   | S     | 106 | VAL  | CA-C-O  | -13.51 | 106.53      | 120.85   |
| 4   | S     | 66  | ASP  | N-CA-C  | -13.48 | 88.63       | 109.25   |
| 2   | B     | 183 | ALA  | N-CA-C  | 13.47  | 130.75      | 114.04   |
| 2   | B     | 185 | LYS  | CA-C-N  | -13.41 | 92.83       | 121.80   |
| 2   | B     | 185 | LYS  | C-N-CA  | -13.41 | 92.83       | 121.80   |
| 1   | A     | 301 | GLY  | N-CA-C  | -13.40 | 95.69       | 113.24   |
| 1   | A     | 320 | HIS  | O-C-N   | -13.37 | 106.91      | 122.15   |
| 2   | B     | 102 | HIS  | CA-C-O  | 13.33  | 134.68      | 120.55   |
| 2   | B     | 154 | ILE  | CA-C-O  | -13.29 | 106.15      | 120.64   |
| 3   | M     | 450 | GLU  | CA-C-O  | 13.29  | 135.79      | 119.31   |
| 1   | A     | 415 | ARG  | N-CA-C  | -13.29 | 89.19       | 110.32   |
| 1   | A     | 405 | THR  | N-CA-C  | 13.29  | 130.85      | 113.18   |
| 1   | A     | 420 | ILE  | CA-C-N  | 13.28  | 132.96      | 120.21   |
| 1   | A     | 420 | ILE  | C-N-CA  | 13.28  | 132.96      | 120.21   |
| 2   | B     | 457 | HIS  | CA-C-O  | 13.28  | 134.49      | 120.42   |
| 1   | A     | 86  | TRP  | CA-C-N  | -13.27 | 99.31       | 122.26   |
| 1   | A     | 86  | TRP  | C-N-CA  | -13.27 | 99.31       | 122.26   |
| 2   | B     | 260 | LEU  | N-CA-C  | -13.27 | 80.49       | 109.81   |
| 3   | M     | 54  | SER  | O-C-N   | 13.26  | 135.85      | 122.19   |
| 2   | B     | 460 | SER  | N-CA-C  | 13.25  | 128.93      | 112.23   |
| 1   | A     | 365 | VAL  | CA-C-N  | -13.25 | 98.59       | 120.72   |
| 1   | A     | 365 | VAL  | C-N-CA  | -13.25 | 98.59       | 120.72   |
| 1   | A     | 162 | ILE  | CA-C-O  | -13.25 | 107.17      | 120.95   |
| 4   | S     | 58  | LEU  | CA-C-O  | 13.22  | 136.10      | 121.16   |
| 2   | B     | 325 | LEU  | CA-C-O  | 13.22  | 135.64      | 119.38   |
| 2   | B     | 515 | PHE  | CA-C-N  | -13.21 | 105.54      | 119.94   |
| 2   | B     | 515 | PHE  | C-N-CA  | -13.21 | 105.54      | 119.94   |
| 1   | A     | 110 | ALA  | CA-C-N  | -13.20 | 98.67       | 120.72   |
| 1   | A     | 110 | ALA  | C-N-CA  | -13.20 | 98.67       | 120.72   |
| 1   | A     | 504 | ILE  | CA-C-N  | -13.19 | 98.25       | 120.68   |
| 1   | A     | 504 | ILE  | C-N-CA  | -13.19 | 98.25       | 120.68   |
| 3   | M     | 83  | SER  | CA-C-N  | 13.19  | 146.73      | 121.54   |
| 3   | M     | 83  | SER  | C-N-CA  | 13.19  | 146.73      | 121.54   |
| 4   | S     | 6   | LEU  | O-C-N   | -13.16 | 107.63      | 123.30   |
| 3   | M     | 293 | PRO  | CA-N-CD | -13.13 | 93.62       | 112.00   |
| 1   | A     | 212 | ILE  | CA-C-N  | -13.12 | 98.18       | 121.14   |
| 1   | A     | 212 | ILE  | C-N-CA  | -13.12 | 98.18       | 121.14   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 607 | LEU  | CA-C-O | -13.11 | 107.20      | 120.70   |
| 3   | M     | 279 | ASN  | N-CA-C | 13.11  | 138.72      | 110.80   |
| 1   | A     | 225 | LEU  | CA-C-O | -13.10 | 105.29      | 120.10   |
| 1   | A     | 440 | ASN  | CA-C-N | 13.10  | 145.94      | 122.62   |
| 1   | A     | 440 | ASN  | C-N-CA | 13.10  | 145.94      | 122.62   |
| 2   | B     | 146 | LYS  | CA-C-N | -13.08 | 100.70      | 122.29   |
| 2   | B     | 146 | LYS  | C-N-CA | -13.08 | 100.70      | 122.29   |
| 1   | A     | 450 | TYR  | O-C-N  | 13.07  | 135.53      | 122.07   |
| 4   | S     | 54  | PRO  | N-CA-C | -13.06 | 94.76       | 110.70   |
| 3   | M     | 379 | LEU  | O-C-N  | -13.05 | 107.77      | 123.30   |
| 2   | B     | 505 | ASP  | CA-C-N | -13.03 | 98.53       | 120.68   |
| 2   | B     | 505 | ASP  | C-N-CA | -13.03 | 98.53       | 120.68   |
| 2   | B     | 472 | VAL  | O-C-N  | -13.00 | 109.26      | 121.87   |
| 4   | S     | 150 | VAL  | CA-C-O | -12.97 | 107.46      | 120.95   |
| 4   | S     | 58  | LEU  | CA-C-N | -12.96 | 102.81      | 120.95   |
| 4   | S     | 58  | LEU  | C-N-CA | -12.96 | 102.81      | 120.95   |
| 1   | A     | 405 | THR  | CA-C-N | -12.95 | 96.03       | 121.41   |
| 1   | A     | 405 | THR  | C-N-CA | -12.95 | 96.03       | 121.41   |
| 2   | B     | 205 | PRO  | CA-C-N | -12.95 | 98.94       | 122.38   |
| 2   | B     | 205 | PRO  | C-N-CA | -12.95 | 98.94       | 122.38   |
| 1   | A     | 569 | ASP  | CA-C-N | -12.94 | 96.92       | 120.99   |
| 1   | A     | 569 | ASP  | C-N-CA | -12.94 | 96.92       | 120.99   |
| 2   | B     | 35  | TYR  | O-C-N  | 12.91  | 135.37      | 122.07   |
| 2   | B     | 497 | LEU  | CA-C-N | -12.90 | 99.17       | 120.72   |
| 2   | B     | 497 | LEU  | C-N-CA | -12.90 | 99.17       | 120.72   |
| 1   | A     | 162 | ILE  | O-C-N  | 12.88  | 134.37      | 121.87   |
| 1   | A     | 511 | VAL  | O-C-N  | 12.87  | 134.35      | 121.87   |
| 3   | M     | 281 | GLY  | N-CA-C | -12.87 | 97.12       | 115.27   |
| 1   | A     | 631 | SER  | O-C-N  | 12.86  | 135.76      | 122.12   |
| 2   | B     | 230 | PHE  | CA-C-N | -12.86 | 96.98       | 121.54   |
| 2   | B     | 230 | PHE  | C-N-CA | -12.86 | 96.98       | 121.54   |
| 1   | A     | 319 | LEU  | O-C-N  | -12.86 | 107.49      | 122.15   |
| 2   | B     | 237 | ILE  | CA-C-N | -12.85 | 103.07      | 120.28   |
| 2   | B     | 237 | ILE  | C-N-CA | -12.85 | 103.07      | 120.28   |
| 1   | A     | 140 | VAL  | CA-C-O | 12.84  | 134.46      | 120.85   |
| 2   | B     | 388 | PRO  | CA-C-N | 12.84  | 138.05      | 120.46   |
| 2   | B     | 388 | PRO  | C-N-CA | 12.84  | 138.05      | 120.46   |
| 1   | A     | 601 | VAL  | CA-C-O | 12.81  | 134.27      | 120.57   |
| 2   | B     | 306 | LEU  | CA-C-O | -12.80 | 106.80      | 120.63   |
| 3   | M     | 477 | GLY  | CA-C-N | -12.79 | 99.46       | 122.74   |
| 3   | M     | 477 | GLY  | C-N-CA | -12.79 | 99.46       | 122.74   |
| 1   | A     | 629 | LEU  | CA-C-O | 12.79  | 130.40      | 118.63   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 155 | THR  | CA-C-N | 12.78  | 134.30      | 119.47   |
| 1   | A     | 155 | THR  | C-N-CA | 12.78  | 134.30      | 119.47   |
| 2   | B     | 442 | LEU  | CA-C-N | -12.78 | 103.06      | 122.74   |
| 2   | B     | 442 | LEU  | C-N-CA | -12.78 | 103.06      | 122.74   |
| 1   | A     | 158 | LEU  | O-C-N  | 12.76  | 135.21      | 122.07   |
| 1   | A     | 350 | SER  | O-C-N  | -12.74 | 108.61      | 122.12   |
| 1   | A     | 518 | CYS  | CA-C-O | -12.72 | 107.47      | 120.82   |
| 1   | A     | 508 | LEU  | O-C-N  | 12.71  | 132.99      | 121.42   |
| 2   | B     | 285 | GLU  | N-CA-C | -12.70 | 93.08       | 110.35   |
| 1   | A     | 107 | TYR  | CA-C-O | -12.70 | 107.49      | 120.82   |
| 1   | A     | 158 | LEU  | CA-C-O | -12.68 | 107.50      | 120.82   |
| 1   | A     | 600 | SER  | CA-C-O | -12.66 | 107.66      | 120.70   |
| 1   | A     | 434 | SER  | O-C-N  | 12.65  | 135.53      | 122.12   |
| 2   | B     | 162 | VAL  | CA-C-N | -12.65 | 97.00       | 122.31   |
| 2   | B     | 162 | VAL  | C-N-CA | -12.65 | 97.00       | 122.31   |
| 1   | A     | 533 | ILE  | CA-C-O | -12.65 | 107.01      | 121.05   |
| 2   | B     | 328 | LEU  | CA-C-N | -12.63 | 103.26      | 120.95   |
| 2   | B     | 328 | LEU  | C-N-CA | -12.63 | 103.26      | 120.95   |
| 1   | A     | 155 | THR  | CA-C-O | -12.61 | 106.75      | 120.88   |
| 1   | A     | 298 | ILE  | CA-C-O | 12.62  | 135.05      | 121.05   |
| 2   | B     | 267 | ASP  | CA-C-O | 12.60  | 134.02      | 120.92   |
| 3   | M     | 59  | ASP  | N-CA-C | -12.60 | 96.36       | 112.23   |
| 2   | B     | 334 | MET  | N-CA-C | 12.58  | 127.89      | 112.54   |
| 3   | M     | 265 | ASN  | CA-C-O | -12.56 | 107.94      | 122.13   |
| 1   | A     | 260 | PHE  | CA-C-N | -12.53 | 103.49      | 120.28   |
| 1   | A     | 260 | PHE  | C-N-CA | -12.53 | 103.49      | 120.28   |
| 4   | S     | 25  | LEU  | CA-C-N | -12.53 | 105.50      | 119.28   |
| 4   | S     | 25  | LEU  | C-N-CA | -12.53 | 105.50      | 119.28   |
| 4   | S     | 143 | GLU  | N-CA-C | -12.52 | 85.94       | 108.48   |
| 1   | A     | 71  | VAL  | CA-C-O | -12.52 | 107.58      | 120.85   |
| 1   | A     | 192 | TYR  | CA-C-O | -12.52 | 103.01      | 120.16   |
| 2   | B     | 566 | ALA  | CA-C-N | 12.51  | 141.61      | 120.71   |
| 2   | B     | 566 | ALA  | C-N-CA | 12.51  | 141.61      | 120.71   |
| 3   | M     | 306 | LEU  | O-C-N  | -12.49 | 107.96      | 122.20   |
| 2   | B     | 111 | ASN  | N-CA-C | 12.49  | 127.97      | 112.23   |
| 1   | A     | 388 | VAL  | O-C-N  | 12.49  | 134.15      | 121.91   |
| 1   | A     | 529 | GLY  | CA-C-O | -12.48 | 104.77      | 119.50   |
| 3   | M     | 367 | ALA  | CA-C-N | 12.48  | 142.94      | 121.35   |
| 3   | M     | 367 | ALA  | C-N-CA | 12.48  | 142.94      | 121.35   |
| 2   | B     | 497 | LEU  | O-C-N  | -12.48 | 105.61      | 122.33   |
| 1   | A     | 487 | MET  | O-C-N  | -12.47 | 109.72      | 121.56   |
| 2   | B     | 575 | ASN  | N-CA-C | -12.46 | 98.07       | 113.28   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 152 | THR  | CA-C-N | -12.44 | 107.26      | 122.93   |
| 1   | A     | 152 | THR  | C-N-CA | -12.44 | 107.26      | 122.93   |
| 1   | A     | 290 | VAL  | CA-C-O | -12.44 | 107.04      | 120.47   |
| 1   | A     | 596 | VAL  | O-C-N  | 12.44  | 134.64      | 121.83   |
| 1   | A     | 196 | LEU  | CA-C-O | 12.43  | 134.26      | 119.97   |
| 1   | A     | 633 | PHE  | CA-C-O | -12.43 | 107.38      | 120.55   |
| 3   | M     | 368 | ASP  | CA-C-O | -12.43 | 107.33      | 119.51   |
| 2   | B     | 271 | GLU  | N-CA-C | 12.40  | 128.23      | 109.25   |
| 2   | B     | 339 | PHE  | O-C-N  | 12.40  | 136.28      | 122.15   |
| 1   | A     | 454 | ILE  | CA-C-O | -12.38 | 107.31      | 121.05   |
| 2   | B     | 204 | ASP  | O-C-N  | 12.38  | 132.70      | 121.18   |
| 2   | B     | 408 | VAL  | O-C-N  | 12.38  | 134.37      | 121.87   |
| 2   | B     | 303 | LEU  | CA-C-O | -12.35 | 107.86      | 120.82   |
| 1   | A     | 218 | ALA  | O-C-N  | 12.34  | 135.20      | 122.12   |
| 4   | S     | 83  | LEU  | CA-C-O | 12.34  | 135.11      | 121.16   |
| 4   | S     | 96  | LEU  | CA-C-O | -12.34 | 107.99      | 120.70   |
| 3   | M     | 279 | ASN  | CA-C-N | 12.34  | 145.11      | 121.54   |
| 3   | M     | 279 | ASN  | C-N-CA | 12.34  | 145.11      | 121.54   |
| 1   | A     | 631 | SER  | CA-C-O | -12.34 | 107.47      | 120.55   |
| 1   | A     | 601 | VAL  | CA-C-N | -12.33 | 102.78      | 120.29   |
| 1   | A     | 601 | VAL  | C-N-CA | -12.33 | 102.78      | 120.29   |
| 1   | A     | 453 | VAL  | O-C-N  | 12.31  | 133.81      | 121.87   |
| 1   | A     | 135 | ASP  | CA-C-N | -12.30 | 97.30       | 121.41   |
| 1   | A     | 135 | ASP  | C-N-CA | -12.30 | 97.30       | 121.41   |
| 2   | B     | 99  | ARG  | CA-C-O | -12.30 | 108.03      | 120.70   |
| 2   | B     | 299 | LEU  | O-C-N  | 12.30  | 135.38      | 122.09   |
| 1   | A     | 573 | GLU  | CA-C-N | -12.29 | 103.62      | 120.46   |
| 1   | A     | 573 | GLU  | C-N-CA | -12.29 | 103.62      | 120.46   |
| 1   | A     | 143 | VAL  | O-C-N  | 12.28  | 133.78      | 121.87   |
| 1   | A     | 271 | ARG  | CA-C-O | -12.27 | 107.38      | 120.63   |
| 1   | A     | 296 | ASN  | CA-C-O | -12.27 | 107.55      | 120.55   |
| 2   | B     | 469 | ASP  | CA-C-O | -12.27 | 107.55      | 120.55   |
| 2   | B     | 508 | ARG  | CA-C-O | 12.24  | 133.93      | 120.10   |
| 1   | A     | 70  | ALA  | O-C-N  | 12.23  | 135.08      | 122.12   |
| 1   | A     | 220 | SER  | O-C-N  | 12.22  | 135.08      | 122.12   |
| 1   | A     | 586 | GLU  | O-C-N  | -12.22 | 107.24      | 122.27   |
| 2   | B     | 296 | ASP  | CA-C-O | -12.21 | 103.43      | 120.16   |
| 2   | B     | 108 | PHE  | O-C-N  | -12.21 | 109.39      | 122.09   |
| 2   | B     | 366 | LEU  | CA-C-N | -12.20 | 101.08      | 120.60   |
| 2   | B     | 366 | LEU  | C-N-CA | -12.20 | 101.08      | 120.60   |
| 1   | A     | 94  | VAL  | O-C-N  | -12.19 | 109.27      | 121.83   |
| 1   | A     | 603 | VAL  | CA-C-O | -12.19 | 107.93      | 120.85   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 223 | LEU  | CA-C-N | -12.18 | 100.37      | 120.72   |
| 2   | B     | 223 | LEU  | C-N-CA | -12.18 | 100.37      | 120.72   |
| 1   | A     | 145 | ILE  | CA-C-O | -12.15 | 108.29      | 121.17   |
| 2   | B     | 147 | MET  | O-C-N  | -12.15 | 109.17      | 123.27   |
| 2   | B     | 66  | ILE  | O-C-N  | 12.14  | 133.64      | 121.87   |
| 1   | A     | 305 | GLU  | N-CA-C | 12.13  | 136.64      | 110.80   |
| 2   | B     | 123 | LEU  | CA-C-O | -12.13 | 106.40      | 120.10   |
| 1   | A     | 491 | THR  | CA-C-O | -12.12 | 108.21      | 120.70   |
| 2   | B     | 389 | ILE  | O-C-N  | -12.12 | 110.11      | 121.87   |
| 3   | M     | 15  | ILE  | N-CA-C | -12.12 | 102.08      | 111.90   |
| 1   | A     | 281 | LEU  | CA-C-N | -12.11 | 101.90      | 120.31   |
| 1   | A     | 281 | LEU  | C-N-CA | -12.11 | 101.90      | 120.31   |
| 1   | A     | 573 | GLU  | O-C-N  | -12.11 | 109.60      | 122.07   |
| 3   | M     | 426 | LYS  | CA-C-N | 12.10  | 139.84      | 122.77   |
| 3   | M     | 426 | LYS  | C-N-CA | 12.10  | 139.84      | 122.77   |
| 1   | A     | 295 | VAL  | CA-C-O | -12.10 | 107.15      | 121.18   |
| 4   | S     | 60  | SER  | N-CA-C | -12.08 | 90.39       | 109.72   |
| 1   | A     | 316 | LEU  | CA-C-O | -12.06 | 108.27      | 120.70   |
| 2   | B     | 314 | ASN  | O-C-N  | 12.06  | 132.53      | 121.19   |
| 4   | S     | 149 | ILE  | O-C-N  | 12.06  | 134.25      | 121.83   |
| 1   | A     | 233 | PHE  | O-C-N  | -12.02 | 109.12      | 122.34   |
| 4   | S     | 85  | PHE  | CA-C-O | 12.02  | 133.16      | 120.30   |
| 1   | A     | 421 | PRO  | CA-C-O | -12.02 | 105.36      | 122.31   |
| 1   | A     | 177 | ILE  | O-C-N  | 12.02  | 134.40      | 121.90   |
| 1   | A     | 496 | ILE  | O-C-N  | 12.00  | 133.51      | 121.87   |
| 2   | B     | 560 | ILE  | CA-C-N | -12.00 | 98.62       | 121.54   |
| 2   | B     | 560 | ILE  | C-N-CA | -12.00 | 98.62       | 121.54   |
| 1   | A     | 333 | ILE  | CA-C-O | -11.99 | 108.48      | 120.95   |
| 1   | A     | 64  | LEU  | CA-C-O | 11.99  | 133.65      | 120.10   |
| 2   | B     | 581 | TYR  | N-CA-C | -11.99 | 92.85       | 110.23   |
| 1   | A     | 297 | CYS  | CA-C-O | 11.98  | 133.25      | 120.55   |
| 2   | B     | 554 | LYS  | O-C-N  | 11.98  | 134.41      | 122.07   |
| 3   | M     | 97  | ASP  | O-C-N  | 11.97  | 135.80      | 122.15   |
| 1   | A     | 572 | PHE  | CA-C-N | 11.97  | 136.00      | 120.44   |
| 1   | A     | 572 | PHE  | C-N-CA | 11.97  | 136.00      | 120.44   |
| 2   | B     | 82  | TYR  | N-CA-C | -11.97 | 98.70       | 113.18   |
| 3   | M     | 368 | ASP  | O-C-N  | 11.96  | 131.71      | 121.31   |
| 1   | A     | 289 | SER  | CA-C-O | 11.94  | 133.71      | 119.97   |
| 1   | A     | 257 | LEU  | CA-C-O | -11.94 | 107.77      | 120.42   |
| 2   | B     | 105 | LEU  | O-C-N  | -11.94 | 109.68      | 122.09   |
| 2   | B     | 270 | SER  | N-CA-C | -11.93 | 91.34       | 109.60   |
| 1   | A     | 407 | SER  | N-CA-C | -11.92 | 93.69       | 110.50   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 605 | PHE  | CA-C-O | -11.92 | 108.31      | 120.82   |
| 1   | A     | 233 | PHE  | CA-C-O | 11.90  | 131.98      | 118.77   |
| 2   | B     | 302 | PHE  | CA-C-O | -11.90 | 108.44      | 120.70   |
| 4   | S     | 150 | VAL  | O-C-N  | 11.90  | 133.41      | 121.87   |
| 2   | B     | 120 | ILE  | CA-C-O | -11.89 | 107.99      | 120.71   |
| 1   | A     | 103 | LYS  | O-C-N  | -11.89 | 108.31      | 122.22   |
| 2   | B     | 416 | LYS  | O-C-N  | 11.89  | 134.72      | 122.12   |
| 3   | M     | 407 | THR  | N-CA-C | -11.88 | 91.06       | 109.95   |
| 1   | A     | 433 | ILE  | CA-C-O | -11.87 | 108.92      | 121.27   |
| 3   | M     | 99  | ILE  | O-C-N  | 11.87  | 137.60      | 122.05   |
| 3   | M     | 261 | ASN  | CA-C-N | -11.86 | 107.00      | 122.77   |
| 3   | M     | 261 | ASN  | C-N-CA | -11.86 | 107.00      | 122.77   |
| 2   | B     | 355 | ASN  | CA-C-O | -11.86 | 107.86      | 120.55   |
| 2   | B     | 318 | ILE  | CA-C-O | -11.84 | 108.04      | 120.71   |
| 2   | B     | 555 | LEU  | CA-C-O | -11.84 | 107.84      | 120.63   |
| 3   | M     | 3   | LEU  | O-C-N  | -11.83 | 107.85      | 123.23   |
| 1   | A     | 282 | MET  | O-C-N  | -11.83 | 107.72      | 122.27   |
| 1   | A     | 100 | LEU  | O-C-N  | -11.82 | 109.59      | 122.12   |
| 3   | M     | 131 | ALA  | N-CA-C | 11.82  | 127.61      | 111.54   |
| 2   | B     | 472 | VAL  | CA-C-O | 11.81  | 133.23      | 120.95   |
| 2   | B     | 333 | GLN  | N-CA-C | -11.80 | 95.05       | 112.04   |
| 4   | S     | 4   | ALA  | CA-C-O | 11.79  | 133.86      | 120.89   |
| 4   | S     | 8   | PHE  | CA-C-O | 11.78  | 134.43      | 121.11   |
| 1   | A     | 237 | SER  | CA-C-O | -11.77 | 107.50      | 118.33   |
| 4   | S     | 139 | GLY  | N-CA-C | -11.77 | 97.90       | 115.32   |
| 2   | B     | 216 | LYS  | CA-C-N | -11.76 | 104.20      | 122.42   |
| 2   | B     | 216 | LYS  | C-N-CA | -11.76 | 104.20      | 122.42   |
| 1   | A     | 91  | ILE  | O-C-N  | 11.76  | 133.27      | 121.87   |
| 2   | B     | 494 | ALA  | O-C-N  | 11.76  | 134.58      | 122.12   |
| 3   | M     | 351 | SER  | CA-C-N | 11.75  | 143.98      | 121.54   |
| 3   | M     | 351 | SER  | C-N-CA | 11.75  | 143.98      | 121.54   |
| 1   | A     | 394 | GLN  | O-C-N  | 11.75  | 134.57      | 122.12   |
| 2   | B     | 362 | ALA  | O-C-N  | 11.74  | 134.56      | 122.12   |
| 2   | B     | 430 | ILE  | CA-C-O | -11.73 | 108.74      | 121.17   |
| 1   | A     | 91  | ILE  | CA-C-O | -11.73 | 108.75      | 120.95   |
| 2   | B     | 573 | GLU  | CA-C-N | -11.72 | 104.33      | 122.49   |
| 2   | B     | 573 | GLU  | C-N-CA | -11.72 | 104.33      | 122.49   |
| 1   | A     | 582 | ILE  | CA-C-O | -11.71 | 108.05      | 121.05   |
| 3   | M     | 16  | PHE  | CA-C-O | 11.70  | 134.10      | 120.99   |
| 1   | A     | 486 | SER  | N-CA-C | -11.70 | 95.11       | 110.43   |
| 1   | A     | 606 | PHE  | O-C-N  | 11.70  | 134.52      | 122.12   |
| 1   | A     | 328 | PRO  | CA-C-N | -11.68 | 100.60      | 120.58   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 328 | PRO  | C-N-CA | -11.68 | 100.60      | 120.58   |
| 2   | B     | 237 | ILE  | O-C-N  | -11.67 | 110.46      | 121.89   |
| 1   | A     | 338 | PHE  | O-C-N  | 11.66  | 134.69      | 122.09   |
| 1   | A     | 108 | LEU  | CA-C-O | -11.66 | 108.19      | 120.55   |
| 2   | B     | 67  | ILE  | CA-C-O | -11.65 | 108.50      | 120.85   |
| 1   | A     | 582 | ILE  | O-C-N  | 11.64  | 134.01      | 121.90   |
| 2   | B     | 505 | ASP  | O-C-N  | -11.64 | 109.78      | 122.12   |
| 3   | M     | 284 | SER  | O-C-N  | -11.64 | 108.39      | 121.66   |
| 2   | B     | 412 | PHE  | CA-C-O | -11.64 | 108.06      | 120.63   |
| 2   | B     | 344 | VAL  | O-C-N  | 11.62  | 133.15      | 121.87   |
| 1   | A     | 217 | ALA  | CA-C-O | -11.62 | 108.23      | 120.55   |
| 1   | A     | 575 | LYS  | CA-C-O | -11.62 | 108.23      | 120.55   |
| 1   | A     | 611 | LEU  | CA-C-O | -11.62 | 108.73      | 120.70   |
| 3   | M     | 21  | GLY  | N-CA-C | -11.62 | 95.62       | 112.81   |
| 2   | B     | 169 | VAL  | O-C-N  | 11.62  | 133.98      | 121.90   |
| 2   | B     | 341 | GLU  | CA-C-O | -11.61 | 108.09      | 120.63   |
| 2   | B     | 387 | ASP  | N-CA-C | 11.62  | 125.98      | 109.84   |
| 1   | A     | 473 | ILE  | O-C-N  | 11.61  | 133.78      | 121.83   |
| 1   | A     | 621 | LEU  | CA-C-O | 11.61  | 129.60      | 118.34   |
| 3   | M     | 46  | SER  | N-CA-C | -11.60 | 99.38       | 113.19   |
| 1   | A     | 242 | GLU  | O-C-N  | -11.60 | 108.60      | 122.87   |
| 3   | M     | 377 | LYS  | N-CA-C | 11.60  | 126.20      | 111.24   |
| 4   | S     | 108 | SER  | O-C-N  | 11.60  | 135.37      | 122.15   |
| 3   | M     | 51  | LEU  | CA-C-N | -11.58 | 100.99      | 120.68   |
| 3   | M     | 51  | LEU  | C-N-CA | -11.58 | 100.99      | 120.68   |
| 2   | B     | 593 | ASN  | CA-C-O | -11.57 | 108.13      | 120.63   |
| 2   | B     | 105 | LEU  | CA-C-O | 11.57  | 133.28      | 120.90   |
| 1   | A     | 539 | ASN  | CA-C-N | -11.57 | 103.99      | 120.42   |
| 1   | A     | 539 | ASN  | C-N-CA | -11.57 | 103.99      | 120.42   |
| 1   | A     | 461 | CYS  | O-C-N  | -11.57 | 108.69      | 122.22   |
| 1   | A     | 313 | MET  | CA-C-O | -11.56 | 108.69      | 120.82   |
| 2   | B     | 174 | ALA  | CA-C-N | -11.55 | 104.80      | 120.28   |
| 2   | B     | 174 | ALA  | C-N-CA | -11.55 | 104.80      | 120.28   |
| 3   | M     | 394 | GLN  | CA-C-O | 11.55  | 133.94      | 120.66   |
| 2   | B     | 489 | ILE  | O-C-N  | 11.54  | 133.53      | 121.87   |
| 1   | A     | 635 | ALA  | CA-C-O | -11.54 | 108.32      | 120.55   |
| 3   | M     | 6   | TYR  | O-C-N  | -11.54 | 108.15      | 123.15   |
| 1   | A     | 422 | GLU  | CA-C-O | -11.53 | 108.19      | 120.42   |
| 2   | B     | 138 | ALA  | CA-C-O | -11.50 | 108.36      | 120.55   |
| 3   | M     | 41  | LEU  | O-C-N  | 11.50  | 137.18      | 122.23   |
| 4   | S     | 96  | LEU  | O-C-N  | 11.49  | 134.50      | 122.09   |
| 1   | A     | 387 | ILE  | CA-C-O | -11.47 | 108.44      | 120.71   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 389 | ILE  | CA-C-N | -11.47 | 104.14      | 120.42   |
| 2   | B     | 389 | ILE  | C-N-CA | -11.47 | 104.14      | 120.42   |
| 2   | B     | 526 | CYS  | O-C-N  | 11.47  | 134.51      | 121.32   |
| 1   | A     | 145 | ILE  | O-C-N  | 11.45  | 133.13      | 121.91   |
| 1   | A     | 365 | VAL  | O-C-N  | -11.45 | 110.30      | 121.87   |
| 1   | A     | 551 | LEU  | CA-C-O | -11.45 | 108.41      | 120.55   |
| 1   | A     | 492 | ILE  | O-C-N  | 11.44  | 133.12      | 121.91   |
| 3   | M     | 237 | THR  | CA-C-N | -11.44 | 106.05      | 120.92   |
| 3   | M     | 237 | THR  | C-N-CA | -11.44 | 106.05      | 120.92   |
| 2   | B     | 574 | ASN  | CA-C-N | -11.43 | 100.80      | 122.06   |
| 2   | B     | 574 | ASN  | C-N-CA | -11.43 | 100.80      | 122.06   |
| 2   | B     | 211 | ALA  | O-C-N  | 11.43  | 137.25      | 122.39   |
| 2   | B     | 586 | SER  | CA-C-O | -11.42 | 108.68      | 120.90   |
| 3   | M     | 53  | HIS  | O-C-N  | -11.42 | 111.20      | 123.42   |
| 1   | A     | 496 | ILE  | CA-C-O | -11.41 | 109.09      | 120.95   |
| 1   | A     | 578 | LEU  | CA-C-O | -11.40 | 108.46      | 120.55   |
| 1   | A     | 574 | ILE  | O-C-N  | 11.40  | 132.93      | 121.87   |
| 2   | B     | 439 | CYS  | CA-C-O | -11.40 | 108.96      | 120.70   |
| 2   | B     | 209 | SER  | CA-C-O | -11.38 | 107.24      | 120.10   |
| 4   | S     | 74  | GLN  | O-C-N  | -11.38 | 109.88      | 123.19   |
| 1   | A     | 545 | HIS  | O-C-N  | -11.38 | 110.06      | 122.12   |
| 2   | B     | 568 | VAL  | CA-C-N | 11.36  | 138.91      | 121.99   |
| 2   | B     | 568 | VAL  | C-N-CA | 11.36  | 138.91      | 121.99   |
| 3   | M     | 371 | GLU  | CA-C-N | -11.36 | 110.98      | 121.65   |
| 3   | M     | 371 | GLU  | C-N-CA | -11.36 | 110.98      | 121.65   |
| 1   | A     | 177 | ILE  | CA-C-O | -11.35 | 108.45      | 121.05   |
| 3   | M     | 3   | LEU  | CA-C-O | 11.35  | 132.96      | 120.70   |
| 3   | M     | 111 | ILE  | O-C-N  | 11.33  | 132.86      | 121.87   |
| 4   | S     | 68  | VAL  | CA-C-N | -11.32 | 104.46      | 122.24   |
| 4   | S     | 68  | VAL  | C-N-CA | -11.32 | 104.46      | 122.24   |
| 1   | A     | 539 | ASN  | O-C-N  | -11.32 | 108.75      | 122.34   |
| 1   | A     | 125 | THR  | CA-C-O | -11.32 | 109.04      | 120.70   |
| 1   | A     | 604 | LEU  | CA-C-O | -11.32 | 108.79      | 120.90   |
| 2   | B     | 511 | ILE  | CA-C-O | 11.32  | 132.82      | 121.05   |
| 2   | B     | 204 | ASP  | CA-C-O | -11.31 | 108.29      | 119.49   |
| 1   | A     | 84  | MET  | O-C-N  | -11.30 | 106.77      | 122.37   |
| 3   | M     | 55  | MET  | CA-C-N | -11.30 | 106.02      | 120.60   |
| 3   | M     | 55  | MET  | C-N-CA | -11.30 | 106.02      | 120.60   |
| 1   | A     | 552 | ILE  | O-C-N  | 11.30  | 132.83      | 121.87   |
| 2   | B     | 132 | SER  | CA-C-N | -11.29 | 101.48      | 120.68   |
| 2   | B     | 132 | SER  | C-N-CA | -11.29 | 101.48      | 120.68   |
| 2   | B     | 337 | THR  | N-CA-C | -11.29 | 98.98       | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 384 | LEU  | O-C-N  | 11.29  | 134.28      | 122.09   |
| 1   | A     | 335 | CYS  | CA-C-O | -11.28 | 108.98      | 120.82   |
| 1   | A     | 601 | VAL  | O-C-N  | -11.28 | 110.48      | 121.87   |
| 1   | A     | 637 | GLU  | CA-C-N | -11.27 | 101.41      | 121.70   |
| 1   | A     | 637 | GLU  | C-N-CA | -11.27 | 101.41      | 121.70   |
| 1   | A     | 514 | GLU  | CA-C-O | -11.27 | 108.47      | 120.42   |
| 4   | S     | 53  | THR  | CA-C-N | -11.27 | 108.77      | 120.38   |
| 4   | S     | 53  | THR  | C-N-CA | -11.27 | 108.77      | 120.38   |
| 1   | A     | 441 | TYR  | N-CA-C | -11.26 | 96.12       | 111.55   |
| 1   | A     | 139 | ASP  | CA-C-O | -11.26 | 108.49      | 120.42   |
| 1   | A     | 254 | ILE  | CA-C-O | -11.26 | 109.56      | 121.27   |
| 1   | A     | 298 | ILE  | O-C-N  | -11.26 | 110.19      | 121.90   |
| 2   | B     | 478 | LEU  | O-C-N  | -11.25 | 110.48      | 122.07   |
| 3   | M     | 77  | LEU  | CA-C-O | 11.25  | 132.64      | 120.71   |
| 2   | B     | 346 | THR  | CA-C-O | -11.24 | 109.02      | 120.82   |
| 1   | A     | 513 | ARG  | CA-C-O | -11.22 | 108.65      | 120.55   |
| 1   | A     | 516 | ILE  | CA-C-O | -11.22 | 108.95      | 120.85   |
| 4   | S     | 103 | GLN  | O-C-N  | 11.22  | 136.08      | 122.27   |
| 2   | B     | 444 | THR  | CA-C-O | 11.22  | 132.31      | 120.42   |
| 2   | B     | 554 | LYS  | CA-C-O | -11.22 | 109.04      | 120.82   |
| 2   | B     | 531 | ARG  | CA-C-O | -11.21 | 108.53      | 120.42   |
| 4   | S     | 98  | ILE  | CA-C-O | -11.21 | 108.14      | 120.25   |
| 1   | A     | 327 | ASP  | CA-C-O | -11.21 | 111.03      | 119.32   |
| 1   | A     | 429 | VAL  | O-C-N  | 11.21  | 132.74      | 121.87   |
| 2   | B     | 555 | LEU  | O-C-N  | 11.20  | 134.00      | 122.12   |
| 3   | M     | 126 | ASN  | CA-C-O | -11.21 | 107.08      | 119.97   |
| 1   | A     | 474 | GLY  | O-C-N  | 11.20  | 132.94      | 122.19   |
| 2   | B     | 589 | SER  | CA-C-O | -11.20 | 109.06      | 120.82   |
| 2   | B     | 158 | VAL  | O-C-N  | 11.19  | 132.86      | 121.89   |
| 2   | B     | 486 | HIS  | O-C-N  | 11.19  | 134.91      | 122.15   |
| 2   | B     | 97  | VAL  | O-C-N  | 11.19  | 133.91      | 121.94   |
| 4   | S     | 36  | TYR  | O-C-N  | 11.19  | 134.91      | 122.15   |
| 2   | B     | 451 | MET  | CA-C-O | -11.18 | 109.08      | 120.82   |
| 1   | A     | 635 | ALA  | O-C-N  | 11.18  | 133.97      | 122.12   |
| 3   | M     | 282 | VAL  | N-CA-C | -11.18 | 99.97       | 110.82   |
| 2   | B     | 272 | GLY  | N-CA-C | -11.18 | 97.69       | 114.90   |
| 2   | B     | 455 | ILE  | O-C-N  | 11.17  | 132.85      | 121.91   |
| 2   | B     | 467 | VAL  | CA-C-O | -11.16 | 109.02      | 120.85   |
| 2   | B     | 475 | ILE  | O-C-N  | 11.16  | 133.17      | 121.90   |
| 1   | A     | 279 | LEU  | CA-C-N | -11.15 | 104.46      | 120.29   |
| 1   | A     | 279 | LEU  | C-N-CA | -11.15 | 104.46      | 120.29   |
| 2   | B     | 363 | ILE  | CA-C-O | -11.15 | 108.64      | 120.57   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 444 | THR  | O-C-N  | -11.15 | 109.44      | 122.15   |
| 1   | A     | 80  | TYR  | CA-C-N | 11.14  | 141.76      | 121.70   |
| 1   | A     | 80  | TYR  | C-N-CA | 11.14  | 141.76      | 121.70   |
| 2   | B     | 172 | GLU  | O-C-N  | -11.14 | 110.31      | 122.12   |
| 2   | B     | 86  | VAL  | CA-C-O | -11.14 | 109.37      | 120.95   |
| 1   | A     | 462 | GLN  | O-C-N  | -11.13 | 107.51      | 122.43   |
| 2   | B     | 615 | SER  | CA-C-O | -11.14 | 109.23      | 120.70   |
| 1   | A     | 495 | ILE  | O-C-N  | 11.13  | 133.30      | 121.83   |
| 2   | B     | 363 | ILE  | O-C-N  | 11.13  | 133.11      | 121.87   |
| 1   | A     | 392 | MET  | CA-C-O | -11.13 | 108.62      | 120.42   |
| 1   | A     | 632 | PHE  | O-C-N  | 11.12  | 133.52      | 122.07   |
| 1   | A     | 559 | PHE  | O-C-N  | 11.12  | 134.87      | 122.20   |
| 1   | A     | 304 | LEU  | O-C-N  | -11.11 | 110.34      | 122.12   |
| 2   | B     | 592 | TYR  | CA-C-O | -11.11 | 109.25      | 120.70   |
| 2   | B     | 366 | LEU  | CA-C-O | 11.11  | 132.32      | 120.55   |
| 1   | A     | 545 | HIS  | CA-C-O | 11.11  | 132.32      | 120.55   |
| 1   | A     | 138 | ASN  | N-CA-C | -11.10 | 89.25       | 108.56   |
| 1   | A     | 517 | TRP  | O-C-N  | 11.09  | 134.07      | 122.09   |
| 2   | B     | 145 | MET  | CA-C-N | -11.07 | 105.56      | 122.16   |
| 2   | B     | 145 | MET  | C-N-CA | -11.07 | 105.56      | 122.16   |
| 3   | M     | 4   | SER  | CA-C-O | 11.07  | 133.90      | 121.06   |
| 1   | A     | 605 | GLU  | O-C-N  | 11.07  | 133.85      | 122.12   |
| 1   | A     | 188 | VAL  | O-C-N  | 11.06  | 133.78      | 121.94   |
| 1   | A     | 562 | TRP  | CA-C-O | -11.06 | 109.20      | 120.82   |
| 3   | M     | 54  | SER  | CA-C-N | 11.06  | 139.59      | 122.78   |
| 3   | M     | 54  | SER  | C-N-CA | 11.06  | 139.59      | 122.78   |
| 1   | A     | 624 | LEU  | CA-C-O | -11.06 | 108.83      | 120.55   |
| 2   | B     | 614 | ILE  | O-C-N  | 11.06  | 132.73      | 121.89   |
| 2   | B     | 475 | ILE  | CA-C-O | -11.05 | 108.59      | 120.64   |
| 2   | B     | 548 | ILE  | O-C-N  | 11.05  | 133.03      | 121.87   |
| 1   | A     | 166 | LEU  | O-C-N  | 11.05  | 133.83      | 122.12   |
| 2   | B     | 174 | ALA  | CA-C-O | 11.05  | 132.13      | 120.42   |
| 4   | S     | 106 | VAL  | O-C-N  | 11.05  | 133.21      | 121.83   |
| 1   | A     | 271 | ARG  | O-C-N  | 11.04  | 133.83      | 122.12   |
| 1   | A     | 569 | ASP  | O-C-N  | -11.04 | 111.61      | 123.42   |
| 2   | B     | 402 | LEU  | N-CA-C | 11.04  | 126.56      | 113.20   |
| 2   | B     | 154 | ILE  | O-C-N  | 11.04  | 133.04      | 121.90   |
| 3   | M     | 420 | THR  | CA-C-N | -11.04 | 104.55      | 121.87   |
| 3   | M     | 420 | THR  | C-N-CA | -11.04 | 104.55      | 121.87   |
| 1   | A     | 390 | THR  | CA-C-O | -11.02 | 108.87      | 120.55   |
| 3   | M     | 124 | ILE  | O-C-N  | 11.01  | 133.18      | 121.83   |
| 2   | B     | 325 | LEU  | CA-C-N | -11.01 | 101.97      | 120.68   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | B     | 325 | LEU  | C-N-CA  | -11.01 | 101.97      | 120.68   |
| 1   | A     | 216 | SER  | CA-C-O  | -11.00 | 108.89      | 120.55   |
| 2   | B     | 255 | TYR  | O-C-N   | 11.00  | 133.53      | 122.09   |
| 4   | S     | 54  | PRO  | CA-N-CD | -11.00 | 96.60       | 112.00   |
| 1   | A     | 367 | ILE  | O-C-N   | 10.99  | 136.35      | 121.84   |
| 1   | A     | 457 | LEU  | O-C-N   | 10.99  | 133.77      | 122.12   |
| 1   | A     | 461 | CYS  | CA-C-N  | -10.99 | 102.37      | 120.72   |
| 1   | A     | 461 | CYS  | C-N-CA  | -10.99 | 102.37      | 120.72   |
| 2   | B     | 324 | ALA  | CA-C-O  | -10.99 | 107.34      | 119.97   |
| 2   | B     | 60  | ARG  | CA-C-O  | -10.98 | 109.59      | 120.90   |
| 1   | A     | 555 | LEU  | O-C-N   | 10.98  | 133.76      | 122.12   |
| 1   | A     | 341 | ILE  | CA-C-O  | -10.98 | 109.22      | 120.85   |
| 3   | M     | 425 | THR  | CA-C-N  | 10.97  | 139.12      | 122.23   |
| 3   | M     | 425 | THR  | C-N-CA  | 10.97  | 139.12      | 122.23   |
| 1   | A     | 242 | GLU  | CA-C-O  | -10.96 | 109.13      | 121.19   |
| 2   | B     | 467 | VAL  | O-C-N   | 10.96  | 133.12      | 121.83   |
| 3   | M     | 458 | LEU  | N-CA-C  | -10.95 | 93.45       | 110.42   |
| 2   | B     | 294 | VAL  | N-CA-C  | -10.94 | 102.40      | 111.81   |
| 3   | M     | 104 | PHE  | CA-C-N  | 10.94  | 142.44      | 121.54   |
| 3   | M     | 104 | PHE  | C-N-CA  | 10.94  | 142.44      | 121.54   |
| 1   | A     | 534 | LYS  | O-C-N   | -10.94 | 109.42      | 122.87   |
| 2   | B     | 474 | VAL  | O-C-N   | 10.94  | 133.21      | 121.94   |
| 2   | B     | 157 | THR  | CA-C-O  | -10.94 | 109.64      | 120.90   |
| 1   | A     | 311 | THR  | O-C-N   | 10.93  | 134.61      | 122.15   |
| 4   | S     | 117 | ASN  | CA-C-O  | -10.93 | 107.79      | 121.78   |
| 1   | A     | 454 | ILE  | O-C-N   | 10.93  | 133.26      | 121.90   |
| 2   | B     | 490 | ILE  | CA-C-O  | -10.93 | 107.96      | 120.96   |
| 3   | M     | 126 | ASN  | O-C-N   | 10.92  | 135.70      | 122.27   |
| 2   | B     | 482 | ASN  | O-C-N   | 10.92  | 131.36      | 121.42   |
| 1   | A     | 312 | ALA  | CA-C-O  | -10.91 | 108.99      | 120.55   |
| 1   | A     | 522 | PHE  | CA-C-O  | -10.91 | 106.80      | 119.56   |
| 2   | B     | 79  | VAL  | CA-C-O  | -10.91 | 106.83      | 120.03   |
| 2   | B     | 391 | ALA  | CA-C-O  | -10.91 | 109.37      | 120.82   |
| 1   | A     | 338 | PHE  | CA-C-O  | -10.90 | 109.47      | 120.70   |
| 2   | B     | 589 | SER  | O-C-N   | 10.90  | 133.30      | 122.07   |
| 2   | B     | 99  | ARG  | O-C-N   | 10.90  | 133.86      | 122.09   |
| 4   | S     | 168 | GLY  | N-CA-C  | 10.89  | 144.90      | 113.30   |
| 2   | B     | 104 | TYR  | O-C-N   | 10.89  | 133.73      | 122.08   |
| 2   | B     | 105 | LEU  | CA-C-N  | -10.89 | 104.60      | 120.28   |
| 2   | B     | 105 | LEU  | C-N-CA  | -10.89 | 104.60      | 120.28   |
| 1   | A     | 105 | VAL  | O-C-N   | 10.89  | 134.10      | 121.80   |
| 2   | B     | 356 | LYS  | O-C-N   | 10.89  | 133.41      | 122.09   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | M     | 47  | SER  | N-CA-C | -10.89 | 92.64       | 110.17   |
| 1   | A     | 516 | ILE  | O-C-N  | 10.88  | 133.03      | 121.83   |
| 2   | B     | 614 | ILE  | CA-C-O | -10.88 | 109.74      | 121.05   |
| 1   | A     | 403 | LEU  | CA-C-N | -10.88 | 98.31       | 121.80   |
| 1   | A     | 403 | LEU  | C-N-CA | -10.88 | 98.31       | 121.80   |
| 2   | B     | 544 | THR  | CA-C-O | -10.88 | 108.89      | 120.42   |
| 1   | A     | 624 | LEU  | O-C-N  | 10.87  | 133.64      | 122.12   |
| 1   | A     | 107 | TYR  | O-C-N  | 10.87  | 133.26      | 122.07   |
| 3   | M     | 7   | ILE  | CA-C-O | -10.87 | 108.84      | 120.36   |
| 2   | B     | 595 | VAL  | CA-C-O | -10.87 | 108.99      | 121.05   |
| 3   | M     | 330 | GLY  | CA-C-N | 10.86  | 142.28      | 121.54   |
| 3   | M     | 330 | GLY  | C-N-CA | 10.86  | 142.28      | 121.54   |
| 1   | A     | 434 | SER  | CA-C-O | -10.86 | 109.04      | 120.55   |
| 1   | A     | 102 | GLN  | O-C-N  | 10.85  | 133.62      | 122.12   |
| 3   | M     | 107 | ASP  | CA-C-O | -10.85 | 106.98      | 119.79   |
| 3   | M     | 96  | ILE  | O-C-N  | 10.84  | 134.05      | 121.80   |
| 1   | A     | 140 | VAL  | CA-C-N | -10.84 | 106.69      | 120.56   |
| 1   | A     | 140 | VAL  | C-N-CA | -10.84 | 106.69      | 120.56   |
| 4   | S     | 31  | LEU  | O-C-N  | 10.84  | 134.50      | 122.15   |
| 1   | A     | 212 | ILE  | O-C-N  | -10.83 | 109.71      | 122.06   |
| 1   | A     | 188 | VAL  | CA-C-O | -10.83 | 108.62      | 121.18   |
| 2   | B     | 212 | VAL  | O-C-N  | -10.82 | 108.73      | 121.94   |
| 1   | A     | 336 | ILE  | O-C-N  | 10.82  | 132.51      | 121.91   |
| 2   | B     | 67  | ILE  | O-C-N  | 10.82  | 132.97      | 121.83   |
| 2   | B     | 452 | LYS  | O-C-N  | 10.82  | 133.59      | 122.12   |
| 1   | A     | 146 | ALA  | CA-C-O | -10.81 | 109.09      | 120.55   |
| 1   | A     | 429 | VAL  | CA-C-O | -10.81 | 109.70      | 120.95   |
| 1   | A     | 252 | ILE  | O-C-N  | 10.81  | 132.96      | 121.83   |
| 2   | B     | 346 | THR  | O-C-N  | 10.81  | 133.20      | 122.07   |
| 1   | A     | 445 | ASN  | N-CA-C | -10.80 | 97.43       | 112.45   |
| 3   | M     | 323 | MET  | CA-C-N | -10.80 | 108.80      | 122.84   |
| 3   | M     | 323 | MET  | C-N-CA | -10.80 | 108.80      | 122.84   |
| 1   | A     | 493 | ALA  | CA-C-O | -10.80 | 109.10      | 120.55   |
| 1   | A     | 607 | LEU  | O-C-N  | 10.78  | 133.73      | 122.09   |
| 1   | A     | 263 | LEU  | CA-C-N | -10.78 | 103.93      | 120.31   |
| 1   | A     | 263 | LEU  | C-N-CA | -10.78 | 103.93      | 120.31   |
| 2   | B     | 365 | PHE  | CA-C-O | -10.78 | 109.37      | 120.90   |
| 1   | A     | 526 | VAL  | CA-C-N | 10.78  | 134.72      | 120.28   |
| 1   | A     | 526 | VAL  | C-N-CA | 10.78  | 134.72      | 120.28   |
| 2   | B     | 513 | TRP  | O-C-N  | 10.78  | 133.30      | 122.09   |
| 2   | B     | 169 | VAL  | CA-C-O | -10.77 | 109.09      | 121.05   |
| 2   | B     | 430 | ILE  | O-C-N  | 10.77  | 132.47      | 121.91   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 507 | ALA  | O-C-N  | 10.77  | 133.16      | 122.07   |
| 2   | B     | 588 | ILE  | CA-C-O | -10.77 | 109.19      | 120.71   |
| 4   | S     | 95  | GLU  | CA-C-O | -10.76 | 109.15      | 120.55   |
| 1   | A     | 319 | LEU  | CA-C-O | 10.75  | 131.82      | 120.42   |
| 4   | S     | 153 | VAL  | O-C-N  | 10.75  | 132.91      | 121.83   |
| 1   | A     | 252 | ILE  | CA-C-O | -10.75 | 109.46      | 120.85   |
| 2   | B     | 344 | VAL  | CA-C-O | -10.75 | 109.77      | 120.95   |
| 2   | B     | 474 | VAL  | CA-C-O | -10.75 | 109.79      | 121.29   |
| 2   | B     | 115 | LEU  | O-C-N  | 10.74  | 135.48      | 122.27   |
| 2   | B     | 147 | MET  | CA-C-N | -10.74 | 102.34      | 121.14   |
| 2   | B     | 147 | MET  | C-N-CA | -10.74 | 102.34      | 121.14   |
| 2   | B     | 584 | SER  | CA-C-N | -10.74 | 100.36      | 121.41   |
| 2   | B     | 584 | SER  | C-N-CA | -10.74 | 100.36      | 121.41   |
| 1   | A     | 550 | VAL  | O-C-N  | 10.74  | 133.06      | 121.90   |
| 2   | B     | 229 | HIS  | CA-C-N | 10.73  | 137.77      | 120.60   |
| 2   | B     | 229 | HIS  | C-N-CA | 10.73  | 137.77      | 120.60   |
| 1   | A     | 380 | ASP  | CA-C-O | -10.73 | 109.28      | 121.40   |
| 2   | B     | 101 | ILE  | O-C-N  | 10.72  | 132.42      | 121.91   |
| 1   | A     | 372 | ILE  | O-C-N  | 10.71  | 132.39      | 121.89   |
| 2   | B     | 489 | ILE  | CA-C-O | -10.71 | 109.11      | 120.57   |
| 1   | A     | 67  | LYS  | O-C-N  | 10.71  | 133.47      | 122.12   |
| 4   | S     | 127 | THR  | O-C-N  | 10.70  | 134.35      | 122.15   |
| 2   | B     | 353 | GLN  | N-CA-C | 10.70  | 122.94      | 111.28   |
| 1   | A     | 554 | ALA  | O-C-N  | 10.69  | 133.09      | 122.07   |
| 2   | B     | 421 | SER  | N-CA-C | 10.68  | 124.83      | 111.69   |
| 2   | B     | 48  | VAL  | CA-C-O | -10.68 | 109.86      | 121.29   |
| 2   | B     | 412 | PHE  | O-C-N  | 10.68  | 133.44      | 122.12   |
| 2   | B     | 531 | ARG  | O-C-N  | 10.68  | 134.32      | 122.15   |
| 1   | A     | 270 | LEU  | O-C-N  | 10.67  | 136.11      | 122.23   |
| 2   | B     | 494 | ALA  | CA-C-O | -10.67 | 109.24      | 120.55   |
| 3   | M     | 65  | TYR  | CA-C-N | -10.66 | 105.86      | 122.59   |
| 3   | M     | 65  | TYR  | C-N-CA | -10.66 | 105.86      | 122.59   |
| 2   | B     | 100 | LEU  | O-C-N  | 10.66  | 133.42      | 122.12   |
| 1   | A     | 332 | TYR  | O-C-N  | 10.65  | 133.17      | 122.09   |
| 1   | A     | 634 | ASN  | CA-C-O | -10.64 | 109.14      | 120.42   |
| 1   | A     | 603 | VAL  | O-C-N  | 10.64  | 132.79      | 121.83   |
| 1   | A     | 508 | LEU  | CA-C-O | -10.63 | 106.77      | 120.80   |
| 2   | B     | 255 | TYR  | CA-C-O | -10.63 | 109.53      | 120.90   |
| 2   | B     | 540 | GLU  | N-CA-C | 10.63  | 126.00      | 110.59   |
| 1   | A     | 562 | TRP  | O-C-N  | 10.62  | 133.01      | 122.07   |
| 4   | S     | 98  | ILE  | O-C-N  | 10.62  | 136.37      | 121.82   |
| 2   | B     | 522 | GLU  | N-CA-C | 10.62  | 126.00      | 108.49   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 319 | LEU  | CA-C-O | -10.61 | 109.17      | 120.42   |
| 1   | A     | 105 | VAL  | CA-C-O | -10.60 | 109.02      | 120.47   |
| 1   | A     | 253 | ILE  | CA-C-O | -10.60 | 109.29      | 121.05   |
| 1   | A     | 391 | LEU  | CA-C-O | 10.60  | 131.66      | 120.42   |
| 3   | M     | 306 | LEU  | CA-C-O | 10.60  | 132.07      | 120.20   |
| 3   | M     | 122 | SER  | CA-C-O | -10.58 | 109.20      | 120.42   |
| 1   | A     | 125 | THR  | O-C-N  | 10.57  | 133.51      | 122.09   |
| 3   | M     | 60  | LEU  | N-CA-C | -10.57 | 94.70       | 110.24   |
| 2   | B     | 435 | SER  | CA-C-O | -10.57 | 110.02      | 120.90   |
| 3   | M     | 105 | ASP  | CA-C-N | -10.56 | 101.36      | 121.54   |
| 3   | M     | 105 | ASP  | C-N-CA | -10.56 | 101.36      | 121.54   |
| 4   | S     | 84  | TYR  | CA-C-O | 10.56  | 132.11      | 120.70   |
| 1   | A     | 221 | VAL  | CA-C-O | -10.56 | 109.33      | 121.05   |
| 2   | B     | 204 | ASP  | CA-C-N | 10.54  | 130.31      | 119.56   |
| 2   | B     | 204 | ASP  | C-N-CA | 10.54  | 130.31      | 119.56   |
| 1   | A     | 204 | VAL  | CA-C-N | -10.54 | 104.29      | 120.31   |
| 1   | A     | 204 | VAL  | C-N-CA | -10.54 | 104.29      | 120.31   |
| 2   | B     | 550 | VAL  | O-C-N  | 10.54  | 132.55      | 121.90   |
| 1   | A     | 327 | ASP  | O-C-N  | 10.54  | 131.04      | 121.35   |
| 2   | B     | 552 | SER  | O-C-N  | 10.53  | 133.29      | 122.12   |
| 1   | A     | 488 | ARG  | O-C-N  | 10.53  | 134.15      | 122.15   |
| 1   | A     | 237 | SER  | O-C-N  | 10.53  | 131.12      | 120.70   |
| 2   | B     | 511 | ILE  | O-C-N  | -10.52 | 111.58      | 121.89   |
| 1   | A     | 141 | VAL  | CA-C-O | -10.52 | 109.37      | 121.05   |
| 1   | A     | 313 | MET  | O-C-N  | 10.52  | 132.90      | 122.07   |
| 2   | B     | 361 | GLN  | O-C-N  | 10.52  | 133.45      | 122.09   |
| 2   | B     | 116 | THR  | CA-C-O | -10.51 | 109.41      | 120.55   |
| 1   | A     | 400 | VAL  | CA-C-O | -10.51 | 109.71      | 120.85   |
| 1   | A     | 182 | ILE  | O-C-N  | 10.50  | 132.82      | 121.90   |
| 4   | S     | 132 | LEU  | O-C-N  | 10.50  | 135.19      | 122.27   |
| 1   | A     | 372 | ILE  | CA-C-O | -10.50 | 110.13      | 121.05   |
| 2   | B     | 454 | LEU  | O-C-N  | 10.49  | 133.42      | 122.09   |
| 4   | S     | 37  | GLU  | CA-C-O | -10.49 | 109.90      | 120.70   |
| 2   | B     | 359 | LEU  | CA-C-O | -10.48 | 109.90      | 120.70   |
| 1   | A     | 577 | VAL  | CA-C-O | -10.48 | 109.75      | 120.85   |
| 2   | B     | 404 | ASN  | O-C-N  | -10.47 | 108.59      | 122.94   |
| 4   | S     | 87  | PHE  | CA-C-O | 10.47  | 131.67      | 120.36   |
| 2   | B     | 447 | GLU  | O-C-N  | 10.47  | 133.22      | 122.12   |
| 1   | A     | 296 | ASN  | O-C-N  | 10.46  | 133.21      | 122.12   |
| 1   | A     | 121 | LEU  | CA-C-O | -10.46 | 109.47      | 120.55   |
| 1   | A     | 308 | ASP  | N-CA-C | 10.46  | 125.59      | 113.15   |
| 1   | A     | 555 | LEU  | CA-C-O | -10.46 | 109.34      | 120.63   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | B     | 189 | HIS  | CA-C-O  | -10.45 | 108.29      | 120.10   |
| 2   | B     | 288 | TYR  | N-CA-C  | -10.45 | 91.70       | 109.15   |
| 2   | B     | 584 | SER  | O-C-N   | -10.45 | 110.24      | 122.15   |
| 2   | B     | 323 | ASN  | CA-C-O  | -10.45 | 108.64      | 120.24   |
| 1   | A     | 600 | SER  | O-C-N   | 10.44  | 133.37      | 122.09   |
| 2   | B     | 508 | ARG  | O-C-N   | -10.44 | 110.01      | 122.22   |
| 1   | A     | 341 | ILE  | O-C-N   | 10.43  | 132.58      | 121.83   |
| 2   | B     | 592 | TYR  | O-C-N   | 10.43  | 133.35      | 122.09   |
| 1   | A     | 146 | ALA  | O-C-N   | 10.43  | 133.17      | 122.12   |
| 1   | A     | 447 | PHE  | O-C-N   | 10.42  | 134.03      | 122.15   |
| 2   | B     | 65  | ARG  | O-C-N   | 10.42  | 133.17      | 122.12   |
| 1   | A     | 573 | GLU  | N-CA-C  | -10.41 | 99.93       | 111.07   |
| 1   | A     | 596 | VAL  | CA-C-O  | -10.41 | 109.81      | 120.85   |
| 2   | B     | 126 | SER  | O-C-N   | -10.41 | 110.04      | 122.22   |
| 2   | B     | 86  | VAL  | O-C-N   | 10.40  | 131.96      | 121.87   |
| 2   | B     | 134 | LEU  | CA-C-O  | -10.40 | 109.42      | 120.55   |
| 2   | B     | 329 | ALA  | CB-CA-C | -10.40 | 93.24       | 109.89   |
| 4   | S     | 130 | SER  | O-C-N   | 10.40  | 133.15      | 122.12   |
| 1   | A     | 594 | PHE  | CA-C-O  | -10.39 | 109.53      | 120.55   |
| 2   | B     | 616 | SER  | CA-C-O  | -10.39 | 109.91      | 120.82   |
| 2   | B     | 253 | ILE  | CA-C-O  | -10.39 | 109.59      | 120.71   |
| 2   | B     | 613 | MET  | O-C-N   | 10.39  | 132.77      | 122.07   |
| 1   | A     | 588 | LEU  | CA-C-O  | 10.38  | 132.55      | 119.05   |
| 1   | A     | 512 | LEU  | CA-C-O  | -10.38 | 109.42      | 120.42   |
| 1   | A     | 602 | GLU  | CA-C-O  | -10.37 | 109.43      | 120.42   |
| 2   | B     | 251 | LEU  | O-C-N   | 10.37  | 133.29      | 122.09   |
| 4   | S     | 100 | ASP  | O-C-N   | 10.37  | 136.33      | 122.43   |
| 2   | B     | 596 | LEU  | CA-C-O  | -10.37 | 109.93      | 120.82   |
| 1   | A     | 330 | LEU  | O-C-N   | 10.36  | 135.02      | 122.27   |
| 2   | B     | 150 | LEU  | CA-C-O  | -10.36 | 106.89      | 119.43   |
| 3   | M     | 111 | ILE  | CA-C-O  | -10.36 | 110.17      | 120.95   |
| 4   | S     | 104 | THR  | O-C-N   | 10.36  | 136.65      | 122.46   |
| 2   | B     | 359 | LEU  | O-C-N   | 10.35  | 133.27      | 122.09   |
| 2   | B     | 557 | SER  | O-C-N   | -10.35 | 108.82      | 122.59   |
| 2   | B     | 174 | ALA  | O-C-N   | -10.34 | 110.36      | 122.15   |
| 1   | A     | 218 | ALA  | CA-C-O  | -10.34 | 109.59      | 120.55   |
| 1   | A     | 602 | GLU  | O-C-N   | 10.34  | 133.93      | 122.15   |
| 1   | A     | 69  | ASN  | CA-C-O  | -10.33 | 109.47      | 120.42   |
| 2   | B     | 525 | ILE  | O-C-N   | 10.33  | 132.36      | 122.23   |
| 2   | B     | 83  | PHE  | O-C-N   | 10.33  | 135.66      | 122.23   |
| 1   | A     | 612 | GLU  | O-C-N   | 10.32  | 133.06      | 122.12   |
| 2   | B     | 219 | TYR  | N-CA-C  | 10.32  | 125.40      | 113.01   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | S     | 153 | VAL  | CA-C-O | -10.32 | 109.91      | 120.85   |
| 1   | A     | 141 | VAL  | O-C-N  | 10.32  | 132.63      | 121.90   |
| 2   | B     | 548 | ILE  | CA-C-O | -10.32 | 109.53      | 120.57   |
| 2   | B     | 604 | GLU  | CA-C-N | 10.32  | 133.85      | 120.44   |
| 2   | B     | 604 | GLU  | C-N-CA | 10.32  | 133.85      | 120.44   |
| 4   | S     | 62  | GLU  | N-CA-C | 10.32  | 132.77      | 110.80   |
| 3   | M     | 92  | PHE  | O-C-N  | 10.31  | 136.15      | 122.33   |
| 1   | A     | 465 | SER  | CA-C-O | 10.31  | 132.79      | 121.56   |
| 1   | A     | 517 | TRP  | CA-C-O | -10.31 | 110.08      | 120.70   |
| 2   | B     | 426 | GLU  | CA-C-O | -10.30 | 109.63      | 120.55   |
| 2   | B     | 361 | GLN  | CA-C-O | -10.30 | 110.09      | 120.70   |
| 1   | A     | 476 | GLN  | O-C-N  | 10.30  | 133.89      | 122.15   |
| 2   | B     | 340 | ILE  | CA-C-O | -10.30 | 109.23      | 121.18   |
| 1   | A     | 400 | VAL  | O-C-N  | 10.29  | 132.43      | 121.83   |
| 2   | B     | 523 | PHE  | O-C-N  | -10.29 | 108.90      | 122.59   |
| 2   | B     | 552 | SER  | CA-C-O | -10.29 | 109.64      | 120.55   |
| 2   | B     | 605 | PHE  | O-C-N  | 10.29  | 132.67      | 122.07   |
| 3   | M     | 429 | ASP  | CA-C-N | -10.28 | 106.56      | 120.95   |
| 3   | M     | 429 | ASP  | C-N-CA | -10.28 | 106.56      | 120.95   |
| 3   | M     | 425 | THR  | N-CA-C | -10.27 | 92.91       | 109.76   |
| 2   | B     | 354 | GLY  | N-CA-C | -10.27 | 99.79       | 113.24   |
| 4   | S     | 30  | LEU  | O-C-N  | 10.26  | 133.85      | 122.15   |
| 2   | B     | 364 | HIS  | CA-C-O | -10.26 | 110.03      | 120.80   |
| 3   | M     | 56  | VAL  | CA-C-O | -10.26 | 110.60      | 121.27   |
| 2   | B     | 127 | LEU  | N-CA-C | -10.26 | 99.31       | 112.23   |
| 1   | A     | 428 | MET  | O-C-N  | 10.26  | 132.63      | 122.07   |
| 2   | B     | 509 | ALA  | CA-C-O | -10.25 | 110.14      | 120.70   |
| 2   | B     | 595 | VAL  | O-C-N  | 10.25  | 132.56      | 121.90   |
| 1   | A     | 166 | LEU  | CA-C-O | -10.25 | 109.69      | 120.55   |
| 2   | B     | 337 | THR  | O-C-N  | 10.24  | 132.62      | 122.07   |
| 4   | S     | 28  | GLN  | O-C-N  | 10.24  | 134.86      | 122.27   |
| 2   | B     | 66  | ILE  | CA-C-O | -10.23 | 110.31      | 120.95   |
| 1   | A     | 398 | GLU  | N-CA-C | 10.23  | 125.30      | 113.02   |
| 2   | B     | 137 | PHE  | O-C-N  | 10.23  | 132.97      | 122.12   |
| 2   | B     | 151 | ALA  | O-C-N  | 10.23  | 133.08      | 121.32   |
| 3   | M     | 306 | LEU  | CA-C-N | -10.23 | 107.14      | 120.44   |
| 3   | M     | 306 | LEU  | C-N-CA | -10.23 | 107.14      | 120.44   |
| 1   | A     | 256 | LEU  | O-C-N  | 10.23  | 134.19      | 122.22   |
| 1   | A     | 611 | LEU  | O-C-N  | 10.22  | 133.13      | 122.09   |
| 2   | B     | 322 | CYS  | CA-C-O | -10.22 | 108.21      | 119.97   |
| 3   | M     | 125 | PHE  | O-C-N  | 10.22  | 132.96      | 122.12   |
| 1   | A     | 334 | SER  | CA-C-O | -10.22 | 110.17      | 120.70   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 556 | VAL  | O-C-N  | 10.22  | 133.35      | 121.80   |
| 2   | B     | 102 | HIS  | CA-C-N | -10.21 | 105.80      | 120.29   |
| 2   | B     | 102 | HIS  | C-N-CA | -10.21 | 105.80      | 120.29   |
| 1   | A     | 309 | PHE  | O-C-N  | 10.20  | 132.58      | 122.07   |
| 1   | A     | 613 | ALA  | CA-C-O | -10.20 | 109.74      | 120.55   |
| 2   | B     | 185 | LYS  | O-C-N  | -10.20 | 111.31      | 122.12   |
| 2   | B     | 454 | LEU  | CA-C-O | -10.20 | 110.19      | 120.70   |
| 4   | S     | 108 | SER  | CA-C-O | -10.19 | 109.61      | 120.42   |
| 2   | B     | 46  | GLN  | O-C-N  | 10.18  | 134.80      | 122.27   |
| 1   | A     | 117 | ASP  | CA-C-O | -10.18 | 109.69      | 120.58   |
| 1   | A     | 335 | CYS  | O-C-N  | 10.18  | 132.55      | 122.07   |
| 2   | B     | 320 | SER  | CA-C-O | -10.18 | 109.76      | 120.55   |
| 1   | A     | 257 | LEU  | O-C-N  | 10.17  | 133.75      | 122.15   |
| 2   | B     | 431 | MET  | CA-C-O | -10.17 | 110.14      | 120.82   |
| 4   | S     | 36  | TYR  | CA-C-O | -10.17 | 109.64      | 120.42   |
| 4   | S     | 78  | LYS  | CA-C-O | 10.17  | 131.61      | 120.32   |
| 1   | A     | 233 | PHE  | N-CA-C | -10.17 | 101.19      | 114.31   |
| 1   | A     | 527 | GLU  | CA-C-N | 10.17  | 140.72      | 122.62   |
| 1   | A     | 527 | GLU  | C-N-CA | 10.17  | 140.72      | 122.62   |
| 1   | A     | 604 | LEU  | O-C-N  | 10.17  | 132.67      | 122.09   |
| 3   | M     | 94  | GLU  | O-C-N  | 10.17  | 133.07      | 122.09   |
| 1   | A     | 90  | HIS  | CA-C-O | -10.17 | 109.64      | 120.42   |
| 1   | A     | 608 | ARG  | O-C-N  | 10.15  | 133.78      | 122.20   |
| 1   | A     | 559 | PHE  | CA-C-O | -10.15 | 108.83      | 120.20   |
| 2   | B     | 375 | LEU  | CA-C-O | 10.15  | 128.68      | 118.73   |
| 2   | B     | 341 | GLU  | O-C-N  | 10.15  | 132.88      | 122.12   |
| 1   | A     | 214 | VAL  | O-C-N  | 10.14  | 132.27      | 121.83   |
| 1   | A     | 560 | SER  | CA-C-O | -10.14 | 109.67      | 120.42   |
| 1   | A     | 333 | ILE  | O-C-N  | 10.14  | 131.70      | 121.87   |
| 2   | B     | 153 | ILE  | O-C-N  | 10.14  | 135.24      | 122.57   |
| 2   | B     | 455 | ILE  | CA-C-O | -10.13 | 110.43      | 121.17   |
| 1   | A     | 609 | LEU  | CA-C-O | -10.13 | 110.27      | 120.70   |
| 2   | B     | 43  | ASN  | O-C-N  | 10.13  | 132.97      | 121.32   |
| 1   | A     | 384 | LEU  | CA-C-O | -10.13 | 110.27      | 120.70   |
| 2   | B     | 126 | SER  | CA-C-O | 10.13  | 131.54      | 120.10   |
| 1   | A     | 425 | LYS  | CA-C-O | -10.12 | 110.27      | 120.70   |
| 2   | B     | 251 | LEU  | CA-C-O | -10.12 | 110.27      | 120.70   |
| 1   | A     | 309 | PHE  | CA-C-O | -10.12 | 110.19      | 120.82   |
| 2   | B     | 512 | VAL  | O-C-N  | 10.12  | 132.42      | 121.90   |
| 2   | B     | 471 | TYR  | CA-C-O | -10.11 | 110.08      | 120.90   |
| 4   | S     | 99  | LEU  | O-C-N  | 10.11  | 133.68      | 122.15   |
| 2   | B     | 290 | SER  | N-CA-C | 10.11  | 125.76      | 113.23   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 544 | THR  | O-C-N  | 10.11  | 133.67      | 122.15   |
| 1   | A     | 548 | GLN  | CA-C-O | -10.11 | 109.84      | 120.55   |
| 1   | A     | 331 | ARG  | O-C-N  | 10.10  | 132.94      | 122.03   |
| 1   | A     | 577 | VAL  | O-C-N  | 10.10  | 132.24      | 121.83   |
| 3   | M     | 110 | SER  | CA-C-O | -10.10 | 109.80      | 121.72   |
| 3   | M     | 372 | ILE  | N-CA-C | 10.09  | 117.01      | 106.21   |
| 4   | S     | 16  | LEU  | CA-C-O | 10.09  | 132.71      | 120.60   |
| 2   | B     | 594 | ALA  | O-C-N  | 10.09  | 133.65      | 122.15   |
| 2   | B     | 230 | PHE  | N-CA-C | -10.08 | 100.08      | 112.38   |
| 2   | B     | 546 | CYS  | CA-C-O | -10.08 | 110.24      | 120.82   |
| 2   | B     | 343 | LEU  | O-C-N  | 10.07  | 132.45      | 122.07   |
| 3   | M     | 87  | LEU  | CA-C-O | -10.07 | 109.87      | 120.55   |
| 1   | A     | 200 | PHE  | O-C-N  | 10.07  | 132.80      | 122.12   |
| 1   | A     | 303 | MET  | N-CA-C | -10.07 | 99.31       | 111.69   |
| 1   | A     | 578 | LEU  | O-C-N  | 10.07  | 132.79      | 122.12   |
| 1   | A     | 68  | THR  | O-C-N  | 10.06  | 132.78      | 122.12   |
| 2   | B     | 611 | ALA  | O-C-N  | 10.06  | 133.99      | 122.22   |
| 1   | A     | 543 | TYR  | N-CA-C | 10.05  | 126.31      | 110.32   |
| 2   | B     | 54  | ARG  | N-CA-C | 10.05  | 125.16      | 113.19   |
| 1   | A     | 244 | LEU  | CA-C-O | 10.05  | 131.45      | 120.20   |
| 1   | A     | 110 | ALA  | CA-C-O | 10.05  | 131.20      | 120.55   |
| 1   | A     | 186 | PHE  | O-C-N  | 10.04  | 132.88      | 122.03   |
| 4   | S     | 74  | GLN  | CA-C-O | 10.04  | 131.94      | 120.80   |
| 4   | S     | 37  | GLU  | O-C-N  | 10.04  | 132.93      | 122.09   |
| 2   | B     | 306 | LEU  | O-C-N  | 10.03  | 132.75      | 122.12   |
| 1   | A     | 477 | PHE  | O-C-N  | 10.03  | 133.59      | 122.15   |
| 2   | B     | 608 | ARG  | CA-C-O | -10.03 | 110.37      | 120.70   |
| 1   | A     | 438 | ALA  | N-CA-C | 10.02  | 124.76      | 110.23   |
| 1   | A     | 431 | VAL  | CA-C-O | -10.02 | 109.93      | 121.05   |
| 2   | B     | 302 | PHE  | O-C-N  | 10.02  | 132.91      | 122.09   |
| 1   | A     | 579 | LYS  | O-C-N  | 10.02  | 132.74      | 122.12   |
| 4   | S     | 137 | GLN  | CA-C-O | 10.01  | 131.87      | 120.96   |
| 1   | A     | 225 | LEU  | O-C-N  | 10.01  | 133.93      | 122.22   |
| 1   | A     | 385 | LYS  | O-C-N  | 10.00  | 132.72      | 122.12   |
| 2   | B     | 296 | ASP  | O-C-N  | 10.00  | 132.82      | 121.32   |
| 1   | A     | 142 | LYS  | CA-C-O | -10.00 | 109.83      | 120.63   |
| 1   | A     | 613 | ALA  | O-C-N  | 10.00  | 132.72      | 122.12   |
| 2   | B     | 393 | ILE  | CA-C-O | -10.00 | 110.01      | 120.71   |
| 3   | M     | 307 | SER  | CA-C-O | -9.99  | 110.33      | 120.82   |
| 3   | M     | 296 | LYS  | CA-C-N | -9.99  | 107.96      | 122.94   |
| 3   | M     | 296 | LYS  | C-N-CA | -9.99  | 107.96      | 122.94   |
| 2   | B     | 571 | SER  | CA-C-O | -9.98  | 110.68      | 121.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 426 | ILE  | O-C-N  | 9.98  | 131.55      | 121.87   |
| 1   | A     | 462 | GLN  | CA-C-N | -9.98 | 105.15      | 120.31   |
| 1   | A     | 462 | GLN  | C-N-CA | -9.98 | 105.15      | 120.31   |
| 3   | M     | 379 | LEU  | CA-C-O | 9.97  | 131.13      | 120.36   |
| 2   | B     | 116 | THR  | O-C-N  | 9.97  | 132.69      | 122.12   |
| 3   | M     | 81  | SER  | O-C-N  | -9.96 | 109.34      | 122.59   |
| 3   | M     | 424 | PHE  | N-CA-C | -9.96 | 92.92       | 109.46   |
| 1   | A     | 497 | LYS  | CA-C-O | -9.96 | 109.99      | 120.55   |
| 1   | A     | 465 | SER  | O-C-N  | 9.96  | 134.61      | 122.86   |
| 2   | B     | 362 | ALA  | CA-C-O | -9.95 | 109.88      | 120.63   |
| 1   | A     | 140 | VAL  | O-C-N  | -9.95 | 111.58      | 121.83   |
| 1   | A     | 163 | ALA  | CA-C-O | 9.95  | 131.10      | 120.55   |
| 2   | B     | 396 | ILE  | CA-C-O | -9.95 | 110.06      | 120.71   |
| 2   | B     | 451 | MET  | O-C-N  | 9.95  | 132.32      | 122.07   |
| 2   | B     | 305 | SER  | O-C-N  | 9.95  | 132.83      | 122.09   |
| 4   | S     | 158 | LYS  | O-C-N  | 9.95  | 135.66      | 122.33   |
| 1   | A     | 610 | SER  | O-C-N  | 9.95  | 133.54      | 122.20   |
| 3   | M     | 90  | PHE  | CA-C-O | -9.94 | 109.20      | 120.24   |
| 2   | B     | 350 | THR  | N-CA-C | 9.94  | 124.87      | 109.96   |
| 4   | S     | 18  | LYS  | CA-C-O | 9.94  | 131.25      | 120.71   |
| 1   | A     | 490 | VAL  | O-C-N  | 9.94  | 132.06      | 121.83   |
| 2   | B     | 360 | LEU  | CA-C-O | -9.94 | 108.87      | 120.10   |
| 2   | B     | 222 | HIS  | N-CA-C | 9.93  | 125.18      | 109.39   |
| 1   | A     | 426 | ILE  | CA-C-O | -9.92 | 110.63      | 120.95   |
| 2   | B     | 184 | GLY  | CA-C-N | 9.91  | 133.56      | 120.28   |
| 2   | B     | 184 | GLY  | C-N-CA | 9.91  | 133.56      | 120.28   |
| 1   | A     | 353 | ASP  | O-C-N  | 9.91  | 132.63      | 122.12   |
| 2   | B     | 63  | MET  | CA-C-O | -9.91 | 109.24      | 120.24   |
| 1   | A     | 538 | GLU  | CA-C-N | -9.90 | 106.81      | 122.65   |
| 1   | A     | 538 | GLU  | C-N-CA | -9.90 | 106.81      | 122.65   |
| 1   | A     | 558 | VAL  | CA-C-O | -9.90 | 108.08      | 121.15   |
| 2   | B     | 593 | ASN  | O-C-N  | 9.89  | 132.61      | 122.12   |
| 2   | B     | 64  | LYS  | O-C-N  | 9.89  | 132.25      | 122.07   |
| 3   | M     | 381 | ASN  | N-CA-C | -9.89 | 94.81       | 110.14   |
| 2   | B     | 317 | VAL  | O-C-N  | 9.88  | 135.00      | 122.05   |
| 1   | A     | 186 | PHE  | CA-C-O | -9.88 | 110.72      | 120.90   |
| 1   | A     | 511 | VAL  | CA-C-O | -9.88 | 110.67      | 120.95   |
| 2   | B     | 342 | ALA  | CA-C-O | -9.88 | 110.08      | 120.55   |
| 1   | A     | 392 | MET  | O-C-N  | 9.88  | 133.41      | 122.15   |
| 1   | A     | 479 | ASN  | CA-C-O | -9.88 | 110.08      | 120.55   |
| 3   | M     | 277 | GLU  | O-C-N  | -9.88 | 111.64      | 123.29   |
| 4   | S     | 127 | THR  | CA-C-O | -9.88 | 109.95      | 120.42   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | M     | 128 | CYS  | CA-C-N | -9.87 | 104.45      | 120.64   |
| 3   | M     | 128 | CYS  | C-N-CA | -9.87 | 104.45      | 120.64   |
| 4   | S     | 146 | VAL  | CA-C-O | -9.87 | 109.88      | 120.64   |
| 2   | B     | 112 | ASP  | CA-C-O | -9.87 | 109.33      | 119.49   |
| 1   | A     | 316 | LEU  | O-C-N  | 9.86  | 132.74      | 122.09   |
| 3   | M     | 75  | TRP  | O-C-N  | -9.86 | 110.68      | 123.21   |
| 2   | B     | 142 | LEU  | CA-C-N | -9.85 | 103.39      | 121.52   |
| 2   | B     | 142 | LEU  | C-N-CA | -9.85 | 103.39      | 121.52   |
| 2   | B     | 468 | LEU  | O-C-N  | 9.85  | 132.56      | 122.12   |
| 1   | A     | 156 | PRO  | O-C-N  | -9.85 | 110.25      | 122.17   |
| 1   | A     | 519 | LEU  | O-C-N  | -9.84 | 110.70      | 122.22   |
| 2   | B     | 515 | PHE  | O-C-N  | -9.84 | 110.70      | 122.22   |
| 2   | B     | 596 | LEU  | O-C-N  | 9.84  | 132.21      | 122.07   |
| 2   | B     | 514 | LEU  | CA-C-O | -9.83 | 109.91      | 120.92   |
| 4   | S     | 4   | ALA  | O-C-N  | -9.83 | 112.47      | 123.48   |
| 2   | B     | 139 | LEU  | CA-C-O | -9.82 | 107.30      | 119.38   |
| 2   | B     | 471 | TYR  | O-C-N  | 9.82  | 132.31      | 122.09   |
| 1   | A     | 281 | LEU  | O-C-N  | -9.82 | 110.19      | 122.27   |
| 1   | A     | 455 | MET  | CA-C-O | -9.81 | 110.15      | 120.55   |
| 2   | B     | 342 | ALA  | O-C-N  | 9.81  | 132.52      | 122.12   |
| 3   | M     | 110 | SER  | O-C-N  | 9.81  | 133.93      | 122.94   |
| 4   | S     | 167 | ILE  | CA-C-N | -9.81 | 104.05      | 121.70   |
| 4   | S     | 167 | ILE  | C-N-CA | -9.81 | 104.05      | 121.70   |
| 1   | A     | 551 | LEU  | O-C-N  | 9.81  | 132.51      | 122.12   |
| 2   | B     | 357 | GLU  | CA-C-O | -9.80 | 110.16      | 120.55   |
| 4   | S     | 157 | ASN  | O-C-N  | 9.80  | 133.69      | 122.22   |
| 1   | A     | 295 | VAL  | O-C-N  | 9.80  | 132.43      | 121.94   |
| 1   | A     | 473 | ILE  | CA-C-O | -9.80 | 110.46      | 120.85   |
| 2   | B     | 56  | SER  | O-C-N  | -9.80 | 109.65      | 122.39   |
| 3   | M     | 458 | LEU  | CA-C-N | 9.80  | 139.28      | 122.81   |
| 3   | M     | 458 | LEU  | C-N-CA | 9.80  | 139.28      | 122.81   |
| 2   | B     | 233 | TYR  | CA-C-O | -9.80 | 110.61      | 120.70   |
| 3   | M     | 335 | SER  | O-C-N  | 9.80  | 135.89      | 123.15   |
| 1   | A     | 67  | LYS  | CA-C-O | -9.80 | 110.17      | 120.55   |
| 2   | B     | 157 | THR  | O-C-N  | 9.80  | 132.61      | 122.03   |
| 2   | B     | 250 | GLU  | CA-C-O | -9.79 | 110.17      | 120.55   |
| 2   | B     | 437 | SER  | O-C-N  | 9.80  | 132.67      | 122.09   |
| 2   | B     | 351 | GLU  | CA-C-O | 9.79  | 131.34      | 119.79   |
| 2   | B     | 425 | PRO  | CA-C-O | -9.79 | 109.71      | 121.95   |
| 2   | B     | 546 | CYS  | O-C-N  | 9.79  | 132.16      | 122.07   |
| 1   | A     | 478 | ARG  | CA-C-O | -9.79 | 110.18      | 120.55   |
| 2   | B     | 476 | ARG  | CA-C-O | -9.79 | 110.04      | 120.42   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 552 | ILE  | CA-C-O | -9.78 | 110.77      | 120.95   |
| 1   | A     | 258 | LYS  | O-C-N  | 9.78  | 132.49      | 122.12   |
| 2   | B     | 437 | SER  | CA-C-O | -9.78 | 110.63      | 120.70   |
| 3   | M     | 290 | PHE  | N-CA-C | -9.77 | 94.08       | 109.23   |
| 4   | S     | 158 | LYS  | CA-C-O | -9.77 | 108.26      | 119.79   |
| 1   | A     | 386 | ALA  | O-C-N  | 9.77  | 133.28      | 122.15   |
| 2   | B     | 233 | TYR  | O-C-N  | 9.77  | 132.64      | 122.09   |
| 2   | B     | 615 | SER  | O-C-N  | 9.77  | 132.64      | 122.09   |
| 2   | B     | 394 | TRP  | CA-C-O | -9.76 | 110.07      | 120.42   |
| 3   | M     | 265 | ASN  | N-CA-C | -9.76 | 90.57       | 108.24   |
| 2   | B     | 138 | ALA  | O-C-N  | 9.76  | 132.47      | 122.12   |
| 1   | A     | 390 | THR  | O-C-N  | 9.75  | 132.46      | 122.12   |
| 2   | B     | 190 | GLU  | O-C-N  | 9.75  | 132.46      | 122.12   |
| 1   | A     | 265 | GLN  | O-C-N  | -9.75 | 112.11      | 123.22   |
| 1   | A     | 348 | PHE  | O-C-N  | 9.75  | 133.62      | 122.22   |
| 2   | B     | 48  | VAL  | O-C-N  | 9.74  | 131.98      | 121.94   |
| 3   | M     | 282 | VAL  | CA-C-N | -9.73 | 109.29      | 122.72   |
| 3   | M     | 282 | VAL  | C-N-CA | -9.73 | 109.29      | 122.72   |
| 1   | A     | 77  | LEU  | CA-C-O | -9.73 | 110.11      | 120.42   |
| 1   | A     | 106 | GLY  | CA-C-O | -9.72 | 110.50      | 121.00   |
| 3   | M     | 406 | GLY  | N-CA-C | -9.72 | 90.14       | 113.18   |
| 1   | A     | 437 | SER  | N-CA-C | 9.72  | 125.14      | 113.28   |
| 1   | A     | 599 | ARG  | CA-C-O | -9.72 | 110.12      | 120.42   |
| 2   | B     | 436 | LEU  | CA-C-O | -9.72 | 108.14      | 119.61   |
| 4   | S     | 5   | VAL  | CA-C-O | 9.71  | 130.59      | 120.39   |
| 1   | A     | 427 | LYS  | CA-C-O | -9.71 | 110.26      | 120.55   |
| 2   | B     | 216 | LYS  | CA-C-O | 9.70  | 131.23      | 119.49   |
| 1   | A     | 554 | ALA  | CA-C-O | -9.70 | 110.64      | 120.82   |
| 2   | B     | 355 | ASN  | O-C-N  | 9.70  | 133.90      | 122.17   |
| 1   | A     | 223 | CYS  | CA-C-O | -9.70 | 110.71      | 120.70   |
| 2   | B     | 193 | LEU  | O-C-N  | 9.69  | 132.85      | 122.38   |
| 4   | S     | 129 | GLU  | CA-C-O | -9.70 | 110.14      | 120.42   |
| 2   | B     | 429 | VAL  | O-C-N  | 9.69  | 132.75      | 121.80   |
| 1   | A     | 391 | LEU  | O-C-N  | -9.69 | 111.11      | 122.15   |
| 1   | A     | 581 | LEU  | O-C-N  | 9.69  | 133.55      | 122.22   |
| 2   | B     | 320 | SER  | O-C-N  | 9.69  | 132.39      | 122.12   |
| 2   | B     | 416 | LYS  | CA-C-O | -9.69 | 110.17      | 120.63   |
| 1   | A     | 102 | GLN  | CA-C-O | -9.67 | 110.30      | 120.55   |
| 2   | B     | 435 | SER  | O-C-N  | 9.66  | 132.47      | 122.03   |
| 3   | M     | 122 | SER  | O-C-N  | 9.66  | 133.16      | 122.15   |
| 3   | M     | 305 | ASP  | CA-C-O | -9.66 | 110.55      | 120.98   |
| 1   | A     | 515 | CYS  | O-C-N  | 9.65  | 133.52      | 122.22   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 325 | LEU  | O-C-N  | -9.65 | 109.50      | 122.43   |
| 1   | A     | 628 | VAL  | CA-C-O | -9.64 | 109.48      | 120.96   |
| 2   | B     | 151 | ALA  | CA-C-O | -9.64 | 106.95      | 120.16   |
| 2   | B     | 250 | GLU  | O-C-N  | 9.64  | 132.34      | 122.12   |
| 1   | A     | 385 | LYS  | CA-C-O | -9.63 | 110.34      | 120.55   |
| 2   | B     | 51  | LEU  | CA-C-N | -9.63 | 102.68      | 121.94   |
| 2   | B     | 51  | LEU  | C-N-CA | -9.63 | 102.68      | 121.94   |
| 4   | S     | 116 | VAL  | O-C-N  | 9.63  | 133.66      | 123.26   |
| 1   | A     | 75  | THR  | CA-C-O | -9.63 | 110.71      | 120.82   |
| 1   | A     | 389 | GLN  | O-C-N  | 9.63  | 132.33      | 122.12   |
| 1   | A     | 493 | ALA  | O-C-N  | 9.63  | 132.33      | 122.12   |
| 2   | B     | 132 | SER  | CA-C-O | 9.62  | 131.22      | 119.38   |
| 2   | B     | 247 | TYR  | CA-C-O | -9.62 | 110.72      | 120.82   |
| 2   | B     | 493 | LEU  | CA-C-O | -9.62 | 108.43      | 119.79   |
| 2   | B     | 543 | GLU  | O-C-N  | 9.63  | 132.32      | 122.12   |
| 1   | A     | 139 | ASP  | O-C-N  | 9.62  | 133.12      | 122.15   |
| 1   | A     | 142 | LYS  | O-C-N  | 9.62  | 132.32      | 122.12   |
| 1   | A     | 356 | ILE  | O-C-N  | 9.62  | 131.91      | 121.90   |
| 3   | M     | 104 | PHE  | O-C-N  | -9.62 | 109.79      | 122.59   |
| 2   | B     | 210 | CYS  | CA-C-O | -9.62 | 109.56      | 120.24   |
| 2   | B     | 444 | THR  | N-CA-C | 9.62  | 121.84      | 111.36   |
| 1   | A     | 339 | TYR  | O-C-N  | 9.62  | 132.37      | 122.08   |
| 1   | A     | 275 | LEU  | O-C-N  | -9.61 | 110.27      | 121.32   |
| 1   | A     | 381 | GLU  | O-C-N  | -9.61 | 111.19      | 122.15   |
| 1   | A     | 156 | PRO  | CA-C-N | -9.61 | 104.67      | 120.71   |
| 1   | A     | 156 | PRO  | C-N-CA | -9.61 | 104.67      | 120.71   |
| 2   | B     | 469 | ASP  | O-C-N  | 9.60  | 132.30      | 122.12   |
| 2   | B     | 549 | LEU  | CA-C-O | -9.60 | 110.72      | 120.80   |
| 1   | A     | 222 | ILE  | O-C-N  | 9.60  | 131.56      | 121.87   |
| 2   | B     | 247 | TYR  | O-C-N  | 9.59  | 131.95      | 122.07   |
| 1   | A     | 121 | LEU  | O-C-N  | 9.59  | 132.29      | 122.12   |
| 2   | B     | 560 | ILE  | O-C-N  | -9.58 | 110.59      | 122.57   |
| 1   | A     | 130 | LYS  | O-C-N  | 9.58  | 132.27      | 122.12   |
| 1   | A     | 184 | ALA  | CA-C-O | -9.57 | 110.77      | 120.82   |
| 1   | A     | 513 | ARG  | O-C-N  | 9.57  | 132.27      | 122.12   |
| 1   | A     | 254 | ILE  | O-C-N  | 9.57  | 131.51      | 121.94   |
| 1   | A     | 633 | PHE  | O-C-N  | 9.57  | 132.26      | 122.12   |
| 2   | B     | 507 | ALA  | CA-C-O | -9.56 | 110.78      | 120.82   |
| 1   | A     | 155 | THR  | O-C-N  | 9.56  | 132.24      | 121.53   |
| 2   | B     | 142 | LEU  | O-C-N  | -9.56 | 109.90      | 122.33   |
| 4   | S     | 8   | PHE  | O-C-N  | -9.56 | 110.76      | 123.19   |
| 1   | A     | 106 | GLY  | O-C-N  | 9.56  | 131.35      | 122.18   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 137 | ASN  | CA-C-N | -9.55 | 107.83      | 122.16   |
| 1   | A     | 137 | ASN  | C-N-CA | -9.55 | 107.83      | 122.16   |
| 2   | B     | 314 | ASN  | CA-C-N | 9.55  | 130.55      | 119.47   |
| 2   | B     | 314 | ASN  | C-N-CA | 9.55  | 130.55      | 119.47   |
| 2   | B     | 528 | ASP  | O-C-N  | 9.55  | 135.13      | 122.33   |
| 2   | B     | 545 | ARG  | CA-C-O | -9.54 | 110.30      | 120.42   |
| 2   | B     | 547 | GLN  | CA-C-O | -9.54 | 110.44      | 120.55   |
| 1   | A     | 355 | LEU  | O-C-N  | 9.54  | 134.00      | 122.27   |
| 2   | B     | 553 | ALA  | CA-C-O | -9.54 | 110.87      | 120.70   |
| 4   | S     | 161 | GLU  | O-C-N  | -9.54 | 109.30      | 122.46   |
| 1   | A     | 312 | ALA  | O-C-N  | 9.54  | 132.23      | 122.12   |
| 1   | A     | 424 | TYR  | O-C-N  | 9.54  | 135.90      | 122.36   |
| 2   | B     | 450 | VAL  | CA-C-O | -9.54 | 109.61      | 120.96   |
| 1   | A     | 94  | VAL  | CA-C-O | 9.53  | 130.96      | 120.85   |
| 2   | B     | 488 | ARG  | O-C-N  | 9.53  | 134.62      | 122.23   |
| 4   | S     | 16  | LEU  | O-C-N  | -9.53 | 111.80      | 123.33   |
| 1   | A     | 122 | MET  | CA-C-O | -9.52 | 110.46      | 120.55   |
| 1   | A     | 138 | ASN  | O-C-N  | 9.52  | 133.78      | 122.46   |
| 2   | B     | 609 | ASP  | CA-C-O | -9.52 | 110.46      | 120.55   |
| 3   | M     | 18  | TYR  | CA-C-O | 9.51  | 132.01      | 120.60   |
| 1   | A     | 147 | LEU  | CA-C-O | -9.51 | 110.34      | 120.42   |
| 2   | B     | 97  | VAL  | CA-C-O | -9.51 | 110.15      | 121.18   |
| 1   | A     | 128 | LEU  | O-C-N  | 9.51  | 133.34      | 122.22   |
| 1   | A     | 471 | SER  | O-C-N  | 9.51  | 132.99      | 122.15   |
| 3   | M     | 55  | MET  | CA-C-O | -9.50 | 110.09      | 122.45   |
| 1   | A     | 100 | LEU  | N-CA-C | -9.50 | 100.92      | 111.28   |
| 3   | M     | 59  | ASP  | CA-C-O | -9.50 | 108.58      | 119.79   |
| 1   | A     | 308 | ASP  | CA-C-N | 9.50  | 132.79      | 120.44   |
| 1   | A     | 308 | ASP  | C-N-CA | 9.50  | 132.79      | 120.44   |
| 2   | B     | 205 | PRO  | O-C-N  | -9.50 | 109.51      | 122.24   |
| 2   | B     | 178 | ILE  | CA-C-O | -9.50 | 108.91      | 120.78   |
| 2   | B     | 530 | LEU  | CA-C-O | -9.50 | 109.37      | 120.10   |
| 3   | M     | 61  | GLU  | O-C-N  | 9.49  | 134.04      | 123.22   |
| 1   | A     | 108 | LEU  | O-C-N  | 9.49  | 132.18      | 122.12   |
| 2   | B     | 358 | MET  | O-C-N  | 9.49  | 132.18      | 122.12   |
| 2   | B     | 586 | SER  | O-C-N  | 9.48  | 131.95      | 122.09   |
| 2   | B     | 223 | LEU  | CA-C-O | 9.48  | 131.04      | 119.38   |
| 3   | M     | 227 | GLU  | CA-C-O | 9.48  | 130.44      | 120.30   |
| 2   | B     | 572 | GLU  | O-C-N  | 9.48  | 133.93      | 122.27   |
| 2   | B     | 411 | ILE  | O-C-N  | 9.47  | 133.50      | 121.94   |
| 2   | B     | 132 | SER  | O-C-N  | -9.47 | 109.74      | 122.43   |
| 2   | B     | 371 | GLN  | N-CA-C | 9.46  | 121.67      | 111.36   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | S     | 43  | ASN  | CA-C-N  | -9.46 | 106.66      | 120.28   |
| 4   | S     | 43  | ASN  | C-N-CA  | -9.46 | 106.66      | 120.28   |
| 2   | B     | 245 | GLN  | CA-C-O  | -9.46 | 108.46      | 120.00   |
| 3   | M     | 385 | ARG  | CA-C-O  | 9.46  | 131.95      | 120.60   |
| 4   | S     | 156 | LEU  | O-C-N   | 9.46  | 132.93      | 122.15   |
| 1   | A     | 370 | LYS  | CA-C-O  | -9.45 | 109.10      | 119.97   |
| 2   | B     | 303 | LEU  | O-C-N   | 9.45  | 131.81      | 122.07   |
| 2   | B     | 468 | LEU  | CA-C-O  | -9.45 | 110.53      | 120.55   |
| 1   | A     | 75  | THR  | O-C-N   | 9.45  | 131.80      | 122.07   |
| 1   | A     | 584 | PHE  | O-C-N   | 9.45  | 132.13      | 122.12   |
| 1   | A     | 574 | ILE  | CA-C-O  | -9.44 | 111.13      | 120.95   |
| 1   | A     | 425 | LYS  | O-C-N   | 9.44  | 132.28      | 122.09   |
| 2   | B     | 134 | LEU  | O-C-N   | 9.44  | 133.59      | 122.17   |
| 4   | S     | 103 | GLN  | CA-C-O  | -9.43 | 109.12      | 119.97   |
| 2   | B     | 345 | ARG  | CA-C-O  | -9.43 | 110.56      | 120.55   |
| 2   | B     | 477 | MET  | CA-C-O  | -9.43 | 110.99      | 120.70   |
| 2   | B     | 391 | ALA  | O-C-N   | 9.43  | 131.78      | 122.07   |
| 3   | M     | 430 | LEU  | CA-C-N  | -9.43 | 113.04      | 123.13   |
| 3   | M     | 430 | LEU  | C-N-CA  | -9.43 | 113.04      | 123.13   |
| 1   | A     | 253 | ILE  | O-C-N   | 9.42  | 131.70      | 121.90   |
| 1   | A     | 178 | ARG  | CA-C-O  | -9.41 | 110.57      | 120.55   |
| 1   | A     | 122 | MET  | O-C-N   | 9.41  | 132.09      | 122.12   |
| 1   | A     | 451 | ASN  | O-C-N   | 9.41  | 133.22      | 122.22   |
| 2   | B     | 465 | ALA  | CA-C-O  | -9.40 | 110.59      | 120.55   |
| 4   | S     | 27  | LYS  | O-C-N   | 9.40  | 134.93      | 122.33   |
| 1   | A     | 336 | ILE  | CA-C-O  | -9.40 | 111.21      | 121.17   |
| 3   | M     | 308 | SER  | CA-C-O  | -9.40 | 110.46      | 120.42   |
| 4   | S     | 29  | LYS  | CA-C-O  | -9.40 | 109.81      | 120.24   |
| 2   | B     | 123 | LEU  | O-C-N   | 9.39  | 133.21      | 122.22   |
| 2   | B     | 500 | GLN  | N-CA-C  | 9.39  | 124.87      | 108.52   |
| 2   | B     | 324 | ALA  | O-C-N   | 9.39  | 133.82      | 122.27   |
| 2   | B     | 119 | SER  | CA-C-O  | -9.39 | 109.49      | 120.10   |
| 2   | B     | 584 | SER  | N-CA-CB | -9.39 | 96.26       | 110.16   |
| 4   | S     | 130 | SER  | CA-C-O  | -9.39 | 110.60      | 120.55   |
| 2   | B     | 119 | SER  | O-C-N   | 9.39  | 133.20      | 122.22   |
| 3   | M     | 385 | ARG  | O-C-N   | -9.39 | 111.97      | 123.33   |
| 1   | A     | 369 | SER  | O-C-N   | 9.38  | 132.07      | 122.12   |
| 3   | M     | 136 | VAL  | CA-C-O  | 9.38  | 131.67      | 121.36   |
| 4   | S     | 129 | GLU  | O-C-N   | 9.38  | 132.84      | 122.15   |
| 3   | M     | 6   | TYR  | CA-C-O  | 9.37  | 132.40      | 121.44   |
| 2   | B     | 73  | ASP  | CA-C-N  | -9.37 | 108.03      | 121.99   |
| 2   | B     | 73  | ASP  | C-N-CA  | -9.37 | 108.03      | 121.99   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 553 | ALA  | O-C-N  | 9.37  | 132.20      | 122.09   |
| 1   | A     | 383 | ASN  | O-C-N  | 9.36  | 133.78      | 122.27   |
| 1   | A     | 479 | ASN  | O-C-N  | 9.36  | 132.04      | 122.12   |
| 1   | A     | 491 | THR  | O-C-N  | 9.36  | 132.20      | 122.09   |
| 3   | M     | 99  | ILE  | CA-C-O | -9.36 | 108.24      | 119.85   |
| 3   | M     | 321 | GLY  | CA-C-N | -9.36 | 107.01      | 122.17   |
| 3   | M     | 321 | GLY  | C-N-CA | -9.36 | 107.01      | 122.17   |
| 1   | A     | 293 | GLU  | O-C-N  | 9.35  | 131.70      | 122.07   |
| 1   | A     | 159 | ALA  | O-C-N  | 9.35  | 132.86      | 122.20   |
| 2   | B     | 211 | ALA  | CA-C-O | -9.35 | 108.18      | 119.49   |
| 1   | A     | 147 | LEU  | O-C-N  | 9.34  | 132.80      | 122.15   |
| 1   | A     | 501 | ASN  | CA-C-N | 9.34  | 135.55      | 120.60   |
| 1   | A     | 501 | ASN  | C-N-CA | 9.34  | 135.55      | 120.60   |
| 2   | B     | 428 | VAL  | O-C-N  | 9.34  | 134.61      | 121.82   |
| 2   | B     | 399 | LEU  | CA-C-N | -9.34 | 105.13      | 120.72   |
| 2   | B     | 399 | LEU  | C-N-CA | -9.34 | 105.13      | 120.72   |
| 2   | B     | 230 | PHE  | CA-C-O | 9.33  | 130.78      | 119.49   |
| 1   | A     | 202 | LYS  | O-C-N  | 9.32  | 132.78      | 122.15   |
| 1   | A     | 337 | LEU  | CA-C-O | -9.32 | 109.57      | 120.10   |
| 2   | B     | 587 | ARG  | O-C-N  | 9.31  | 132.77      | 122.15   |
| 4   | S     | 13  | GLN  | CA-C-O | 9.31  | 130.04      | 119.61   |
| 1   | A     | 477 | PHE  | CA-C-O | -9.31 | 110.55      | 120.42   |
| 4   | S     | 32  | LEU  | CA-C-O | -9.31 | 107.93      | 119.38   |
| 4   | S     | 157 | ASN  | CA-C-O | -9.31 | 109.58      | 120.10   |
| 2   | B     | 301 | LEU  | O-C-N  | 9.31  | 133.11      | 122.22   |
| 1   | A     | 381 | GLU  | CA-C-O | 9.30  | 130.28      | 120.42   |
| 1   | A     | 123 | LEU  | CA-C-O | -9.30 | 111.12      | 120.70   |
| 1   | A     | 126 | ASN  | CA-C-O | -9.30 | 110.69      | 120.55   |
| 1   | A     | 330 | LEU  | CA-C-O | -9.30 | 109.28      | 119.97   |
| 1   | A     | 92  | LEU  | CA-C-O | -9.30 | 110.69      | 120.55   |
| 3   | M     | 20  | LEU  | CA-C-O | 9.29  | 130.24      | 120.30   |
| 1   | A     | 609 | LEU  | O-C-N  | 9.29  | 132.12      | 122.09   |
| 2   | B     | 612 | ARG  | CA-C-O | -9.29 | 110.61      | 120.55   |
| 2   | B     | 274 | PRO  | CA-C-N | -9.29 | 101.57      | 121.45   |
| 2   | B     | 274 | PRO  | C-N-CA | -9.29 | 101.57      | 121.45   |
| 1   | A     | 217 | ALA  | O-C-N  | 9.29  | 131.96      | 122.12   |
| 1   | A     | 317 | GLU  | O-C-N  | 9.29  | 131.96      | 122.12   |
| 2   | B     | 610 | ARG  | O-C-N  | 9.28  | 132.72      | 122.15   |
| 3   | M     | 458 | LEU  | CA-C-O | -9.27 | 110.35      | 121.66   |
| 4   | S     | 159 | ALA  | O-C-N  | 9.27  | 132.10      | 122.09   |
| 1   | A     | 558 | VAL  | O-C-N  | 9.27  | 133.25      | 121.94   |
| 4   | S     | 154 | ASP  | CA-C-O | -9.27 | 109.31      | 119.97   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 189 | HIS  | N-CA-C | 9.26  | 122.36      | 111.71   |
| 2   | B     | 485 | LYS  | N-CA-C | -9.26 | 100.89      | 113.30   |
| 1   | A     | 375 | VAL  | CA-C-O | 9.26  | 130.68      | 121.05   |
| 2   | B     | 29  | LYS  | CA-C-N | -9.26 | 108.05      | 120.54   |
| 2   | B     | 29  | LYS  | C-N-CA | -9.26 | 108.05      | 120.54   |
| 1   | A     | 315 | CYS  | O-C-N  | 9.25  | 132.70      | 122.15   |
| 1   | A     | 416 | ILE  | N-CA-C | 9.24  | 118.61      | 107.61   |
| 1   | A     | 575 | LYS  | O-C-N  | 9.24  | 131.92      | 122.12   |
| 2   | B     | 236 | ILE  | CA-C-O | -9.24 | 110.79      | 121.05   |
| 2   | B     | 244 | SER  | CA-C-O | -9.24 | 107.03      | 119.05   |
| 2   | B     | 486 | HIS  | CA-C-O | -9.24 | 110.63      | 120.42   |
| 1   | A     | 568 | GLU  | N-CA-C | -9.22 | 100.17      | 111.33   |
| 2   | B     | 395 | LYS  | O-C-N  | 9.22  | 133.01      | 122.22   |
| 3   | M     | 135 | ASN  | CA-C-N | 9.22  | 132.85      | 120.50   |
| 3   | M     | 135 | ASN  | C-N-CA | 9.22  | 132.85      | 120.50   |
| 1   | A     | 199 | ASN  | N-CA-C | 9.22  | 124.59      | 113.16   |
| 1   | A     | 216 | SER  | O-C-N  | 9.21  | 131.89      | 122.12   |
| 1   | A     | 368 | ARG  | O-C-N  | 9.21  | 131.56      | 122.07   |
| 3   | M     | 123 | LEU  | O-C-N  | 9.21  | 133.60      | 122.27   |
| 1   | A     | 612 | GLU  | CA-C-O | -9.21 | 110.79      | 120.55   |
| 1   | A     | 346 | THR  | O-C-N  | -9.20 | 110.43      | 122.39   |
| 2   | B     | 172 | GLU  | CA-C-O | 9.20  | 130.30      | 120.55   |
| 3   | M     | 72  | LEU  | CA-C-N | 9.20  | 141.20      | 124.82   |
| 3   | M     | 72  | LEU  | C-N-CA | 9.20  | 141.20      | 124.82   |
| 2   | B     | 389 | ILE  | CA-C-O | 9.20  | 130.52      | 120.95   |
| 2   | B     | 448 | SER  | O-C-N  | 9.20  | 131.87      | 122.12   |
| 3   | M     | 263 | MET  | CA-C-N | 9.19  | 138.61      | 120.77   |
| 3   | M     | 263 | MET  | C-N-CA | 9.19  | 138.61      | 120.77   |
| 1   | A     | 183 | THR  | CA-C-O | -9.19 | 110.81      | 120.55   |
| 2   | B     | 300 | ASP  | O-C-N  | 9.19  | 131.86      | 122.12   |
| 1   | A     | 474 | GLY  | CA-C-O | -9.19 | 111.29      | 120.75   |
| 1   | A     | 478 | ARG  | O-C-N  | 9.19  | 131.86      | 122.12   |
| 2   | B     | 358 | MET  | CA-C-O | -9.18 | 110.82      | 120.55   |
| 4   | S     | 136 | VAL  | N-CA-C | 9.18  | 121.01      | 111.00   |
| 1   | A     | 124 | ALA  | CA-C-O | -9.18 | 109.73      | 120.10   |
| 2   | B     | 334 | MET  | CA-C-N | 9.18  | 132.58      | 120.28   |
| 2   | B     | 334 | MET  | C-N-CA | 9.18  | 132.58      | 120.28   |
| 1   | A     | 148 | SER  | O-C-N  | 9.17  | 131.84      | 122.12   |
| 2   | B     | 61  | ASP  | CA-C-O | -9.17 | 111.09      | 120.90   |
| 1   | A     | 519 | LEU  | CA-C-O | 9.17  | 130.46      | 120.10   |
| 2   | B     | 426 | GLU  | O-C-N  | 9.17  | 131.84      | 122.12   |
| 1   | A     | 184 | ALA  | O-C-N  | 9.17  | 131.51      | 122.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 292 | TYR  | O-C-N  | 9.17  | 131.51      | 122.07   |
| 2   | B     | 60  | ARG  | O-C-N  | 9.17  | 131.93      | 122.03   |
| 2   | B     | 193 | LEU  | CA-C-O | -9.17 | 110.63      | 120.71   |
| 1   | A     | 230 | PRO  | CA-C-O | -9.16 | 106.08      | 119.18   |
| 1   | A     | 522 | PHE  | O-C-N  | 9.16  | 133.34      | 122.34   |
| 3   | M     | 1   | MET  | CA-C-N | -9.16 | 108.42      | 122.81   |
| 3   | M     | 1   | MET  | C-N-CA | -9.16 | 108.42      | 122.81   |
| 2   | B     | 59  | VAL  | CA-C-O | -9.16 | 110.36      | 120.25   |
| 4   | S     | 84  | TYR  | O-C-N  | -9.16 | 111.32      | 123.23   |
| 1   | A     | 625 | LEU  | O-C-N  | -9.16 | 112.64      | 122.07   |
| 2   | B     | 431 | MET  | O-C-N  | 9.16  | 131.50      | 122.07   |
| 3   | M     | 322 | LEU  | CA-C-N | -9.16 | 110.08      | 122.72   |
| 3   | M     | 322 | LEU  | C-N-CA | -9.16 | 110.08      | 122.72   |
| 4   | S     | 128 | LEU  | O-C-N  | 9.15  | 133.53      | 122.27   |
| 4   | S     | 118 | GLU  | O-C-N  | 9.15  | 134.59      | 122.33   |
| 1   | A     | 371 | ALA  | O-C-N  | 9.15  | 131.97      | 122.09   |
| 1   | A     | 487 | MET  | CA-C-O | 9.14  | 128.15      | 119.00   |
| 2   | B     | 492 | LYS  | CA-C-O | -9.14 | 109.45      | 119.97   |
| 2   | B     | 143 | SER  | CA-C-N | -9.14 | 104.08      | 121.54   |
| 2   | B     | 143 | SER  | C-N-CA | -9.14 | 104.08      | 121.54   |
| 1   | A     | 475 | GLU  | O-C-N  | 9.14  | 132.91      | 122.22   |
| 2   | B     | 117 | LEU  | CA-C-O | -9.14 | 110.74      | 120.42   |
| 1   | A     | 297 | CYS  | O-C-N  | -9.13 | 112.44      | 122.12   |
| 2   | B     | 512 | VAL  | CA-C-O | -9.13 | 110.92      | 121.05   |
| 4   | S     | 115 | GLU  | CA-C-N | -9.13 | 111.18      | 123.14   |
| 4   | S     | 115 | GLU  | C-N-CA | -9.13 | 111.18      | 123.14   |
| 1   | A     | 579 | LYS  | CA-C-O | -9.12 | 110.88      | 120.55   |
| 2   | B     | 319 | LEU  | O-C-N  | 9.12  | 132.55      | 122.15   |
| 1   | A     | 255 | ARG  | O-C-N  | 9.12  | 131.47      | 122.07   |
| 2   | B     | 504 | ALA  | O-C-N  | 9.12  | 134.03      | 122.81   |
| 4   | S     | 132 | LEU  | CA-C-O | -9.12 | 109.48      | 119.97   |
| 4   | S     | 102 | ILE  | CA-C-O | -9.11 | 110.96      | 120.71   |
| 2   | B     | 356 | LYS  | CA-C-O | -9.11 | 111.15      | 120.90   |
| 1   | A     | 126 | ASN  | O-C-N  | 9.11  | 131.77      | 122.12   |
| 2   | B     | 510 | GLY  | CA-C-N | 9.11  | 133.37      | 120.53   |
| 2   | B     | 510 | GLY  | C-N-CA | 9.11  | 133.37      | 120.53   |
| 1   | A     | 152 | THR  | N-CA-C | -9.10 | 102.10      | 113.02   |
| 2   | B     | 181 | TYR  | O-C-N  | -9.10 | 112.47      | 122.12   |
| 2   | B     | 567 | GLN  | N-CA-C | 9.10  | 122.50      | 111.40   |
| 3   | M     | 113 | LYS  | O-C-N  | 9.10  | 133.47      | 122.27   |
| 2   | B     | 122 | SER  | O-C-N  | 9.10  | 131.76      | 122.12   |
| 2   | B     | 150 | LEU  | O-C-N  | 9.10  | 134.13      | 122.39   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | M     | 394 | GLN  | O-C-N  | -9.10 | 112.17      | 123.27   |
| 2   | B     | 390 | VAL  | CA-C-O | -9.09 | 111.21      | 120.85   |
| 1   | A     | 383 | ASN  | CA-C-O | -9.09 | 109.51      | 119.97   |
| 1   | A     | 550 | VAL  | CA-C-O | -9.09 | 110.96      | 121.05   |
| 1   | A     | 417 | PRO  | N-CA-C | -9.09 | 96.93       | 111.38   |
| 2   | B     | 340 | ILE  | O-C-N  | 9.09  | 131.66      | 121.94   |
| 1   | A     | 127 | LEU  | O-C-N  | 9.08  | 132.50      | 122.15   |
| 2   | B     | 417 | TYR  | O-C-N  | 9.08  | 132.85      | 122.22   |
| 1   | A     | 411 | GLU  | CA-C-N | 9.08  | 133.18      | 120.29   |
| 1   | A     | 411 | GLU  | C-N-CA | 9.08  | 133.18      | 120.29   |
| 2   | B     | 547 | GLN  | O-C-N  | 9.08  | 131.74      | 122.12   |
| 3   | M     | 319 | SER  | CA-C-N | 9.08  | 138.31      | 121.97   |
| 3   | M     | 319 | SER  | C-N-CA | 9.08  | 138.31      | 121.97   |
| 3   | M     | 377 | LYS  | CA-C-O | 9.08  | 130.33      | 120.80   |
| 1   | A     | 597 | GLN  | CA-C-O | -9.08 | 110.93      | 120.55   |
| 3   | M     | 308 | SER  | O-C-N  | 9.07  | 132.49      | 122.15   |
| 2   | B     | 314 | ASN  | CA-C-O | -9.07 | 111.74      | 119.36   |
| 2   | B     | 383 | VAL  | N-CA-C | 9.06  | 122.47      | 109.51   |
| 4   | S     | 31  | LEU  | CA-C-O | -9.06 | 110.82      | 120.42   |
| 1   | A     | 123 | LEU  | O-C-N  | 9.06  | 131.87      | 122.09   |
| 2   | B     | 215 | TYR  | O-C-N  | 9.05  | 134.63      | 122.59   |
| 2   | B     | 360 | LEU  | O-C-N  | 9.05  | 132.81      | 122.22   |
| 3   | M     | 396 | GLN  | CA-C-O | 9.06  | 130.37      | 120.32   |
| 3   | M     | 307 | SER  | O-C-N  | 9.05  | 131.40      | 122.07   |
| 4   | S     | 18  | LYS  | O-C-N  | -9.05 | 111.71      | 123.21   |
| 1   | A     | 389 | GLN  | CA-C-O | -9.05 | 110.96      | 120.55   |
| 2   | B     | 35  | TYR  | CA-C-O | -9.05 | 111.32      | 120.82   |
| 2   | B     | 526 | CYS  | CA-C-O | -9.05 | 107.77      | 120.16   |
| 1   | A     | 397 | ASP  | CA-C-O | 9.04  | 128.65      | 118.97   |
| 1   | A     | 356 | ILE  | CA-C-O | -9.04 | 111.01      | 121.05   |
| 2   | B     | 249 | ILE  | CA-C-O | -9.04 | 110.20      | 120.96   |
| 3   | M     | 455 | VAL  | CA-C-N | -9.04 | 104.82      | 122.62   |
| 3   | M     | 455 | VAL  | C-N-CA | -9.04 | 104.82      | 122.62   |
| 4   | S     | 24  | ASP  | O-C-N  | 9.04  | 133.67      | 123.01   |
| 1   | A     | 255 | ARG  | CA-C-O | -9.03 | 111.33      | 120.82   |
| 1   | A     | 109 | ALA  | O-C-N  | 9.03  | 131.84      | 122.09   |
| 3   | M     | 87  | LEU  | O-C-N  | 9.03  | 131.69      | 122.12   |
| 2   | B     | 447 | GLU  | CA-C-O | -9.03 | 110.98      | 120.55   |
| 2   | B     | 389 | ILE  | N-CA-C | -9.02 | 101.42      | 110.62   |
| 4   | S     | 70  | ASN  | CA-C-O | 9.02  | 133.41      | 120.51   |
| 1   | A     | 571 | ARG  | CA-C-N | 9.02  | 133.27      | 120.28   |
| 1   | A     | 571 | ARG  | C-N-CA | 9.02  | 133.27      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 583 | GLU  | CA-C-O | -9.02 | 110.99      | 120.55   |
| 1   | A     | 629 | LEU  | O-C-N  | -9.02 | 111.98      | 120.55   |
| 2   | B     | 493 | LEU  | O-C-N  | 9.02  | 134.42      | 122.33   |
| 1   | A     | 621 | LEU  | O-C-N  | -9.02 | 112.23      | 120.71   |
| 4   | S     | 66  | ASP  | CA-C-N | 9.02  | 140.25      | 121.32   |
| 4   | S     | 66  | ASP  | C-N-CA | 9.02  | 140.25      | 121.32   |
| 1   | A     | 279 | LEU  | O-C-N  | -9.01 | 110.60      | 122.59   |
| 2   | B     | 323 | ASN  | O-C-N  | 9.01  | 133.95      | 122.23   |
| 3   | M     | 319 | SER  | N-CA-C | -9.01 | 91.61       | 110.80   |
| 3   | M     | 447 | ILE  | CA-C-O | 9.01  | 132.04      | 120.78   |
| 3   | M     | 277 | GLU  | CA-C-N | -9.01 | 105.76      | 121.97   |
| 3   | M     | 277 | GLU  | C-N-CA | -9.01 | 105.76      | 121.97   |
| 3   | M     | 426 | LYS  | N-CA-C | -9.01 | 95.07       | 109.39   |
| 1   | A     | 371 | ALA  | CA-C-O | -9.00 | 111.43      | 120.70   |
| 2   | B     | 409 | LYS  | O-C-N  | 9.00  | 132.75      | 122.22   |
| 2   | B     | 343 | LEU  | CA-C-O | -9.00 | 111.37      | 120.82   |
| 4   | S     | 107 | GLU  | O-C-N  | 8.99  | 132.74      | 122.22   |
| 2   | B     | 411 | ILE  | CA-C-O | -8.99 | 109.29      | 121.15   |
| 1   | A     | 452 | ALA  | CA-C-O | -8.98 | 110.90      | 120.42   |
| 2   | B     | 192 | LEU  | O-C-N  | 8.98  | 134.38      | 122.43   |
| 2   | B     | 98  | LYS  | O-C-N  | 8.98  | 132.44      | 122.20   |
| 1   | A     | 580 | GLU  | O-C-N  | 8.98  | 131.64      | 122.12   |
| 2   | B     | 68  | SER  | CA-C-O | -8.98 | 111.45      | 120.70   |
| 2   | B     | 305 | SER  | CA-C-O | -8.97 | 111.46      | 120.70   |
| 3   | M     | 367 | ALA  | N-CA-C | -8.97 | 94.62       | 109.24   |
| 1   | A     | 337 | LEU  | O-C-N  | 8.97  | 132.71      | 122.22   |
| 2   | B     | 43  | ASN  | CA-C-O | -8.97 | 107.88      | 120.16   |
| 4   | S     | 125 | TRP  | O-C-N  | 8.96  | 131.41      | 122.09   |
| 1   | A     | 588 | LEU  | O-C-N  | -8.96 | 110.09      | 122.46   |
| 2   | B     | 84  | ALA  | CA-C-O | -8.96 | 111.05      | 120.55   |
| 2   | B     | 267 | ASP  | O-C-N  | -8.96 | 111.30      | 122.68   |
| 2   | B     | 513 | TRP  | CA-C-O | -8.96 | 111.31      | 120.90   |
| 4   | S     | 151 | ALA  | O-C-N  | 8.96  | 132.36      | 122.15   |
| 4   | S     | 105 | PHE  | CA-C-O | -8.96 | 110.30      | 120.24   |
| 1   | A     | 320 | HIS  | CA-C-O | 8.95  | 129.91      | 120.42   |
| 1   | A     | 472 | LYS  | O-C-N  | 8.95  | 133.28      | 122.27   |
| 3   | M     | 403 | THR  | N-CA-C | -8.95 | 92.09       | 108.02   |
| 4   | S     | 165 | SER  | CA-C-N | -8.95 | 105.77      | 120.72   |
| 4   | S     | 165 | SER  | C-N-CA | -8.95 | 105.77      | 120.72   |
| 2   | B     | 96  | LYS  | O-C-N  | 8.95  | 132.35      | 122.15   |
| 1   | A     | 518 | CYS  | O-C-N  | 8.95  | 131.29      | 122.07   |
| 2   | B     | 433 | VAL  | CA-C-O | -8.95 | 109.91      | 120.83   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 466 | SER  | O-C-N   | 8.95  | 132.35      | 122.15   |
| 1   | A     | 68  | THR  | CA-C-O  | -8.94 | 111.08      | 120.55   |
| 3   | M     | 22  | ALA  | CB-CA-C | 8.94  | 128.21      | 110.42   |
| 2   | B     | 549 | LEU  | O-C-N   | 8.94  | 132.48      | 122.11   |
| 2   | B     | 491 | PHE  | CA-C-O  | -8.94 | 110.98      | 120.63   |
| 3   | M     | 124 | ILE  | CA-C-O  | -8.94 | 111.38      | 120.85   |
| 3   | M     | 272 | LEU  | CA-C-N  | 8.94  | 137.23      | 120.97   |
| 3   | M     | 272 | LEU  | C-N-CA  | 8.94  | 137.23      | 120.97   |
| 1   | A     | 346 | THR  | CA-C-O  | 8.93  | 130.30      | 119.49   |
| 1   | A     | 130 | LYS  | CA-C-O  | -8.93 | 111.08      | 120.55   |
| 1   | A     | 215 | VAL  | O-C-N   | -8.93 | 112.63      | 121.83   |
| 4   | S     | 42  | ARG  | CA-C-N  | 8.93  | 134.23      | 120.75   |
| 4   | S     | 42  | ARG  | C-N-CA  | 8.93  | 134.23      | 120.75   |
| 3   | M     | 386 | PHE  | CA-C-O  | 8.93  | 130.00      | 120.36   |
| 1   | A     | 124 | ALA  | O-C-N   | 8.92  | 132.66      | 122.22   |
| 1   | A     | 129 | LYS  | O-C-N   | 8.92  | 132.32      | 122.15   |
| 2   | B     | 246 | SER  | O-C-N   | 8.92  | 132.66      | 122.22   |
| 1   | A     | 553 | LEU  | CA-C-O  | -8.92 | 110.97      | 120.42   |
| 1   | A     | 317 | GLU  | CA-C-O  | -8.91 | 111.10      | 120.55   |
| 4   | S     | 135 | ILE  | CA-C-O  | 8.91  | 129.88      | 120.25   |
| 1   | A     | 399 | ASP  | O-C-N   | 8.91  | 134.33      | 122.30   |
| 3   | M     | 284 | SER  | CA-C-O  | 8.91  | 131.21      | 120.87   |
| 2   | B     | 209 | SER  | O-C-N   | 8.91  | 132.65      | 122.22   |
| 3   | M     | 283 | PHE  | N-CA-C  | -8.91 | 94.72       | 109.24   |
| 2   | B     | 58  | GLU  | O-C-N   | 8.91  | 132.64      | 122.22   |
| 3   | M     | 460 | ILE  | CA-C-N  | 8.91  | 137.52      | 121.85   |
| 3   | M     | 460 | ILE  | C-N-CA  | 8.91  | 137.52      | 121.85   |
| 1   | A     | 419 | ILE  | N-CA-C  | 8.90  | 127.86      | 109.34   |
| 1   | A     | 302 | ASN  | CA-C-O  | 8.90  | 133.24      | 120.51   |
| 2   | B     | 439 | CYS  | O-C-N   | 8.90  | 131.70      | 122.09   |
| 3   | M     | 387 | GLU  | CA-C-O  | 8.90  | 130.20      | 120.32   |
| 4   | S     | 161 | GLU  | CA-C-O  | 8.90  | 130.35      | 119.31   |
| 1   | A     | 71  | VAL  | O-C-N   | 8.89  | 130.99      | 121.83   |
| 2   | B     | 103 | LEU  | O-C-N   | 8.89  | 132.28      | 122.15   |
| 1   | A     | 553 | LEU  | O-C-N   | 8.88  | 132.28      | 122.15   |
| 1   | A     | 72  | LEU  | CA-C-O  | -8.88 | 111.14      | 120.55   |
| 1   | A     | 556 | VAL  | CA-C-O  | -8.88 | 110.88      | 120.47   |
| 1   | A     | 288 | THR  | CA-C-N  | 8.88  | 133.80      | 120.31   |
| 1   | A     | 288 | THR  | C-N-CA  | 8.88  | 133.80      | 120.31   |
| 4   | S     | 86  | THR  | CA-C-O  | 8.88  | 130.06      | 120.38   |
| 2   | B     | 61  | ASP  | O-C-N   | 8.88  | 131.32      | 122.09   |
| 2   | B     | 365 | PHE  | O-C-N   | 8.88  | 131.32      | 122.09   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 425 | PRO  | O-C-N  | 8.87  | 133.65      | 122.91   |
| 2   | B     | 453 | TRP  | O-C-N  | 8.87  | 133.18      | 122.27   |
| 1   | A     | 610 | SER  | CA-C-O | -8.86 | 110.28      | 120.20   |
| 2   | B     | 248 | LEU  | CA-C-O | -8.86 | 108.77      | 119.49   |
| 2   | B     | 293 | VAL  | O-C-N  | -8.86 | 113.27      | 121.87   |
| 2   | B     | 551 | LEU  | CA-C-O | -8.86 | 109.23      | 119.60   |
| 2   | B     | 612 | ARG  | O-C-N  | 8.86  | 132.89      | 122.17   |
| 3   | M     | 91  | THR  | O-C-N  | 8.86  | 133.17      | 122.27   |
| 4   | S     | 137 | GLN  | N-CA-C | 8.86  | 123.27      | 110.24   |
| 2   | B     | 582 | ASP  | O-C-N  | -8.86 | 112.84      | 123.29   |
| 2   | B     | 103 | LEU  | CA-C-O | -8.85 | 111.04      | 120.42   |
| 2   | B     | 299 | LEU  | CA-C-O | -8.84 | 111.59      | 120.70   |
| 2   | B     | 371 | GLN  | O-C-N  | 8.84  | 132.23      | 122.15   |
| 1   | A     | 323 | CYS  | N-CA-C | 8.84  | 123.47      | 112.87   |
| 2   | B     | 64  | LYS  | CA-C-O | -8.84 | 111.54      | 120.82   |
| 2   | B     | 472 | VAL  | CA-C-N | -8.84 | 107.75      | 120.29   |
| 2   | B     | 472 | VAL  | C-N-CA | -8.84 | 107.75      | 120.29   |
| 1   | A     | 576 | MET  | O-C-N  | 8.83  | 132.22      | 122.15   |
| 3   | M     | 372 | ILE  | CA-C-N | -8.83 | 110.67      | 122.42   |
| 3   | M     | 372 | ILE  | C-N-CA | -8.83 | 110.67      | 122.42   |
| 2   | B     | 253 | ILE  | O-C-N  | 8.83  | 133.49      | 121.84   |
| 2   | B     | 36  | THR  | CA-C-O | -8.83 | 108.52      | 119.38   |
| 1   | A     | 495 | ILE  | CA-C-O | -8.82 | 111.50      | 120.85   |
| 1   | A     | 583 | GLU  | O-C-N  | 8.82  | 131.47      | 122.12   |
| 1   | A     | 72  | LEU  | O-C-N  | 8.82  | 131.47      | 122.12   |
| 1   | A     | 334 | SER  | O-C-N  | 8.82  | 131.61      | 122.09   |
| 2   | B     | 47  | LEU  | CA-C-O | -8.82 | 111.12      | 120.55   |
| 1   | A     | 182 | ILE  | CA-C-O | -8.81 | 111.27      | 121.05   |
| 3   | M     | 294 | ASP  | CA-C-N | 8.81  | 138.68      | 121.41   |
| 3   | M     | 294 | ASP  | C-N-CA | 8.81  | 138.68      | 121.41   |
| 1   | A     | 74  | LEU  | CA-C-O | -8.81 | 111.21      | 120.55   |
| 1   | A     | 456 | ASP  | O-C-N  | 8.81  | 131.60      | 122.09   |
| 1   | A     | 240 | LEU  | O-C-N  | -8.80 | 111.92      | 122.22   |
| 2   | B     | 300 | ASP  | CA-C-O | -8.80 | 111.13      | 120.63   |
| 1   | A     | 328 | PRO  | O-C-N  | -8.80 | 110.45      | 122.24   |
| 2   | B     | 491 | PHE  | O-C-N  | 8.80  | 131.44      | 122.12   |
| 1   | A     | 598 | GLU  | CA-C-O | -8.79 | 109.86      | 119.97   |
| 2   | B     | 616 | SER  | O-C-N  | 8.79  | 131.12      | 122.07   |
| 1   | A     | 428 | MET  | CA-C-O | -8.78 | 111.60      | 120.82   |
| 3   | M     | 266 | ASP  | CA-C-N | 8.78  | 134.35      | 121.18   |
| 3   | M     | 266 | ASP  | C-N-CA | 8.78  | 134.35      | 121.18   |
| 1   | A     | 98  | ASN  | O-C-N  | -8.78 | 113.04      | 122.96   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 156 | PRO  | CA-C-O | 8.78  | 133.51      | 119.64   |
| 1   | A     | 514 | GLU  | O-C-N  | 8.78  | 132.15      | 122.15   |
| 2   | B     | 98  | LYS  | CA-C-O | -8.77 | 110.38      | 120.20   |
| 3   | M     | 223 | HIS  | O-C-N  | -8.77 | 112.66      | 123.36   |
| 1   | A     | 214 | VAL  | CA-C-O | -8.77 | 111.56      | 120.85   |
| 1   | A     | 260 | PHE  | N-CA-C | -8.77 | 101.80      | 111.36   |
| 2   | B     | 252 | LEU  | O-C-N  | 8.77  | 133.79      | 122.39   |
| 2   | B     | 415 | LEU  | O-C-N  | 8.76  | 134.25      | 122.59   |
| 4   | S     | 85  | PHE  | O-C-N  | -8.76 | 113.11      | 123.27   |
| 1   | A     | 395 | PHE  | CA-C-N | -8.76 | 106.10      | 120.64   |
| 1   | A     | 395 | PHE  | C-N-CA | -8.76 | 106.10      | 120.64   |
| 4   | S     | 116 | VAL  | CA-C-O | 8.76  | 129.58      | 120.39   |
| 1   | A     | 315 | CYS  | CA-C-O | -8.75 | 111.14      | 120.42   |
| 3   | M     | 117 | ASN  | CA-C-O | -8.75 | 109.26      | 119.59   |
| 3   | M     | 93  | LEU  | CA-C-O | -8.75 | 111.14      | 120.42   |
| 1   | A     | 224 | GLU  | CA-C-N | -8.75 | 107.68      | 120.28   |
| 1   | A     | 224 | GLU  | C-N-CA | -8.75 | 107.68      | 120.28   |
| 2   | B     | 345 | ARG  | O-C-N  | 8.75  | 131.39      | 122.12   |
| 1   | A     | 331 | ARG  | CA-C-O | -8.75 | 111.89      | 120.90   |
| 1   | A     | 427 | LYS  | O-C-N  | 8.74  | 131.39      | 122.12   |
| 3   | M     | 129 | VAL  | CA-C-N | 8.74  | 139.64      | 122.07   |
| 3   | M     | 129 | VAL  | C-N-CA | 8.74  | 139.64      | 122.07   |
| 1   | A     | 165 | ASP  | O-C-N  | 8.74  | 132.11      | 122.15   |
| 1   | A     | 512 | LEU  | O-C-N  | 8.74  | 132.11      | 122.15   |
| 1   | A     | 462 | GLN  | N-CA-C | -8.74 | 101.88      | 112.54   |
| 1   | A     | 632 | PHE  | CA-C-O | -8.74 | 111.65      | 120.82   |
| 1   | A     | 457 | LEU  | CA-C-O | -8.73 | 111.20      | 120.63   |
| 3   | M     | 396 | GLN  | CA-C-N | -8.73 | 110.68      | 123.00   |
| 3   | M     | 396 | GLN  | C-N-CA | -8.73 | 110.68      | 123.00   |
| 4   | S     | 151 | ALA  | CA-C-O | -8.73 | 111.16      | 120.42   |
| 4   | S     | 33  | GLU  | O-C-N  | 8.73  | 133.58      | 122.23   |
| 1   | A     | 455 | MET  | O-C-N  | 8.73  | 131.37      | 122.12   |
| 1   | A     | 117 | ASP  | O-C-N  | 8.72  | 133.40      | 122.93   |
| 3   | M     | 400 | ASP  | CA-C-O | -8.72 | 111.44      | 121.47   |
| 2   | B     | 477 | MET  | O-C-N  | 8.72  | 131.51      | 122.09   |
| 1   | A     | 113 | SER  | N-CA-C | 8.72  | 124.56      | 112.45   |
| 1   | A     | 369 | SER  | CA-C-O | -8.72 | 111.31      | 120.55   |
| 1   | A     | 436 | CYS  | CA-C-O | 8.71  | 129.99      | 119.97   |
| 1   | A     | 533 | ILE  | O-C-N  | 8.71  | 130.96      | 121.90   |
| 1   | A     | 73  | LYS  | CA-C-O | -8.71 | 111.19      | 120.42   |
| 2   | B     | 476 | ARG  | O-C-N  | 8.71  | 132.08      | 122.15   |
| 2   | B     | 607 | ILE  | O-C-N  | 8.71  | 133.22      | 121.90   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 101 | GLN  | CA-C-O  | -8.71 | 111.32      | 120.55   |
| 2   | B     | 79  | VAL  | O-C-N   | 8.70  | 131.97      | 122.06   |
| 3   | M     | 317 | MET  | CA-C-N  | -8.70 | 104.55      | 121.94   |
| 3   | M     | 317 | MET  | C-N-CA  | -8.70 | 104.55      | 121.94   |
| 2   | B     | 58  | GLU  | CA-C-O  | -8.69 | 110.28      | 120.10   |
| 2   | B     | 95  | THR  | CA-C-O  | -8.69 | 111.21      | 120.42   |
| 2   | B     | 523 | PHE  | CA-C-N  | -8.69 | 107.10      | 120.31   |
| 2   | B     | 523 | PHE  | C-N-CA  | -8.69 | 107.10      | 120.31   |
| 3   | M     | 41  | LEU  | CA-C-O  | -8.69 | 110.60      | 120.24   |
| 1   | A     | 293 | GLU  | CA-C-O  | -8.69 | 111.70      | 120.82   |
| 2   | B     | 357 | GLU  | O-C-N   | 8.68  | 131.32      | 122.12   |
| 2   | B     | 485 | LYS  | O-C-N   | 8.68  | 132.74      | 122.24   |
| 1   | A     | 104 | ARG  | CA-C-O  | -8.67 | 110.61      | 120.24   |
| 2   | B     | 609 | ASP  | O-C-N   | 8.67  | 131.31      | 122.12   |
| 1   | A     | 467 | LYS  | O-C-N   | 8.67  | 132.93      | 122.27   |
| 1   | A     | 549 | GLU  | O-C-N   | 8.67  | 132.03      | 122.15   |
| 1   | A     | 339 | TYR  | CA-C-O  | -8.67 | 111.54      | 121.07   |
| 1   | A     | 487 | MET  | CA-C-N  | -8.65 | 108.01      | 120.29   |
| 1   | A     | 487 | MET  | C-N-CA  | -8.65 | 108.01      | 120.29   |
| 2   | B     | 111 | ASN  | CA-C-N  | 8.65  | 133.45      | 122.64   |
| 2   | B     | 111 | ASN  | C-N-CA  | 8.65  | 133.45      | 122.64   |
| 2   | B     | 118 | LEU  | O-C-N   | 8.65  | 130.98      | 122.07   |
| 2   | B     | 418 | TYR  | CA-C-O  | 8.64  | 129.84      | 120.24   |
| 2   | B     | 170 | ARG  | O-C-N   | -8.64 | 112.35      | 122.20   |
| 2   | B     | 329 | ALA  | N-CA-C  | 8.64  | 122.92      | 109.96   |
| 1   | A     | 64  | LEU  | CA-C-N  | -8.63 | 107.19      | 120.31   |
| 1   | A     | 64  | LEU  | C-N-CA  | -8.63 | 107.19      | 120.31   |
| 2   | B     | 394 | TRP  | O-C-N   | 8.63  | 131.99      | 122.15   |
| 2   | B     | 613 | MET  | CA-C-O  | -8.62 | 111.77      | 120.82   |
| 1   | A     | 363 | VAL  | N-CA-C  | 8.62  | 124.21      | 113.00   |
| 4   | S     | 68  | VAL  | N-CA-CB | -8.62 | 100.43      | 111.64   |
| 1   | A     | 134 | TYR  | CA-C-N  | -8.62 | 108.73      | 120.28   |
| 1   | A     | 134 | TYR  | C-N-CA  | -8.62 | 108.73      | 120.28   |
| 2   | B     | 280 | PRO  | N-CA-C  | -8.62 | 98.49       | 111.41   |
| 4   | S     | 131 | VAL  | O-C-N   | 8.61  | 131.53      | 121.80   |
| 2   | B     | 63  | MET  | O-C-N   | 8.61  | 133.42      | 122.23   |
| 2   | B     | 590 | GLN  | CA-C-O  | -8.61 | 109.45      | 119.61   |
| 2   | B     | 68  | SER  | O-C-N   | 8.60  | 131.38      | 122.09   |
| 2   | B     | 226 | LEU  | O-C-N   | 8.60  | 134.03      | 122.59   |
| 1   | A     | 608 | ARG  | CA-C-O  | -8.60 | 110.57      | 120.20   |
| 2   | B     | 422 | ALA  | N-CA-C  | -8.60 | 99.83       | 110.41   |
| 1   | A     | 598 | GLU  | O-C-N   | 8.60  | 132.84      | 122.27   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 398 | ILE  | O-C-N  | 8.60  | 130.79      | 121.94   |
| 1   | A     | 181 | ALA  | O-C-N  | 8.59  | 131.23      | 122.12   |
| 2   | B     | 533 | LEU  | O-C-N  | 8.59  | 131.23      | 122.12   |
| 2   | B     | 456 | ASP  | CA-C-O | -8.59 | 110.58      | 120.20   |
| 1   | A     | 298 | ILE  | CA-C-N | -8.59 | 106.22      | 120.30   |
| 1   | A     | 298 | ILE  | C-N-CA | -8.59 | 106.22      | 120.30   |
| 1   | A     | 163 | ALA  | O-C-N  | -8.58 | 113.02      | 122.12   |
| 1   | A     | 314 | ALA  | O-C-N  | 8.58  | 131.22      | 122.12   |
| 3   | M     | 232 | HIS  | O-C-N  | -8.58 | 113.15      | 123.19   |
| 2   | B     | 246 | SER  | CA-C-O | -8.58 | 110.41      | 120.10   |
| 2   | B     | 47  | LEU  | O-C-N  | 8.58  | 132.55      | 122.17   |
| 2   | B     | 321 | CYS  | O-C-N  | 8.57  | 132.82      | 122.27   |
| 2   | B     | 588 | ILE  | O-C-N  | 8.57  | 133.16      | 121.84   |
| 2   | B     | 321 | CYS  | CA-C-O | -8.57 | 110.12      | 119.97   |
| 1   | A     | 288 | THR  | N-CA-C | 8.56  | 134.97      | 111.00   |
| 1   | A     | 70  | ALA  | CA-C-O | -8.56 | 111.48      | 120.55   |
| 2   | B     | 434 | LYS  | CA-C-O | -8.56 | 110.43      | 120.10   |
| 2   | B     | 399 | LEU  | CA-C-O | 8.55  | 129.87      | 120.63   |
| 2   | B     | 55  | ASN  | CA-C-N | 8.55  | 134.28      | 120.60   |
| 2   | B     | 55  | ASN  | C-N-CA | 8.55  | 134.28      | 120.60   |
| 2   | B     | 223 | LEU  | O-C-N  | -8.55 | 110.98      | 122.43   |
| 2   | B     | 482 | ASN  | CA-C-O | -8.55 | 109.52      | 120.80   |
| 2   | B     | 470 | ALA  | CA-C-O | -8.54 | 112.10      | 120.90   |
| 3   | M     | 60  | LEU  | O-C-N  | 8.54  | 133.31      | 123.06   |
| 1   | A     | 623 | MET  | O-C-N  | 8.54  | 133.78      | 122.33   |
| 1   | A     | 452 | ALA  | O-C-N  | 8.54  | 131.88      | 122.15   |
| 2   | B     | 408 | VAL  | CA-C-O | -8.54 | 111.43      | 120.57   |
| 4   | S     | 124 | ASN  | O-C-N  | 8.54  | 133.13      | 122.20   |
| 3   | M     | 40  | GLN  | CA-C-O | -8.54 | 111.37      | 120.42   |
| 4   | S     | 83  | LEU  | O-C-N  | -8.54 | 112.41      | 123.16   |
| 2   | B     | 413 | LYS  | O-C-N  | 8.53  | 132.20      | 122.22   |
| 2   | B     | 213 | LEU  | O-C-N  | 8.53  | 133.93      | 122.59   |
| 1   | A     | 276 | PRO  | CA-C-O | 8.53  | 130.20      | 118.86   |
| 2   | B     | 112 | ASP  | N-CA-C | 8.53  | 127.14      | 108.73   |
| 2   | B     | 155 | LEU  | CA-C-O | -8.52 | 108.32      | 120.51   |
| 2   | B     | 415 | LEU  | CA-C-O | -8.52 | 108.32      | 120.51   |
| 2   | B     | 169 | VAL  | N-CA-C | -8.52 | 102.52      | 110.53   |
| 2   | B     | 207 | VAL  | CA-C-O | -8.52 | 111.00      | 120.46   |
| 1   | A     | 456 | ASP  | CA-C-O | -8.52 | 111.93      | 120.70   |
| 2   | B     | 410 | GLU  | O-C-N  | 8.52  | 132.75      | 122.27   |
| 4   | S     | 38  | LEU  | O-C-N  | 8.51  | 132.74      | 122.27   |
| 1   | A     | 306 | GLU  | O-C-N  | -8.51 | 111.27      | 122.59   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 539 | ASN  | CA-C-O | 8.51  | 129.51      | 119.56   |
| 1   | A     | 458 | ALA  | O-C-N  | 8.51  | 132.17      | 122.22   |
| 2   | B     | 173 | VAL  | O-C-N  | 8.51  | 131.76      | 122.06   |
| 2   | B     | 545 | ARG  | O-C-N  | 8.51  | 131.85      | 122.15   |
| 2   | B     | 530 | LEU  | O-C-N  | 8.51  | 132.17      | 122.22   |
| 2   | B     | 215 | TYR  | CA-C-O | -8.50 | 108.36      | 120.51   |
| 4   | S     | 159 | ALA  | CA-C-O | -8.50 | 111.94      | 120.70   |
| 2   | B     | 44  | PRO  | O-C-N  | 8.50  | 132.43      | 122.23   |
| 2   | B     | 490 | ILE  | O-C-N  | 8.50  | 132.95      | 121.90   |
| 1   | A     | 476 | GLN  | CA-C-O | -8.49 | 111.42      | 120.42   |
| 4   | S     | 94  | SER  | CA-C-O | -8.49 | 111.79      | 121.81   |
| 1   | A     | 292 | TYR  | CA-C-O | -8.49 | 111.90      | 120.82   |
| 1   | A     | 548 | GLN  | O-C-N  | 8.49  | 131.12      | 122.12   |
| 1   | A     | 128 | LEU  | CA-C-O | -8.48 | 110.51      | 120.10   |
| 1   | A     | 222 | ILE  | CA-C-O | -8.48 | 111.49      | 120.57   |
| 1   | A     | 256 | LEU  | CA-C-O | -8.48 | 110.51      | 120.10   |
| 2   | B     | 464 | SER  | O-C-N  | 8.47  | 132.66      | 122.75   |
| 3   | M     | 117 | ASN  | CA-C-N | 8.46  | 133.52      | 120.82   |
| 3   | M     | 117 | ASN  | C-N-CA | 8.46  | 133.52      | 120.82   |
| 2   | B     | 378 | THR  | CA-C-O | -8.46 | 112.12      | 121.00   |
| 4   | S     | 152 | SER  | O-C-N  | 8.46  | 131.79      | 122.15   |
| 2   | B     | 128 | SER  | CA-C-N | 8.45  | 133.51      | 120.75   |
| 2   | B     | 128 | SER  | C-N-CA | 8.45  | 133.51      | 120.75   |
| 1   | A     | 544 | SER  | CA-C-O | -8.45 | 112.07      | 121.87   |
| 2   | B     | 91  | THR  | CA-C-N | 8.44  | 133.50      | 120.75   |
| 2   | B     | 91  | THR  | C-N-CA | 8.44  | 133.50      | 120.75   |
| 1   | A     | 508 | LEU  | CA-C-N | 8.44  | 128.56      | 119.28   |
| 1   | A     | 508 | LEU  | C-N-CA | 8.44  | 128.56      | 119.28   |
| 2   | B     | 142 | LEU  | CA-C-O | 8.43  | 129.56      | 119.61   |
| 2   | B     | 295 | ASN  | CA-C-N | 8.43  | 142.37      | 121.80   |
| 2   | B     | 295 | ASN  | C-N-CA | 8.43  | 142.37      | 121.80   |
| 1   | A     | 241 | TYR  | O-C-N  | 8.43  | 131.76      | 122.15   |
| 1   | A     | 628 | VAL  | O-C-N  | 8.43  | 132.86      | 121.90   |
| 2   | B     | 452 | LYS  | CA-C-O | -8.43 | 111.62      | 120.55   |
| 2   | B     | 456 | ASP  | O-C-N  | 8.43  | 131.81      | 122.20   |
| 4   | S     | 148 | ARG  | O-C-N  | 8.42  | 133.62      | 122.33   |
| 3   | M     | 279 | ASN  | CA-C-O | -8.42 | 108.47      | 120.51   |
| 1   | A     | 219 | VAL  | O-C-N  | 8.40  | 130.64      | 121.90   |
| 2   | B     | 449 | HIS  | CA-C-O | -8.40 | 110.31      | 119.97   |
| 2   | B     | 550 | VAL  | CA-C-O | -8.40 | 111.48      | 120.64   |
| 1   | A     | 547 | VAL  | CA-C-O | -8.39 | 112.22      | 120.95   |
| 4   | S     | 141 | VAL  | CA-C-N | -8.39 | 111.59      | 122.16   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | S     | 141 | VAL  | C-N-CA | -8.39 | 111.59      | 122.16   |
| 1   | A     | 294 | SER  | O-C-N  | 8.38  | 132.03      | 122.22   |
| 3   | M     | 89  | CYS  | O-C-N  | 8.38  | 133.56      | 122.33   |
| 1   | A     | 87  | CYS  | O-C-N  | 8.38  | 133.40      | 122.42   |
| 1   | A     | 226 | SER  | CA-C-N | -8.38 | 108.39      | 120.29   |
| 1   | A     | 226 | SER  | C-N-CA | -8.38 | 108.39      | 120.29   |
| 1   | A     | 374 | LEU  | CA-C-O | -8.38 | 111.58      | 120.55   |
| 3   | M     | 86  | PRO  | O-C-N  | 8.38  | 132.70      | 122.23   |
| 2   | B     | 80  | GLN  | N-CA-C | 8.38  | 120.41      | 111.28   |
| 2   | B     | 236 | ILE  | CA-C-N | 8.37  | 132.34      | 120.53   |
| 2   | B     | 236 | ILE  | C-N-CA | 8.37  | 132.34      | 120.53   |
| 2   | B     | 249 | ILE  | O-C-N  | 8.37  | 132.78      | 121.90   |
| 2   | B     | 104 | TYR  | CA-C-O | -8.37 | 111.86      | 121.07   |
| 3   | M     | 123 | LEU  | CA-C-O | -8.37 | 110.35      | 119.97   |
| 2   | B     | 177 | ILE  | O-C-N  | 8.36  | 133.02      | 122.57   |
| 1   | A     | 467 | LYS  | CA-C-O | -8.36 | 110.36      | 119.97   |
| 2   | B     | 398 | ILE  | CA-C-O | -8.35 | 112.35      | 121.29   |
| 1   | A     | 201 | ASP  | CA-C-O | -8.35 | 111.57      | 120.42   |
| 1   | A     | 580 | GLU  | CA-C-O | -8.35 | 111.70      | 120.55   |
| 2   | B     | 62  | ALA  | O-C-N  | 8.35  | 133.24      | 122.39   |
| 3   | M     | 121 | ILE  | CA-C-O | -8.35 | 111.78      | 120.71   |
| 3   | M     | 256 | VAL  | O-C-N  | 8.35  | 132.03      | 123.10   |
| 4   | S     | 35  | VAL  | O-C-N  | 8.35  | 133.26      | 121.82   |
| 2   | B     | 567 | GLN  | CA-C-N | -8.35 | 106.95      | 121.97   |
| 2   | B     | 567 | GLN  | C-N-CA | -8.35 | 106.95      | 121.97   |
| 3   | M     | 16  | PHE  | O-C-N  | -8.35 | 113.90      | 123.33   |
| 4   | S     | 156 | LEU  | CA-C-O | -8.35 | 111.57      | 120.42   |
| 2   | B     | 82  | TYR  | CA-C-O | 8.34  | 129.79      | 119.11   |
| 1   | A     | 528 | ASN  | CA-C-O | 8.34  | 136.06      | 121.38   |
| 1   | A     | 597 | GLN  | O-C-N  | 8.34  | 130.96      | 122.12   |
| 1   | A     | 90  | HIS  | O-C-N  | 8.33  | 131.65      | 122.15   |
| 1   | A     | 174 | ARG  | O-C-N  | 8.33  | 130.90      | 121.32   |
| 1   | A     | 310 | GLU  | CA-C-O | -8.33 | 111.64      | 120.63   |
| 3   | M     | 309 | GLN  | O-C-N  | 8.32  | 131.08      | 122.09   |
| 1   | A     | 350 | SER  | CA-C-O | 8.32  | 129.37      | 120.55   |
| 2   | B     | 175 | LEU  | O-C-N  | 8.32  | 130.94      | 122.12   |
| 2   | B     | 395 | LYS  | CA-C-O | -8.32 | 110.70      | 120.10   |
| 2   | B     | 181 | TYR  | CA-C-O | 8.32  | 129.37      | 120.55   |
| 2   | B     | 429 | VAL  | CA-C-O | -8.32 | 111.48      | 120.47   |
| 2   | B     | 434 | LYS  | O-C-N  | 8.32  | 131.96      | 122.22   |
| 2   | B     | 470 | ALA  | O-C-N  | 8.31  | 131.01      | 122.03   |
| 4   | S     | 155 | GLU  | CA-C-O | -8.31 | 109.98      | 119.79   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | M     | 290 | PHE  | CA-C-N | 8.30  | 137.49      | 122.13   |
| 3   | M     | 290 | PHE  | C-N-CA | 8.30  | 137.49      | 122.13   |
| 1   | A     | 137 | ASN  | N-CA-C | 8.30  | 122.66      | 112.54   |
| 2   | B     | 49  | THR  | CA-C-O | -8.29 | 111.67      | 120.63   |
| 3   | M     | 92  | PHE  | CA-C-O | -8.29 | 110.00      | 119.79   |
| 3   | M     | 105 | ASP  | O-C-N  | -8.29 | 111.56      | 122.59   |
| 2   | B     | 101 | ILE  | CA-C-O | -8.29 | 112.38      | 121.17   |
| 2   | B     | 27  | THR  | CA-C-N | 8.29  | 137.09      | 122.42   |
| 2   | B     | 27  | THR  | C-N-CA | 8.29  | 137.09      | 122.42   |
| 2   | B     | 166 | SER  | CA-C-N | 8.29  | 134.76      | 120.58   |
| 2   | B     | 166 | SER  | C-N-CA | 8.29  | 134.76      | 120.58   |
| 1   | A     | 278 | ILE  | CA-C-N | 8.29  | 137.38      | 121.54   |
| 1   | A     | 278 | ILE  | C-N-CA | 8.29  | 137.38      | 121.54   |
| 3   | M     | 125 | PHE  | CA-C-O | -8.29 | 111.76      | 120.55   |
| 4   | S     | 29  | LYS  | O-C-N  | 8.29  | 133.00      | 122.23   |
| 4   | S     | 131 | VAL  | CA-C-O | -8.28 | 111.52      | 120.47   |
| 1   | A     | 328 | PRO  | CA-C-O | 8.28  | 131.02      | 119.18   |
| 2   | B     | 84  | ALA  | O-C-N  | 8.27  | 130.89      | 122.12   |
| 3   | M     | 88  | ASP  | CA-C-O | -8.27 | 110.75      | 120.10   |
| 1   | A     | 515 | CYS  | CA-C-O | -8.27 | 110.75      | 120.10   |
| 2   | B     | 243 | TRP  | O-C-N  | 8.27  | 134.27      | 122.20   |
| 1   | A     | 178 | ARG  | O-C-N  | 8.27  | 130.88      | 122.12   |
| 2   | B     | 117 | LEU  | O-C-N  | 8.26  | 131.57      | 122.15   |
| 3   | M     | 377 | LYS  | CA-C-N | -8.26 | 111.51      | 122.99   |
| 3   | M     | 377 | LYS  | C-N-CA | -8.26 | 111.51      | 122.99   |
| 1   | A     | 581 | LEU  | CA-C-O | -8.26 | 110.77      | 120.10   |
| 2   | B     | 515 | PHE  | CA-C-O | 8.26  | 129.43      | 120.10   |
| 3   | M     | 379 | LEU  | CA-C-N | -8.26 | 111.34      | 122.99   |
| 3   | M     | 379 | LEU  | C-N-CA | -8.26 | 111.34      | 122.99   |
| 1   | A     | 332 | TYR  | CA-C-O | -8.26 | 112.06      | 120.90   |
| 2   | B     | 178 | ILE  | O-C-N  | 8.26  | 132.89      | 122.57   |
| 2   | B     | 189 | HIS  | O-C-N  | 8.26  | 131.88      | 122.22   |
| 1   | A     | 430 | ASN  | O-C-N  | 8.26  | 131.88      | 122.22   |
| 2   | B     | 181 | TYR  | CA-C-N | -8.26 | 105.77      | 121.54   |
| 2   | B     | 181 | TYR  | C-N-CA | -8.26 | 105.77      | 121.54   |
| 2   | B     | 417 | TYR  | CA-C-O | -8.25 | 110.77      | 120.10   |
| 1   | A     | 436 | CYS  | CA-C-N | -8.25 | 106.72      | 122.06   |
| 1   | A     | 436 | CYS  | C-N-CA | -8.25 | 106.72      | 122.06   |
| 1   | A     | 160 | ARG  | O-C-N  | 8.25  | 131.55      | 122.15   |
| 1   | A     | 165 | ASP  | CA-C-O | -8.24 | 111.68      | 120.42   |
| 2   | B     | 450 | VAL  | O-C-N  | 8.24  | 132.62      | 121.90   |
| 1   | A     | 110 | ALA  | O-C-N  | -8.23 | 113.39      | 122.12   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 137 | PHE  | CA-C-O  | -8.23 | 111.74      | 120.63   |
| 1   | A     | 230 | PRO  | N-CA-C  | 8.23  | 124.53      | 113.84   |
| 3   | M     | 396 | GLN  | O-C-N   | -8.23 | 113.69      | 123.31   |
| 2   | B     | 56  | SER  | CA-C-O  | 8.22  | 129.44      | 119.49   |
| 2   | B     | 100 | LEU  | CA-C-O  | -8.22 | 111.83      | 120.55   |
| 2   | B     | 69  | ILE  | CA-C-N  | -8.22 | 109.26      | 120.28   |
| 2   | B     | 69  | ILE  | C-N-CA  | -8.22 | 109.26      | 120.28   |
| 4   | S     | 112 | CYS  | CA-C-N  | -8.22 | 109.85      | 123.33   |
| 4   | S     | 112 | CYS  | C-N-CA  | -8.22 | 109.85      | 123.33   |
| 1   | A     | 557 | LYS  | O-C-N   | 8.22  | 132.38      | 122.27   |
| 2   | B     | 234 | CYS  | CA-C-O  | -8.22 | 111.71      | 120.42   |
| 1   | A     | 436 | CYS  | O-C-N   | -8.21 | 112.17      | 122.27   |
| 2   | B     | 532 | ARG  | CA-C-O  | -8.21 | 110.52      | 119.97   |
| 1   | A     | 179 | LYS  | CA-C-O  | -8.21 | 111.72      | 120.42   |
| 2   | B     | 611 | ALA  | CA-C-O  | -8.21 | 110.82      | 120.10   |
| 4   | S     | 109 | LEU  | CA-C-N  | -8.21 | 107.83      | 120.31   |
| 4   | S     | 109 | LEU  | C-N-CA  | -8.21 | 107.83      | 120.31   |
| 2   | B     | 465 | ALA  | O-C-N   | 8.21  | 130.82      | 122.12   |
| 2   | B     | 608 | ARG  | O-C-N   | 8.20  | 130.95      | 122.09   |
| 3   | M     | 75  | TRP  | CA-C-O  | 8.20  | 129.41      | 120.71   |
| 1   | A     | 99  | LYS  | CA-C-N  | 8.20  | 131.27      | 120.28   |
| 1   | A     | 99  | LYS  | C-N-CA  | 8.20  | 131.27      | 120.28   |
| 2   | B     | 504 | ALA  | CA-C-N  | 8.20  | 131.27      | 120.28   |
| 2   | B     | 504 | ALA  | C-N-CA  | 8.20  | 131.27      | 120.28   |
| 1   | A     | 453 | VAL  | CA-C-O  | -8.20 | 112.43      | 120.95   |
| 2   | B     | 81  | LEU  | CA-C-N  | -8.20 | 105.60      | 121.58   |
| 2   | B     | 81  | LEU  | C-N-CA  | -8.20 | 105.60      | 121.58   |
| 2   | B     | 101 | ILE  | CA-C-N  | 8.20  | 131.26      | 120.28   |
| 2   | B     | 101 | ILE  | C-N-CA  | 8.20  | 131.26      | 120.28   |
| 4   | S     | 113 | PHE  | N-CA-C  | -8.20 | 89.78       | 107.49   |
| 3   | M     | 104 | PHE  | N-CA-CB | -8.19 | 96.65       | 110.49   |
| 2   | B     | 569 | THR  | CA-C-N  | 8.19  | 133.96      | 121.51   |
| 2   | B     | 569 | THR  | C-N-CA  | 8.19  | 133.96      | 121.51   |
| 1   | A     | 193 | PRO  | CA-C-O  | -8.19 | 107.11      | 119.55   |
| 2   | B     | 135 | ARG  | O-C-N   | 8.18  | 132.97      | 122.33   |
| 2   | B     | 267 | ASP  | CA-C-N  | -8.18 | 104.98      | 121.18   |
| 2   | B     | 267 | ASP  | C-N-CA  | -8.18 | 104.98      | 121.18   |
| 1   | A     | 387 | ILE  | O-C-N   | 8.18  | 132.63      | 121.84   |
| 4   | S     | 145 | ASN  | O-C-N   | 8.18  | 133.08      | 123.02   |
| 2   | B     | 159 | LYS  | CA-C-O  | -8.17 | 111.89      | 120.55   |
| 2   | B     | 213 | LEU  | CA-C-O  | -8.17 | 108.83      | 120.51   |
| 2   | B     | 559 | ASP  | O-C-N   | 8.17  | 133.64      | 122.37   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | M     | 97  | ASP  | CA-C-O | -8.17 | 111.76      | 120.42   |
| 2   | B     | 195 | ILE  | O-C-N  | 8.16  | 132.77      | 122.57   |
| 1   | A     | 241 | TYR  | CA-C-O | -8.16 | 111.77      | 120.42   |
| 2   | B     | 56  | SER  | CA-C-N | -8.16 | 104.27      | 121.64   |
| 2   | B     | 56  | SER  | C-N-CA | -8.16 | 104.27      | 121.64   |
| 1   | A     | 180 | LYS  | CA-C-O | -8.15 | 111.78      | 120.42   |
| 2   | B     | 259 | TYR  | N-CA-C | 8.15  | 122.58      | 113.21   |
| 2   | B     | 392 | SER  | O-C-N  | 8.15  | 131.76      | 122.22   |
| 1   | A     | 67  | LYS  | N-CA-C | -8.15 | 102.40      | 111.28   |
| 1   | A     | 470 | GLY  | O-C-N  | 8.15  | 131.16      | 122.28   |
| 1   | A     | 573 | GLU  | CA-C-O | 8.14  | 129.36      | 120.82   |
| 1   | A     | 634 | ASN  | O-C-N  | 8.14  | 131.43      | 122.15   |
| 2   | B     | 139 | LEU  | O-C-N  | 8.13  | 133.33      | 122.43   |
| 3   | M     | 387 | GLU  | O-C-N  | -8.13 | 113.80      | 123.31   |
| 1   | A     | 458 | ALA  | CA-C-O | -8.12 | 110.92      | 120.10   |
| 2   | B     | 237 | ILE  | CA-C-O | 8.12  | 129.50      | 121.05   |
| 3   | M     | 277 | GLU  | N-CA-C | 8.12  | 122.14      | 109.07   |
| 1   | A     | 260 | PHE  | CA-C-O | 8.11  | 129.02      | 120.42   |
| 1   | A     | 593 | THR  | CA-C-O | -8.12 | 111.34      | 120.43   |
| 2   | B     | 604 | GLU  | O-C-N  | 8.12  | 133.19      | 122.96   |
| 4   | S     | 30  | LEU  | CA-C-O | -8.12 | 111.82      | 120.42   |
| 4   | S     | 145 | ASN  | CA-C-O | -8.11 | 111.08      | 120.49   |
| 3   | M     | 88  | ASP  | O-C-N  | 8.11  | 131.71      | 122.22   |
| 1   | A     | 277 | LYS  | CA-C-O | -8.11 | 113.05      | 122.37   |
| 1   | A     | 375 | VAL  | O-C-N  | -8.11 | 113.94      | 121.89   |
| 2   | B     | 322 | CYS  | O-C-N  | 8.11  | 132.24      | 122.27   |
| 1   | A     | 185 | LEU  | O-C-N  | 8.11  | 132.93      | 122.39   |
| 2   | B     | 505 | ASP  | CA-C-O | 8.11  | 129.14      | 120.55   |
| 2   | B     | 78  | ASP  | O-C-N  | -8.11 | 111.81      | 122.59   |
| 3   | M     | 105 | ASP  | N-CA-C | 8.10  | 128.06      | 110.80   |
| 4   | S     | 101 | LEU  | O-C-N  | 8.10  | 133.56      | 122.46   |
| 2   | B     | 56  | SER  | N-CA-C | -8.10 | 102.50      | 112.38   |
| 1   | A     | 219 | VAL  | CA-C-O | -8.09 | 112.06      | 121.05   |
| 1   | A     | 270 | LEU  | CA-C-O | -8.09 | 111.27      | 120.24   |
| 1   | A     | 100 | LEU  | CA-C-O | 8.08  | 129.12      | 120.55   |
| 4   | S     | 141 | VAL  | N-CA-C | -8.08 | 96.94       | 108.58   |
| 1   | A     | 462 | GLN  | CA-C-O | 8.08  | 129.32      | 119.38   |
| 3   | M     | 98  | ARG  | O-C-N  | 8.07  | 131.35      | 122.15   |
| 2   | B     | 75  | ASP  | N-CA-C | 8.07  | 122.69      | 113.01   |
| 2   | B     | 146 | LYS  | CA-C-O | -8.07 | 113.09      | 122.37   |
| 2   | B     | 34  | SER  | O-C-N  | 8.06  | 130.66      | 122.12   |
| 2   | B     | 191 | GLU  | O-C-N  | 8.06  | 132.71      | 122.23   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 447 | PHE  | N-CA-C | -8.06 | 102.58      | 111.36   |
| 1   | A     | 185 | LEU  | CA-C-O | -8.06 | 109.74      | 119.49   |
| 1   | A     | 350 | SER  | CA-C-N | -8.06 | 107.27      | 120.72   |
| 1   | A     | 350 | SER  | C-N-CA | -8.06 | 107.27      | 120.72   |
| 2   | B     | 248 | LEU  | O-C-N  | 8.05  | 132.86      | 122.39   |
| 4   | S     | 32  | LEU  | O-C-N  | 8.06  | 133.22      | 122.43   |
| 4   | S     | 27  | LYS  | CA-C-O | -8.05 | 110.29      | 119.79   |
| 4   | S     | 105 | PHE  | O-C-N  | 8.05  | 132.70      | 122.23   |
| 1   | A     | 120 | ILE  | CA-C-O | -8.05 | 112.11      | 121.05   |
| 2   | B     | 196 | LEU  | CA-C-O | -8.05 | 109.00      | 120.51   |
| 1   | A     | 605 | GLU  | CA-C-O | -8.05 | 112.02      | 120.55   |
| 1   | A     | 594 | PHE  | O-C-N  | 8.05  | 130.65      | 122.12   |
| 2   | B     | 457 | HIS  | CA-C-N | -8.04 | 107.85      | 120.88   |
| 2   | B     | 457 | HIS  | C-N-CA | -8.04 | 107.85      | 120.88   |
| 2   | B     | 54  | ARG  | CA-C-N | 8.04  | 133.16      | 122.30   |
| 2   | B     | 54  | ARG  | C-N-CA | 8.04  | 133.16      | 122.30   |
| 1   | A     | 566 | PHE  | CA-C-N | 8.03  | 136.88      | 121.54   |
| 1   | A     | 566 | PHE  | C-N-CA | 8.03  | 136.88      | 121.54   |
| 1   | A     | 421 | PRO  | O-C-N  | 8.03  | 132.81      | 122.86   |
| 4   | S     | 86  | THR  | O-C-N  | -8.03 | 113.82      | 123.29   |
| 1   | A     | 489 | GLU  | O-C-N  | 8.03  | 131.61      | 122.22   |
| 1   | A     | 364 | ASP  | O-C-N  | 8.02  | 132.89      | 123.02   |
| 2   | B     | 59  | VAL  | O-C-N  | 8.02  | 132.81      | 121.82   |
| 2   | B     | 170 | ARG  | CA-C-O | 8.01  | 129.18      | 120.20   |
| 3   | M     | 132 | GLY  | CA-C-O | 8.01  | 134.51      | 120.57   |
| 1   | A     | 239 | LEU  | CA-C-N | -8.01 | 108.75      | 120.28   |
| 1   | A     | 239 | LEU  | C-N-CA | -8.01 | 108.75      | 120.28   |
| 1   | A     | 249 | ASN  | CA-C-N | 8.01  | 130.85      | 120.44   |
| 1   | A     | 249 | ASN  | C-N-CA | 8.01  | 130.85      | 120.44   |
| 1   | A     | 353 | ASP  | CA-C-O | -8.01 | 112.06      | 120.55   |
| 1   | A     | 106 | GLY  | N-CA-C | -8.00 | 103.22      | 112.50   |
| 2   | B     | 585 | GLY  | N-CA-C | -8.00 | 94.22       | 113.18   |
| 4   | S     | 95  | GLU  | O-C-N  | 8.00  | 130.60      | 122.12   |
| 4   | S     | 138 | GLY  | CA-C-N | 8.00  | 133.67      | 121.51   |
| 4   | S     | 138 | GLY  | C-N-CA | 8.00  | 133.67      | 121.51   |
| 2   | B     | 382 | TYR  | N-CA-C | -8.00 | 97.96       | 109.96   |
| 3   | M     | 387 | GLU  | CA-C-N | -8.00 | 110.25      | 122.09   |
| 3   | M     | 387 | GLU  | C-N-CA | -8.00 | 110.25      | 122.09   |
| 4   | S     | 49  | SER  | CA-C-O | -8.00 | 108.87      | 119.11   |
| 1   | A     | 340 | LYS  | O-C-N  | 7.99  | 130.59      | 122.12   |
| 2   | B     | 252 | LEU  | CA-C-O | -7.98 | 109.83      | 119.49   |
| 2   | B     | 350 | THR  | CA-C-N | 7.97  | 134.23      | 120.68   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 350 | THR  | C-N-CA  | 7.97  | 134.23      | 120.68   |
| 1   | A     | 494 | ASN  | O-C-N   | 7.97  | 132.07      | 122.27   |
| 2   | B     | 449 | HIS  | O-C-N   | 7.97  | 132.07      | 122.27   |
| 1   | A     | 386 | ALA  | CA-C-O  | -7.97 | 111.97      | 120.42   |
| 3   | M     | 279 | ASN  | N-CA-CB | -7.96 | 97.03       | 110.49   |
| 3   | M     | 324 | SER  | CA-C-O  | 7.96  | 128.82      | 120.54   |
| 2   | B     | 594 | ALA  | CA-C-O  | -7.96 | 111.98      | 120.42   |
| 3   | M     | 230 | LYS  | CA-C-O  | -7.96 | 112.33      | 121.65   |
| 3   | M     | 339 | GLU  | CA-C-O  | 7.96  | 128.67      | 120.24   |
| 1   | A     | 159 | ALA  | CA-C-O  | -7.95 | 111.29      | 120.20   |
| 1   | A     | 413 | SER  | CA-C-N  | -7.95 | 107.44      | 120.72   |
| 1   | A     | 413 | SER  | C-N-CA  | -7.95 | 107.44      | 120.72   |
| 4   | S     | 80  | TYR  | O-C-N   | -7.95 | 112.62      | 123.12   |
| 1   | A     | 240 | LEU  | CA-C-O  | 7.95  | 129.08      | 120.10   |
| 2   | B     | 172 | GLU  | CA-C-N  | -7.95 | 107.58      | 120.86   |
| 2   | B     | 172 | GLU  | C-N-CA  | -7.95 | 107.58      | 120.86   |
| 2   | B     | 173 | VAL  | CA-C-O  | -7.95 | 110.41      | 120.03   |
| 2   | B     | 462 | ASN  | CA-C-N  | -7.95 | 106.50      | 120.97   |
| 2   | B     | 462 | ASN  | C-N-CA  | -7.95 | 106.50      | 120.97   |
| 2   | B     | 446 | TRP  | O-C-N   | 7.94  | 132.27      | 122.34   |
| 2   | B     | 364 | HIS  | O-C-N   | 7.94  | 131.32      | 122.11   |
| 2   | B     | 192 | LEU  | CA-C-O  | -7.94 | 109.10      | 119.10   |
| 2   | B     | 390 | VAL  | O-C-N   | 7.94  | 130.01      | 121.83   |
| 2   | B     | 338 | LYS  | CA-C-O  | -7.93 | 112.14      | 120.55   |
| 4   | S     | 155 | GLU  | O-C-N   | 7.93  | 132.96      | 122.33   |
| 3   | M     | 65  | TYR  | O-C-N   | 7.93  | 132.29      | 123.33   |
| 2   | B     | 241 | ASP  | O-C-N   | 7.92  | 131.91      | 122.96   |
| 2   | B     | 529 | VAL  | CA-C-O  | -7.92 | 111.53      | 120.96   |
| 1   | A     | 290 | VAL  | CA-C-N  | 7.92  | 132.07      | 120.74   |
| 1   | A     | 290 | VAL  | C-N-CA  | 7.92  | 132.07      | 120.74   |
| 1   | A     | 213 | SER  | CA-C-N  | 7.92  | 131.67      | 120.42   |
| 1   | A     | 213 | SER  | C-N-CA  | 7.92  | 131.67      | 120.42   |
| 2   | B     | 436 | LEU  | O-C-N   | 7.92  | 132.62      | 122.33   |
| 2   | B     | 167 | ALA  | CA-C-O  | -7.91 | 111.45      | 120.24   |
| 2   | B     | 140 | SER  | CA-C-O  | -7.91 | 112.56      | 120.70   |
| 1   | A     | 200 | PHE  | CA-C-O  | -7.90 | 112.09      | 120.63   |
| 1   | A     | 265 | GLN  | CA-C-N  | 7.90  | 135.92      | 121.70   |
| 1   | A     | 265 | GLN  | C-N-CA  | 7.90  | 135.92      | 121.70   |
| 1   | A     | 311 | THR  | N-CA-C  | -7.90 | 102.75      | 111.36   |
| 2   | B     | 371 | GLN  | CA-C-O  | -7.90 | 112.05      | 120.42   |
| 1   | A     | 180 | LYS  | O-C-N   | 7.88  | 131.13      | 122.15   |
| 1   | A     | 588 | LEU  | N-CA-C  | 7.88  | 122.47      | 113.01   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | M     | 343 | ASN  | CA-C-N  | -7.88 | 107.78      | 121.97   |
| 3   | M     | 343 | ASN  | C-N-CA  | -7.88 | 107.78      | 121.97   |
| 2   | B     | 572 | GLU  | N-CA-C  | 7.88  | 120.96      | 111.82   |
| 2   | B     | 587 | ARG  | CA-C-O  | -7.88 | 112.07      | 120.42   |
| 2   | B     | 55  | ASN  | O-C-N   | 7.87  | 132.18      | 123.13   |
| 3   | M     | 98  | ARG  | CA-C-O  | -7.87 | 112.08      | 120.42   |
| 2   | B     | 492 | LYS  | O-C-N   | 7.87  | 131.95      | 122.27   |
| 2   | B     | 414 | GLU  | O-C-N   | 7.87  | 132.87      | 122.33   |
| 2   | B     | 378 | THR  | O-C-N   | 7.86  | 130.21      | 122.03   |
| 3   | M     | 324 | SER  | CA-C-N  | -7.86 | 111.87      | 122.72   |
| 3   | M     | 324 | SER  | C-N-CA  | -7.86 | 111.87      | 122.72   |
| 2   | B     | 521 | ILE  | N-CA-C  | -7.86 | 92.99       | 109.34   |
| 3   | M     | 85  | GLY  | N-CA-C  | -7.86 | 96.31       | 112.34   |
| 3   | M     | 117 | ASN  | O-C-N   | 7.86  | 131.60      | 122.25   |
| 3   | M     | 90  | PHE  | O-C-N   | 7.86  | 132.44      | 122.23   |
| 1   | A     | 560 | SER  | O-C-N   | 7.85  | 131.10      | 122.15   |
| 2   | B     | 74  | ASP  | CA-C-N  | 7.85  | 136.73      | 121.18   |
| 2   | B     | 74  | ASP  | C-N-CA  | 7.85  | 136.73      | 121.18   |
| 4   | S     | 83  | LEU  | CA-C-N  | -7.85 | 111.16      | 122.94   |
| 4   | S     | 83  | LEU  | C-N-CA  | -7.85 | 111.16      | 122.94   |
| 2   | B     | 610 | ARG  | CA-C-O  | -7.85 | 112.10      | 120.42   |
| 4   | S     | 33  | GLU  | CA-C-O  | -7.84 | 111.54      | 120.24   |
| 2   | B     | 529 | VAL  | O-C-N   | 7.84  | 132.09      | 121.90   |
| 3   | M     | 349 | LYS  | CA-C-N  | -7.84 | 110.83      | 121.80   |
| 3   | M     | 349 | LYS  | C-N-CA  | -7.84 | 110.83      | 121.80   |
| 1   | A     | 249 | ASN  | O-C-N   | 7.83  | 132.20      | 123.04   |
| 1   | A     | 278 | ILE  | CA-C-O  | -7.83 | 107.48      | 120.80   |
| 2   | B     | 166 | SER  | O-C-N   | 7.83  | 132.44      | 122.89   |
| 1   | A     | 81  | GLY  | CA-C-N  | 7.82  | 136.97      | 122.74   |
| 1   | A     | 81  | GLY  | C-N-CA  | 7.82  | 136.97      | 122.74   |
| 4   | S     | 64  | ASN  | CA-C-N  | -7.82 | 106.61      | 121.54   |
| 4   | S     | 64  | ASN  | C-N-CA  | -7.82 | 106.61      | 121.54   |
| 4   | S     | 55  | PRO  | CA-N-CD | -7.81 | 101.07      | 112.00   |
| 1   | A     | 502 | ASP  | CA-C-O  | -7.81 | 110.04      | 119.49   |
| 1   | A     | 466 | ASP  | O-C-N   | 7.81  | 133.54      | 123.24   |
| 2   | B     | 392 | SER  | CA-C-O  | -7.80 | 111.28      | 120.10   |
| 3   | M     | 404 | ALA  | CA-C-O  | -7.80 | 112.38      | 121.82   |
| 1   | A     | 66  | SER  | CA-C-O  | -7.80 | 112.15      | 120.42   |
| 1   | A     | 267 | GLU  | O-C-N   | 7.80  | 130.29      | 121.32   |
| 1   | A     | 282 | MET  | CA-C-N  | -7.80 | 109.83      | 120.28   |
| 1   | A     | 282 | MET  | C-N-CA  | -7.80 | 109.83      | 120.28   |
| 1   | A     | 183 | THR  | O-C-N   | 7.80  | 130.38      | 122.12   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 188 | TYR  | CA-C-O | -7.80 | 110.47      | 119.05   |
| 3   | M     | 74  | TYR  | O-C-N  | -7.79 | 113.34      | 123.16   |
| 2   | B     | 532 | ARG  | O-C-N  | 7.79  | 131.86      | 122.27   |
| 4   | S     | 149 | ILE  | CA-C-O | -7.78 | 112.60      | 120.85   |
| 3   | M     | 121 | ILE  | O-C-N  | 7.78  | 132.11      | 121.84   |
| 2   | B     | 244 | SER  | O-C-N  | 7.77  | 133.19      | 122.46   |
| 1   | A     | 276 | PRO  | N-CA-C | -7.77 | 103.38      | 114.18   |
| 2   | B     | 396 | ILE  | O-C-N  | 7.77  | 132.10      | 121.84   |
| 3   | M     | 85  | GLY  | CA-C-O | -7.77 | 110.41      | 121.52   |
| 3   | M     | 447 | ILE  | CA-C-N | -7.77 | 110.05      | 121.24   |
| 3   | M     | 447 | ILE  | C-N-CA | -7.77 | 110.05      | 121.24   |
| 4   | S     | 154 | ASP  | O-C-N  | 7.77  | 131.82      | 122.27   |
| 2   | B     | 185 | LYS  | CA-C-O | 7.76  | 128.78      | 120.55   |
| 1   | A     | 211 | ASP  | O-C-N  | 7.76  | 132.56      | 123.02   |
| 2   | B     | 121 | ASN  | CA-C-O | -7.76 | 112.33      | 120.55   |
| 1   | A     | 73  | LYS  | O-C-N  | 7.75  | 130.99      | 122.15   |
| 4   | S     | 87  | PHE  | O-C-N  | -7.75 | 114.08      | 123.30   |
| 2   | B     | 317 | VAL  | CA-C-O | -7.75 | 110.24      | 119.85   |
| 2   | B     | 385 | PRO  | N-CA-C | 7.75  | 124.11      | 113.65   |
| 2   | B     | 495 | ASP  | O-C-N  | 7.75  | 131.80      | 122.27   |
| 1   | A     | 549 | GLU  | CA-C-O | -7.74 | 112.21      | 120.42   |
| 2   | B     | 568 | VAL  | O-C-N  | 7.74  | 132.24      | 122.57   |
| 4   | S     | 136 | VAL  | CA-C-N | 7.74  | 132.12      | 121.05   |
| 4   | S     | 136 | VAL  | C-N-CA | 7.74  | 132.12      | 121.05   |
| 1   | A     | 236 | LEU  | O-C-N  | 7.74  | 133.40      | 122.41   |
| 1   | A     | 170 | LEU  | N-CA-C | -7.72 | 101.86      | 111.75   |
| 3   | M     | 231 | SER  | CA-C-N | -7.72 | 111.14      | 122.65   |
| 3   | M     | 231 | SER  | C-N-CA | -7.72 | 111.14      | 122.65   |
| 1   | A     | 77  | LEU  | O-C-N  | 7.72  | 130.95      | 122.15   |
| 1   | A     | 69  | ASN  | O-C-N  | 7.72  | 130.95      | 122.15   |
| 1   | A     | 104 | ARG  | O-C-N  | 7.72  | 132.26      | 122.23   |
| 1   | A     | 319 | LEU  | CA-C-N | -7.72 | 109.33      | 120.29   |
| 1   | A     | 319 | LEU  | C-N-CA | -7.72 | 109.33      | 120.29   |
| 4   | S     | 28  | GLN  | CA-C-O | -7.72 | 111.09      | 119.97   |
| 2   | B     | 353 | GLN  | CA-C-O | -7.71 | 112.37      | 120.55   |
| 1   | A     | 382 | ASP  | O-C-N  | 7.71  | 131.24      | 122.22   |
| 3   | M     | 4   | SER  | CA-C-N | -7.71 | 111.37      | 122.94   |
| 3   | M     | 4   | SER  | C-N-CA | -7.71 | 111.37      | 122.94   |
| 1   | A     | 139 | ASP  | CA-C-N | 7.71  | 131.37      | 120.42   |
| 1   | A     | 139 | ASP  | C-N-CA | 7.71  | 131.37      | 120.42   |
| 2   | B     | 541 | GLY  | O-C-N  | 7.71  | 129.48      | 121.77   |
| 3   | M     | 310 | VAL  | CA-C-O | 7.70  | 128.96      | 120.95   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | M     | 130 | GLU  | N-CA-CB | 7.69  | 122.77      | 110.46   |
| 2   | B     | 87  | VAL  | N-CA-C  | -7.68 | 103.04      | 110.42   |
| 4   | S     | 144 | THR  | CA-C-O  | 7.68  | 127.50      | 119.05   |
| 2   | B     | 230 | PHE  | O-C-N   | -7.68 | 112.41      | 122.39   |
| 3   | M     | 373 | ALA  | CA-C-N  | -7.68 | 109.91      | 122.81   |
| 3   | M     | 373 | ALA  | C-N-CA  | -7.68 | 109.91      | 122.81   |
| 2   | B     | 195 | ILE  | CA-C-O  | -7.68 | 111.18      | 120.78   |
| 2   | B     | 590 | GLN  | O-C-N   | 7.67  | 132.31      | 122.33   |
| 1   | A     | 305 | GLU  | CA-C-O  | -7.67 | 109.54      | 120.51   |
| 2   | B     | 236 | ILE  | O-C-N   | 7.67  | 129.88      | 121.90   |
| 4   | S     | 76  | ILE  | O-C-N   | -7.67 | 114.12      | 123.10   |
| 2   | B     | 135 | ARG  | CA-C-O  | -7.67 | 110.56      | 119.61   |
| 2   | B     | 241 | ASP  | CA-C-O  | -7.67 | 112.65      | 121.47   |
| 2   | B     | 438 | ARG  | CA-C-O  | -7.67 | 109.95      | 119.38   |
| 4   | S     | 107 | GLU  | CA-C-O  | -7.67 | 111.44      | 120.10   |
| 1   | A     | 207 | LEU  | N-CA-C  | -7.66 | 103.04      | 112.38   |
| 1   | A     | 441 | TYR  | CA-C-O  | 7.66  | 134.86      | 121.38   |
| 2   | B     | 496 | LEU  | O-C-N   | 7.66  | 131.69      | 122.27   |
| 3   | M     | 113 | LYS  | CA-C-O  | -7.66 | 111.17      | 119.97   |
| 4   | S     | 78  | LYS  | O-C-N   | -7.65 | 114.36      | 123.31   |
| 2   | B     | 121 | ASN  | O-C-N   | 7.65  | 130.23      | 122.12   |
| 4   | S     | 49  | SER  | N-CA-C  | -7.65 | 103.92      | 113.18   |
| 2   | B     | 473 | ASN  | CA-C-O  | -7.65 | 112.31      | 120.42   |
| 3   | M     | 112 | LYS  | CA-C-O  | -7.65 | 112.44      | 120.55   |
| 2   | B     | 89  | ASN  | CA-C-N  | 7.64  | 133.62      | 120.86   |
| 2   | B     | 89  | ASN  | C-N-CA  | 7.64  | 133.62      | 120.86   |
| 1   | A     | 340 | LYS  | CA-C-O  | -7.64 | 112.38      | 120.63   |
| 2   | B     | 102 | HIS  | N-CA-C  | -7.63 | 102.96      | 111.28   |
| 2   | B     | 49  | THR  | O-C-N   | 7.63  | 130.21      | 122.12   |
| 2   | B     | 262 | LYS  | N-CA-C  | 7.63  | 122.94      | 109.58   |
| 2   | B     | 432 | ALA  | O-C-N   | 7.63  | 132.74      | 122.59   |
| 1   | A     | 258 | LYS  | CA-C-O  | -7.63 | 112.47      | 120.55   |
| 1   | A     | 265 | GLN  | N-CA-CB | 7.62  | 122.74      | 110.16   |
| 2   | B     | 419 | VAL  | CA-C-N  | -7.62 | 109.94      | 120.38   |
| 2   | B     | 419 | VAL  | C-N-CA  | -7.62 | 109.94      | 120.38   |
| 2   | B     | 457 | HIS  | O-C-N   | -7.62 | 113.47      | 122.15   |
| 4   | S     | 34  | GLN  | O-C-N   | 7.62  | 131.64      | 122.27   |
| 4   | S     | 81  | ALA  | N-CA-C  | -7.62 | 94.58       | 110.80   |
| 3   | M     | 51  | LEU  | O-C-N   | -7.61 | 112.47      | 122.59   |
| 4   | S     | 120 | ASP  | CA-C-O  | -7.61 | 109.87      | 119.31   |
| 3   | M     | 50  | TYR  | N-CA-CB | -7.61 | 98.10       | 110.42   |
| 3   | M     | 394 | GLN  | N-CA-C  | 7.61  | 121.94      | 109.24   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 179 | LYS  | O-C-N  | 7.61  | 130.82      | 122.15   |
| 2   | B     | 256 | CYS  | O-C-N  | -7.60 | 114.06      | 122.12   |
| 2   | B     | 214 | ALA  | O-C-N  | 7.60  | 132.70      | 122.59   |
| 1   | A     | 280 | GLU  | O-C-N  | 7.60  | 130.81      | 122.15   |
| 1   | A     | 219 | VAL  | N-CA-C | 7.60  | 117.67      | 110.53   |
| 2   | B     | 155 | LEU  | O-C-N  | 7.60  | 132.69      | 122.59   |
| 2   | B     | 463 | LEU  | N-CA-C | 7.59  | 120.55      | 110.53   |
| 3   | M     | 120 | ARG  | O-C-N  | 7.59  | 132.26      | 122.39   |
| 2   | B     | 413 | LYS  | CA-C-O | -7.59 | 111.52      | 120.10   |
| 1   | A     | 625 | LEU  | CA-C-N | -7.59 | 106.88      | 120.99   |
| 1   | A     | 625 | LEU  | C-N-CA | -7.59 | 106.88      | 120.99   |
| 1   | A     | 422 | GLU  | O-C-N  | 7.58  | 130.80      | 122.15   |
| 2   | B     | 203 | THR  | N-CA-C | 7.58  | 122.83      | 112.90   |
| 2   | B     | 393 | ILE  | O-C-N  | 7.58  | 131.85      | 121.84   |
| 3   | M     | 130 | GLU  | O-C-N  | 7.58  | 131.43      | 122.94   |
| 1   | A     | 367 | ILE  | CA-C-O | -7.57 | 112.61      | 120.71   |
| 4   | S     | 140 | MET  | CA-C-N | -7.57 | 112.60      | 122.37   |
| 4   | S     | 140 | MET  | C-N-CA | -7.57 | 112.60      | 122.37   |
| 1   | A     | 285 | THR  | CA-C-N | -7.57 | 115.44      | 123.08   |
| 1   | A     | 285 | THR  | C-N-CA | -7.57 | 115.44      | 123.08   |
| 1   | A     | 235 | GLN  | N-CA-C | 7.57  | 119.61      | 111.36   |
| 2   | B     | 318 | ILE  | O-C-N  | 7.57  | 131.83      | 121.84   |
| 1   | A     | 287 | ALA  | N-CA-C | 7.57  | 126.91      | 110.80   |
| 3   | M     | 53  | HIS  | CA-C-O | -7.57 | 113.13      | 121.23   |
| 1   | A     | 129 | LYS  | CA-C-O | -7.56 | 112.41      | 120.42   |
| 2   | B     | 212 | VAL  | CA-C-N | -7.56 | 107.10      | 121.54   |
| 2   | B     | 212 | VAL  | C-N-CA | -7.56 | 107.10      | 121.54   |
| 1   | A     | 599 | ARG  | O-C-N  | 7.56  | 130.76      | 122.15   |
| 4   | S     | 48  | SER  | CA-C-N | -7.56 | 106.84      | 121.58   |
| 4   | S     | 48  | SER  | C-N-CA | -7.56 | 106.84      | 121.58   |
| 1   | A     | 572 | PHE  | O-C-N  | 7.56  | 131.06      | 122.22   |
| 1   | A     | 470 | GLY  | CA-C-O | -7.55 | 111.99      | 120.30   |
| 1   | A     | 459 | MET  | O-C-N  | 7.55  | 130.24      | 122.09   |
| 1   | A     | 115 | TYR  | N-CA-C | -7.55 | 100.43      | 110.24   |
| 2   | B     | 45  | GLN  | O-C-N  | 7.55  | 130.12      | 122.12   |
| 2   | B     | 136 | CYS  | O-C-N  | 7.54  | 132.62      | 122.59   |
| 2   | B     | 176 | ALA  | CA-C-O | -7.54 | 109.72      | 120.51   |
| 1   | A     | 203 | PHE  | O-C-N  | 7.54  | 130.11      | 122.12   |
| 2   | B     | 606 | ASP  | CA-C-O | -7.54 | 111.58      | 120.10   |
| 2   | B     | 285 | GLU  | CA-C-N | 7.54  | 130.89      | 120.49   |
| 2   | B     | 285 | GLU  | C-N-CA | 7.54  | 130.89      | 120.49   |
| 1   | A     | 251 | TRP  | O-C-N  | 7.53  | 131.53      | 122.27   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 223 | CYS  | O-C-N   | 7.52  | 130.21      | 122.09   |
| 3   | M     | 63  | TYR  | O-C-N   | 7.52  | 133.01      | 123.23   |
| 2   | B     | 177 | ILE  | CA-C-O  | -7.52 | 111.38      | 120.78   |
| 2   | B     | 284 | ASN  | N-CA-C  | 7.51  | 121.85      | 112.24   |
| 1   | A     | 467 | LYS  | CA-C-N  | -7.51 | 108.18      | 120.72   |
| 1   | A     | 467 | LYS  | C-N-CA  | -7.51 | 108.18      | 120.72   |
| 3   | M     | 237 | THR  | O-C-N   | -7.51 | 113.50      | 122.96   |
| 1   | A     | 471 | SER  | CA-C-O  | -7.50 | 112.47      | 120.42   |
| 2   | B     | 481 | LYS  | N-CA-C  | 7.50  | 121.68      | 112.23   |
| 3   | M     | 89  | CYS  | CA-C-O  | -7.50 | 110.94      | 119.79   |
| 3   | M     | 280 | ASP  | CB-CA-C | -7.50 | 95.51       | 110.42   |
| 1   | A     | 311 | THR  | CA-C-O  | -7.49 | 112.48      | 120.42   |
| 1   | A     | 378 | ILE  | N-CA-C  | 7.49  | 121.04      | 113.47   |
| 2   | B     | 304 | GLN  | O-C-N   | 7.49  | 130.98      | 122.22   |
| 2   | B     | 607 | ILE  | CA-C-O  | -7.49 | 112.05      | 120.96   |
| 2   | B     | 585 | GLY  | O-C-N   | 7.49  | 132.44      | 122.70   |
| 1   | A     | 154 | ILE  | CA-C-N  | -7.49 | 106.21      | 121.48   |
| 1   | A     | 154 | ILE  | C-N-CA  | -7.49 | 106.21      | 121.48   |
| 3   | M     | 410 | VAL  | CA-C-N  | -7.49 | 112.06      | 123.14   |
| 3   | M     | 410 | VAL  | C-N-CA  | -7.49 | 112.06      | 123.14   |
| 1   | A     | 261 | THR  | CA-C-O  | -7.48 | 112.62      | 120.55   |
| 1   | A     | 118 | SER  | CA-C-O  | -7.48 | 111.36      | 119.97   |
| 1   | A     | 448 | GLU  | CA-C-N  | 7.48  | 135.82      | 121.54   |
| 1   | A     | 448 | GLU  | C-N-CA  | 7.48  | 135.82      | 121.54   |
| 1   | A     | 282 | MET  | CA-C-O  | 7.47  | 128.57      | 119.97   |
| 1   | A     | 215 | VAL  | CA-C-N  | -7.47 | 110.27      | 120.28   |
| 1   | A     | 215 | VAL  | C-N-CA  | -7.47 | 110.27      | 120.28   |
| 3   | M     | 326 | HIS  | CA-C-O  | 7.47  | 128.45      | 120.46   |
| 4   | S     | 61  | ASN  | CA-C-N  | -7.47 | 107.28      | 121.54   |
| 4   | S     | 61  | ASN  | C-N-CA  | -7.47 | 107.28      | 121.54   |
| 4   | S     | 152 | SER  | CA-C-O  | -7.47 | 112.51      | 120.42   |
| 3   | M     | 108 | LYS  | N-CA-C  | 7.46  | 119.63      | 107.32   |
| 4   | S     | 167 | ILE  | CB-CA-C | -7.46 | 102.54      | 111.94   |
| 2   | B     | 140 | SER  | O-C-N   | 7.46  | 130.14      | 122.09   |
| 1   | A     | 499 | ILE  | CA-C-N  | -7.45 | 107.05      | 121.58   |
| 1   | A     | 499 | ILE  | C-N-CA  | -7.45 | 107.05      | 121.58   |
| 2   | B     | 461 | HIS  | N-CA-C  | 7.45  | 121.68      | 112.59   |
| 2   | B     | 579 | PRO  | N-CA-C  | 7.45  | 127.81      | 112.47   |
| 3   | M     | 260 | LEU  | CA-C-N  | -7.45 | 112.13      | 122.93   |
| 3   | M     | 260 | LEU  | C-N-CA  | -7.45 | 112.13      | 122.93   |
| 1   | A     | 522 | PHE  | N-CA-C  | 7.44  | 122.08      | 112.92   |
| 2   | B     | 62  | ALA  | CA-C-O  | -7.44 | 110.48      | 119.49   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 325 | SER  | CA-C-N  | 7.44  | 135.91      | 121.18   |
| 1   | A     | 325 | SER  | C-N-CA  | 7.44  | 135.91      | 121.18   |
| 2   | B     | 428 | VAL  | CA-C-O  | -7.43 | 112.22      | 120.25   |
| 2   | B     | 591 | MET  | O-C-N   | 7.43  | 133.21      | 122.28   |
| 1   | A     | 109 | ALA  | CA-C-O  | -7.43 | 113.05      | 120.70   |
| 1   | A     | 231 | GLN  | CA-C-N  | 7.43  | 128.09      | 119.47   |
| 1   | A     | 231 | GLN  | C-N-CA  | 7.43  | 128.09      | 119.47   |
| 3   | M     | 135 | ASN  | O-C-N   | 7.43  | 131.67      | 123.13   |
| 1   | A     | 239 | LEU  | N-CA-C  | -7.42 | 102.56      | 111.69   |
| 3   | M     | 136 | VAL  | O-C-N   | 7.42  | 130.50      | 122.63   |
| 3   | M     | 271 | SER  | CA-C-N  | -7.42 | 110.92      | 122.87   |
| 3   | M     | 271 | SER  | C-N-CA  | -7.42 | 110.92      | 122.87   |
| 2   | B     | 312 | SER  | N-CA-C  | -7.42 | 99.59       | 110.42   |
| 2   | B     | 402 | LEU  | CA-C-N  | 7.42  | 131.07      | 120.98   |
| 2   | B     | 402 | LEU  | C-N-CA  | 7.42  | 131.07      | 120.98   |
| 4   | S     | 35  | VAL  | CA-C-O  | -7.41 | 112.25      | 120.25   |
| 1   | A     | 119 | ASP  | O-C-N   | 7.41  | 130.60      | 122.15   |
| 3   | M     | 135 | ASN  | CA-C-O  | 7.41  | 128.72      | 120.43   |
| 1   | A     | 87  | CYS  | CA-C-O  | -7.40 | 110.71      | 119.15   |
| 1   | A     | 606 | PHE  | CA-C-O  | -7.40 | 112.70      | 120.55   |
| 2   | B     | 124 | GLN  | CA-C-O  | -7.40 | 112.57      | 120.42   |
| 1   | A     | 187 | LYS  | CA-C-O  | -7.40 | 111.74      | 120.10   |
| 3   | M     | 234 | ARG  | O-C-N   | -7.39 | 114.63      | 123.13   |
| 1   | A     | 576 | MET  | CA-C-O  | -7.39 | 112.59      | 120.42   |
| 2   | B     | 525 | ILE  | CA-C-O  | -7.38 | 112.11      | 119.20   |
| 2   | B     | 283 | TYR  | N-CA-C  | -7.38 | 102.61      | 111.69   |
| 1   | A     | 284 | SER  | N-CA-C  | 7.38  | 122.12      | 113.20   |
| 2   | B     | 533 | LEU  | CA-C-O  | -7.37 | 112.73      | 120.55   |
| 1   | A     | 440 | ASN  | N-CA-C  | -7.37 | 96.61       | 108.55   |
| 4   | S     | 67  | GLU  | CA-C-N  | -7.37 | 113.30      | 123.10   |
| 4   | S     | 67  | GLU  | C-N-CA  | -7.37 | 113.30      | 123.10   |
| 1   | A     | 471 | SER  | N-CA-C  | 7.37  | 119.39      | 111.36   |
| 2   | B     | 275 | ARG  | N-CA-CB | 7.37  | 120.97      | 110.44   |
| 2   | B     | 301 | LEU  | CA-C-O  | -7.37 | 111.78      | 120.10   |
| 3   | M     | 54  | SER  | CB-CA-C | -7.37 | 97.19       | 109.27   |
| 2   | B     | 256 | CYS  | CA-C-O  | 7.36  | 128.36      | 120.55   |
| 3   | M     | 5   | PHE  | O-C-N   | -7.36 | 113.66      | 123.23   |
| 4   | S     | 120 | ASP  | O-C-N   | 7.36  | 132.62      | 122.46   |
| 3   | M     | 230 | LYS  | O-C-N   | -7.36 | 113.75      | 122.58   |
| 2   | B     | 583 | PHE  | CA-C-N  | 7.35  | 130.73      | 120.29   |
| 2   | B     | 583 | PHE  | C-N-CA  | 7.35  | 130.73      | 120.29   |
| 2   | B     | 508 | ARG  | CA-C-N  | -7.34 | 110.45      | 120.44   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 508 | ARG  | C-N-CA  | -7.34 | 110.45      | 120.44   |
| 2   | B     | 568 | VAL  | CA-C-O  | 7.34  | 129.95      | 120.78   |
| 2   | B     | 85  | ASP  | O-C-N   | 7.32  | 130.50      | 122.15   |
| 2   | B     | 196 | LEU  | O-C-N   | 7.32  | 132.33      | 122.59   |
| 2   | B     | 65  | ARG  | CA-C-O  | -7.32 | 112.79      | 120.55   |
| 1   | A     | 297 | CYS  | CA-C-N  | -7.32 | 111.19      | 120.56   |
| 1   | A     | 297 | CYS  | C-N-CA  | -7.32 | 111.19      | 120.56   |
| 2   | B     | 136 | CYS  | CA-C-O  | -7.32 | 110.04      | 120.51   |
| 2   | B     | 194 | ASP  | O-C-N   | 7.31  | 132.32      | 122.59   |
| 2   | B     | 226 | LEU  | CA-C-O  | -7.31 | 110.06      | 120.51   |
| 4   | S     | 89  | VAL  | CA-C-O  | 7.31  | 130.37      | 121.75   |
| 2   | B     | 591 | MET  | CA-C-O  | -7.30 | 111.09      | 120.00   |
| 1   | A     | 89  | PHE  | O-C-N   | 7.30  | 129.86      | 122.12   |
| 1   | A     | 261 | THR  | O-C-N   | 7.30  | 129.86      | 122.12   |
| 2   | B     | 238 | LYS  | CA-C-N  | 7.30  | 136.54      | 121.94   |
| 2   | B     | 238 | LYS  | C-N-CA  | 7.30  | 136.54      | 121.94   |
| 1   | A     | 181 | ALA  | CA-C-O  | -7.29 | 112.82      | 120.55   |
| 1   | A     | 354 | GLN  | O-C-N   | 7.29  | 129.85      | 122.12   |
| 3   | M     | 352 | GLN  | CA-C-N  | 7.29  | 132.51      | 123.10   |
| 3   | M     | 352 | GLN  | C-N-CA  | 7.29  | 132.51      | 123.10   |
| 2   | B     | 159 | LYS  | O-C-N   | 7.29  | 129.85      | 122.12   |
| 2   | B     | 514 | LEU  | O-C-N   | 7.29  | 130.49      | 122.11   |
| 2   | B     | 510 | GLY  | O-C-N   | 7.29  | 132.17      | 122.70   |
| 2   | B     | 410 | GLU  | CA-C-O  | -7.28 | 111.59      | 119.97   |
| 1   | A     | 80  | TYR  | N-CA-CB | 7.27  | 122.48      | 110.85   |
| 2   | B     | 508 | ARG  | N-CA-C  | -7.27 | 103.35      | 111.71   |
| 2   | B     | 239 | GLN  | CA-C-N  | 7.26  | 136.05      | 123.05   |
| 2   | B     | 239 | GLN  | C-N-CA  | 7.26  | 136.05      | 123.05   |
| 1   | A     | 368 | ARG  | CA-C-O  | -7.26 | 113.19      | 120.82   |
| 1   | A     | 95  | MET  | N-CA-C  | -7.26 | 103.40      | 111.82   |
| 2   | B     | 424 | PHE  | CA-C-N  | 7.26  | 127.69      | 119.92   |
| 2   | B     | 424 | PHE  | C-N-CA  | 7.26  | 127.69      | 119.92   |
| 4   | S     | 126 | GLN  | CA-C-O  | -7.26 | 112.86      | 120.55   |
| 4   | S     | 128 | LEU  | CA-C-O  | -7.26 | 111.62      | 119.97   |
| 2   | B     | 444 | THR  | CA-C-N  | -7.25 | 109.28      | 120.31   |
| 2   | B     | 444 | THR  | C-N-CA  | -7.25 | 109.28      | 120.31   |
| 2   | B     | 108 | PHE  | CA-C-N  | -7.25 | 109.85      | 120.28   |
| 2   | B     | 108 | PHE  | C-N-CA  | -7.25 | 109.85      | 120.28   |
| 1   | A     | 365 | VAL  | CA-C-O  | 7.24  | 128.32      | 120.57   |
| 2   | B     | 175 | LEU  | CA-C-O  | -7.24 | 112.88      | 120.55   |
| 2   | B     | 598 | LEU  | CA-C-O  | -7.24 | 111.25      | 119.79   |
| 1   | A     | 177 | ILE  | N-CA-C  | -7.23 | 103.73      | 110.53   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 69  | ILE  | O-C-N  | -7.23 | 114.82      | 121.91   |
| 3   | M     | 104 | PHE  | CA-C-O | 7.23  | 130.85      | 120.51   |
| 2   | B     | 399 | LEU  | O-C-N  | -7.23 | 114.46      | 122.12   |
| 1   | A     | 161 | ASP  | O-C-N  | 7.22  | 129.89      | 122.09   |
| 1   | A     | 375 | VAL  | CA-C-N | -7.22 | 109.88      | 120.28   |
| 1   | A     | 375 | VAL  | C-N-CA | -7.22 | 109.88      | 120.28   |
| 3   | M     | 5   | PHE  | CA-C-O | 7.22  | 128.50      | 120.70   |
| 1   | A     | 206 | LYS  | CA-C-N | 7.21  | 132.14      | 120.60   |
| 1   | A     | 206 | LYS  | C-N-CA | 7.21  | 132.14      | 120.60   |
| 3   | M     | 364 | VAL  | N-CA-C | -7.21 | 106.10      | 113.10   |
| 1   | A     | 320 | HIS  | CA-C-N | -7.21 | 109.86      | 120.38   |
| 1   | A     | 320 | HIS  | C-N-CA | -7.21 | 109.86      | 120.38   |
| 2   | B     | 261 | PRO  | N-CA-C | -7.21 | 99.89       | 111.14   |
| 1   | A     | 379 | VAL  | CA-C-N | 7.21  | 133.88      | 122.21   |
| 1   | A     | 379 | VAL  | C-N-CA | 7.21  | 133.88      | 122.21   |
| 2   | B     | 316 | THR  | O-C-N  | 7.21  | 129.87      | 122.09   |
| 3   | M     | 461 | GLY  | N-CA-C | -7.21 | 105.27      | 115.43   |
| 3   | M     | 67  | SER  | CA-C-N | -7.20 | 112.93      | 122.94   |
| 3   | M     | 67  | SER  | C-N-CA | -7.20 | 112.93      | 122.94   |
| 1   | A     | 98  | ASN  | CA-C-O | -7.20 | 113.19      | 121.47   |
| 1   | A     | 595 | GLU  | CA-C-O | -7.19 | 113.29      | 120.70   |
| 1   | A     | 381 | GLU  | N-CA-C | 7.19  | 119.20      | 111.36   |
| 2   | B     | 106 | LEU  | CA-C-O | -7.19 | 111.97      | 120.10   |
| 1   | A     | 424 | TYR  | CA-C-O | -7.19 | 111.19      | 119.60   |
| 2   | B     | 307 | ASN  | CA-C-O | -7.19 | 113.50      | 120.90   |
| 2   | B     | 120 | ILE  | O-C-N  | 7.19  | 131.32      | 121.84   |
| 2   | B     | 509 | ALA  | O-C-N  | 7.18  | 129.85      | 122.09   |
| 2   | B     | 216 | LYS  | O-C-N  | -7.18 | 113.05      | 122.39   |
| 4   | S     | 47  | GLN  | CA-C-N | -7.18 | 110.69      | 120.82   |
| 4   | S     | 47  | GLN  | C-N-CA | -7.18 | 110.69      | 120.82   |
| 4   | S     | 48  | SER  | N-CA-C | -7.18 | 99.41       | 110.10   |
| 1   | A     | 475 | GLU  | CA-C-O | -7.18 | 111.99      | 120.10   |
| 3   | M     | 133 | GLU  | C-N-CD | 7.18  | 154.43      | 125.00   |
| 1   | A     | 84  | MET  | N-CA-C | -7.17 | 104.26      | 113.16   |
| 1   | A     | 160 | ARG  | CA-C-O | -7.16 | 112.83      | 120.42   |
| 2   | B     | 131 | ASN  | O-C-N  | 7.16  | 132.13      | 122.82   |
| 1   | A     | 289 | SER  | CA-C-N | -7.16 | 108.56      | 120.30   |
| 1   | A     | 289 | SER  | C-N-CA | -7.16 | 108.56      | 120.30   |
| 3   | M     | 55  | MET  | O-C-N  | -7.16 | 114.23      | 123.32   |
| 1   | A     | 451 | ASN  | CA-C-O | -7.15 | 112.02      | 120.10   |
| 2   | B     | 606 | ASP  | O-C-N  | 7.15  | 130.59      | 122.22   |
| 1   | A     | 127 | LEU  | CA-C-O | -7.15 | 112.84      | 120.42   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 342 | GLY  | CA-C-N  | -7.15 | 110.58      | 120.38   |
| 1   | A     | 342 | GLY  | C-N-CA  | -7.15 | 110.58      | 120.38   |
| 3   | M     | 18  | TYR  | O-C-N   | -7.15 | 114.68      | 123.33   |
| 1   | A     | 593 | THR  | O-C-N   | 7.14  | 131.35      | 123.13   |
| 3   | M     | 96  | ILE  | CA-C-O  | -7.14 | 112.76      | 120.47   |
| 4   | S     | 116 | VAL  | N-CA-C  | -7.14 | 98.11       | 108.11   |
| 3   | M     | 86  | PRO  | CA-C-O  | -7.14 | 109.39      | 119.74   |
| 2   | B     | 528 | ASP  | CA-C-O  | -7.13 | 111.37      | 119.79   |
| 2   | B     | 409 | LYS  | CA-C-O  | -7.13 | 112.04      | 120.10   |
| 3   | M     | 405 | THR  | CA-C-O  | 7.13  | 130.70      | 120.51   |
| 1   | A     | 231 | GLN  | O-C-N   | 7.12  | 129.51      | 121.32   |
| 2   | B     | 414 | GLU  | CA-C-O  | -7.12 | 111.38      | 119.79   |
| 1   | A     | 352 | PHE  | O-C-N   | 7.12  | 131.47      | 122.22   |
| 3   | M     | 288 | ILE  | CA-C-N  | -7.11 | 112.28      | 122.94   |
| 3   | M     | 288 | ILE  | C-N-CA  | -7.11 | 112.28      | 122.94   |
| 2   | B     | 458 | MET  | CA-C-N  | -7.11 | 107.97      | 121.54   |
| 2   | B     | 458 | MET  | C-N-CA  | -7.11 | 107.97      | 121.54   |
| 1   | A     | 265 | GLN  | CB-CA-C | 7.11  | 121.45      | 109.80   |
| 2   | B     | 374 | PHE  | CA-C-O  | -7.11 | 110.01      | 119.11   |
| 4   | S     | 58  | LEU  | N-CA-CB | 7.10  | 122.22      | 110.85   |
| 3   | M     | 398 | ILE  | O-C-N   | -7.09 | 113.59      | 122.88   |
| 3   | M     | 131 | ALA  | CA-C-N  | 7.09  | 135.30      | 121.41   |
| 3   | M     | 131 | ALA  | C-N-CA  | 7.09  | 135.30      | 121.41   |
| 2   | B     | 188 | TYR  | O-C-N   | 7.08  | 131.06      | 122.35   |
| 1   | A     | 218 | ALA  | CA-C-N  | 7.08  | 129.62      | 120.56   |
| 1   | A     | 218 | ALA  | C-N-CA  | 7.08  | 129.62      | 120.56   |
| 2   | B     | 179 | LYS  | CA-C-O  | -7.08 | 110.39      | 120.51   |
| 2   | B     | 133 | GLU  | O-C-N   | 7.07  | 131.81      | 122.33   |
| 1   | A     | 74  | LEU  | O-C-N   | 7.07  | 129.61      | 122.12   |
| 2   | B     | 232 | ARG  | O-C-N   | 7.07  | 131.99      | 122.59   |
| 1   | A     | 370 | LYS  | O-C-N   | 7.06  | 130.96      | 122.27   |
| 2   | B     | 205 | PRO  | N-CA-C  | -7.06 | 104.66      | 113.84   |
| 4   | S     | 25  | LEU  | N-CA-C  | -7.06 | 103.13      | 113.16   |
| 3   | M     | 457 | GLY  | O-C-N   | 7.06  | 130.34      | 122.50   |
| 1   | A     | 88  | ASN  | O-C-N   | -7.06 | 113.59      | 122.27   |
| 1   | A     | 191 | GLN  | N-CA-C  | 7.05  | 122.06      | 112.68   |
| 2   | B     | 464 | SER  | CA-C-O  | -7.05 | 114.11      | 121.87   |
| 1   | A     | 168 | THR  | CA-C-O  | -7.05 | 113.42      | 120.82   |
| 2   | B     | 287 | GLU  | O-C-N   | 7.05  | 131.29      | 123.04   |
| 1   | A     | 433 | ILE  | O-C-N   | 7.05  | 128.99      | 121.94   |
| 2   | B     | 229 | HIS  | N-CA-C  | 7.05  | 121.93      | 113.12   |
| 1   | A     | 393 | LYS  | CA-C-N  | -7.04 | 110.84      | 120.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 393 | LYS  | C-N-CA  | -7.04 | 110.84      | 120.28   |
| 4   | S     | 63  | ASN  | CA-C-O  | -7.04 | 112.77      | 120.30   |
| 1   | A     | 439 | ASP  | CA-C-N  | 7.04  | 134.71      | 121.69   |
| 1   | A     | 439 | ASP  | C-N-CA  | 7.04  | 134.71      | 121.69   |
| 2   | B     | 438 | ARG  | O-C-N   | 7.04  | 131.86      | 122.43   |
| 2   | B     | 543 | GLU  | CA-C-O  | -7.04 | 113.09      | 120.55   |
| 1   | A     | 525 | LEU  | N-CA-C  | -7.03 | 103.69      | 112.90   |
| 3   | M     | 112 | LYS  | O-C-N   | 7.03  | 129.57      | 122.12   |
| 3   | M     | 364 | VAL  | CA-C-N  | -7.03 | 110.87      | 120.44   |
| 3   | M     | 364 | VAL  | C-N-CA  | -7.03 | 110.87      | 120.44   |
| 2   | B     | 374 | PHE  | O-C-N   | 7.03  | 132.69      | 122.43   |
| 1   | A     | 291 | ILE  | CA-C-O  | -7.03 | 112.60      | 120.96   |
| 3   | M     | 95  | THR  | O-C-N   | 7.03  | 130.44      | 122.22   |
| 2   | B     | 566 | ALA  | CB-CA-C | 7.02  | 120.23      | 109.34   |
| 1   | A     | 84  | MET  | CA-C-O  | 7.02  | 127.78      | 119.28   |
| 1   | A     | 115 | TYR  | CA-C-N  | 7.01  | 134.94      | 121.54   |
| 1   | A     | 115 | TYR  | C-N-CA  | 7.01  | 134.94      | 121.54   |
| 2   | B     | 87  | VAL  | CA-C-N  | -7.01 | 110.89      | 120.28   |
| 2   | B     | 87  | VAL  | C-N-CA  | -7.01 | 110.89      | 120.28   |
| 2   | B     | 168 | MET  | O-C-N   | 7.01  | 129.29      | 122.07   |
| 3   | M     | 106 | LYS  | CA-C-N  | -7.00 | 108.78      | 120.68   |
| 3   | M     | 106 | LYS  | C-N-CA  | -7.00 | 108.78      | 120.68   |
| 1   | A     | 236 | LEU  | CA-C-O  | -7.00 | 110.85      | 119.18   |
| 2   | B     | 176 | ALA  | O-C-N   | 7.00  | 131.90      | 122.59   |
| 1   | A     | 397 | ASP  | O-C-N   | -7.00 | 114.01      | 122.48   |
| 2   | B     | 234 | CYS  | O-C-N   | 6.99  | 130.12      | 122.15   |
| 1   | A     | 406 | GLY  | N-CA-C  | -6.99 | 96.61       | 113.18   |
| 2   | B     | 422 | ALA  | N-CA-CB | 6.99  | 119.96      | 110.38   |
| 3   | M     | 367 | ALA  | CB-CA-C | 6.99  | 121.29      | 109.75   |
| 2   | B     | 94  | ASP  | O-C-N   | 6.99  | 131.19      | 123.22   |
| 3   | M     | 310 | VAL  | O-C-N   | -6.99 | 115.09      | 121.87   |
| 1   | A     | 489 | GLU  | CA-C-O  | -6.99 | 112.21      | 120.10   |
| 3   | M     | 256 | VAL  | CA-C-N  | -6.98 | 112.81      | 122.93   |
| 3   | M     | 256 | VAL  | C-N-CA  | -6.98 | 112.81      | 122.93   |
| 1   | A     | 294 | SER  | CA-C-O  | -6.98 | 112.22      | 120.10   |
| 3   | M     | 80  | THR  | N-CA-CB | -6.97 | 101.26      | 110.88   |
| 2   | B     | 423 | HIS  | N-CA-C  | -6.97 | 95.62       | 108.24   |
| 3   | M     | 135 | ASN  | N-CA-CB | 6.97  | 121.88      | 110.17   |
| 3   | M     | 328 | GLN  | CA-C-N  | -6.97 | 110.36      | 121.86   |
| 3   | M     | 328 | GLN  | C-N-CA  | -6.97 | 110.36      | 121.86   |
| 1   | A     | 418 | ILE  | CA-C-O  | -6.96 | 113.08      | 120.53   |
| 2   | B     | 254 | LYS  | O-C-N   | 6.95  | 130.58      | 122.17   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | M     | 130 | GLU  | CB-CA-C | 6.95  | 121.99      | 109.83   |
| 4   | S     | 17  | VAL  | CA-C-N  | -6.93 | 112.89      | 122.93   |
| 4   | S     | 17  | VAL  | C-N-CA  | -6.93 | 112.89      | 122.93   |
| 1   | A     | 630 | PRO  | O-C-N   | 6.92  | 131.71      | 122.30   |
| 3   | M     | 469 | GLY  | CA-C-N  | -6.92 | 108.33      | 121.54   |
| 3   | M     | 469 | GLY  | C-N-CA  | -6.92 | 108.33      | 121.54   |
| 2   | B     | 560 | ILE  | CA-C-O  | 6.92  | 129.43      | 120.78   |
| 2   | B     | 127 | LEU  | CA-C-N  | -6.91 | 108.10      | 121.58   |
| 2   | B     | 127 | LEU  | C-N-CA  | -6.91 | 108.10      | 121.58   |
| 4   | S     | 38  | LEU  | CA-C-O  | -6.91 | 112.02      | 119.97   |
| 1   | A     | 227 | LYS  | CA-C-N  | 6.91  | 132.39      | 120.58   |
| 1   | A     | 227 | LYS  | C-N-CA  | 6.91  | 132.39      | 120.58   |
| 1   | A     | 380 | ASP  | O-C-N   | 6.90  | 131.52      | 123.17   |
| 2   | B     | 407 | ASN  | O-C-N   | 6.90  | 131.74      | 122.49   |
| 1   | A     | 437 | SER  | CA-C-N  | 6.90  | 130.50      | 120.71   |
| 1   | A     | 437 | SER  | C-N-CA  | 6.90  | 130.50      | 120.71   |
| 2   | B     | 310 | ILE  | N-CA-C  | -6.89 | 102.47      | 111.09   |
| 2   | B     | 448 | SER  | CA-C-O  | -6.89 | 113.24      | 120.55   |
| 4   | S     | 104 | THR  | CA-C-O  | -6.89 | 111.20      | 119.27   |
| 1   | A     | 404 | GLN  | N-CA-C  | -6.89 | 102.12      | 112.04   |
| 1   | A     | 625 | LEU  | CA-C-O  | 6.89  | 128.06      | 120.82   |
| 2   | B     | 418 | TYR  | O-C-N   | -6.88 | 113.29      | 122.23   |
| 2   | B     | 563 | PHE  | O-C-N   | 6.88  | 130.31      | 122.19   |
| 1   | A     | 85  | ALA  | O-C-N   | 6.87  | 131.17      | 122.23   |
| 2   | B     | 349 | MET  | CA-C-N  | -6.87 | 111.33      | 120.95   |
| 2   | B     | 349 | MET  | C-N-CA  | -6.87 | 111.33      | 120.95   |
| 2   | B     | 497 | LEU  | CA-C-O  | 6.87  | 127.90      | 119.79   |
| 2   | B     | 388 | PRO  | O-C-N   | 6.87  | 131.38      | 122.86   |
| 2   | B     | 291 | TYR  | CA-C-N  | 6.86  | 132.34      | 120.68   |
| 2   | B     | 291 | TYR  | C-N-CA  | 6.86  | 132.34      | 120.68   |
| 3   | M     | 225 | VAL  | O-C-N   | 6.86  | 131.86      | 122.88   |
| 1   | A     | 212 | ILE  | CA-C-O  | 6.85  | 128.32      | 120.03   |
| 2   | B     | 179 | LYS  | O-C-N   | 6.85  | 131.70      | 122.59   |
| 1   | A     | 154 | ILE  | CB-CA-C | -6.85 | 102.50      | 111.88   |
| 1   | A     | 347 | ASP  | CA-C-N  | 6.85  | 130.14      | 120.28   |
| 1   | A     | 347 | ASP  | C-N-CA  | 6.85  | 130.14      | 120.28   |
| 4   | S     | 54  | PRO  | O-C-N   | -6.84 | 113.38      | 121.46   |
| 1   | A     | 175 | PRO  | O-C-N   | 6.84  | 131.40      | 122.24   |
| 2   | B     | 408 | VAL  | N-CA-C  | 6.84  | 119.60      | 111.05   |
| 2   | B     | 317 | VAL  | N-CA-C  | -6.83 | 102.47      | 112.04   |
| 4   | S     | 24  | ASP  | CA-C-O  | -6.83 | 113.26      | 121.05   |
| 1   | A     | 444 | VAL  | N-CA-CB | 6.83  | 120.79      | 110.13   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 536 | ASN  | CA-C-O | -6.83 | 111.42      | 119.48   |
| 3   | M     | 19  | LEU  | CA-C-N | -6.83 | 113.37      | 123.00   |
| 3   | M     | 19  | LEU  | C-N-CA | -6.83 | 113.37      | 123.00   |
| 1   | A     | 103 | LYS  | CA-C-N | -6.82 | 108.91      | 120.58   |
| 1   | A     | 103 | LYS  | C-N-CA | -6.82 | 108.91      | 120.58   |
| 1   | A     | 585 | PHE  | CA-C-O | -6.82 | 112.13      | 119.97   |
| 2   | B     | 499 | VAL  | CA-C-O | 6.82  | 128.62      | 121.05   |
| 1   | A     | 430 | ASN  | CA-C-O | -6.82 | 112.39      | 120.10   |
| 3   | M     | 94  | GLU  | CA-C-O | -6.82 | 113.68      | 120.70   |
| 1   | A     | 101 | GLN  | O-C-N  | 6.82  | 129.35      | 122.12   |
| 1   | A     | 172 | SER  | CA-C-N | -6.82 | 108.56      | 120.97   |
| 1   | A     | 172 | SER  | C-N-CA | -6.82 | 108.56      | 120.97   |
| 2   | B     | 551 | LEU  | O-C-N  | 6.82  | 132.04      | 122.36   |
| 3   | M     | 21  | GLY  | O-C-N  | 6.82  | 130.52      | 122.68   |
| 3   | M     | 303 | SER  | CA-C-N | -6.82 | 114.21      | 123.14   |
| 3   | M     | 303 | SER  | C-N-CA | -6.82 | 114.21      | 123.14   |
| 2   | B     | 487 | LEU  | CA-C-O | -6.82 | 112.40      | 120.10   |
| 2   | B     | 115 | LEU  | CA-C-O | -6.81 | 112.13      | 119.97   |
| 2   | B     | 188 | TYR  | N-CA-C | 6.80  | 122.57      | 113.72   |
| 2   | B     | 95  | THR  | O-C-N  | 6.79  | 129.89      | 122.15   |
| 1   | A     | 557 | LYS  | CA-C-O | -6.78 | 112.17      | 119.97   |
| 2   | B     | 122 | SER  | CA-C-O | -6.78 | 113.36      | 120.55   |
| 3   | M     | 77  | LEU  | O-C-N  | -6.78 | 114.60      | 123.21   |
| 1   | A     | 164 | ASP  | O-C-N  | 6.77  | 130.60      | 122.27   |
| 2   | B     | 113 | PRO  | CA-C-N | -6.77 | 110.68      | 120.29   |
| 2   | B     | 113 | PRO  | C-N-CA | -6.77 | 110.68      | 120.29   |
| 3   | M     | 118 | TYR  | O-C-N  | 6.77  | 129.89      | 122.11   |
| 4   | S     | 1   | MET  | CA-C-O | 6.76  | 132.30      | 120.80   |
| 1   | A     | 193 | PRO  | O-C-N  | 6.76  | 130.94      | 122.22   |
| 4   | S     | 164 | ASP  | O-C-N  | -6.76 | 113.60      | 122.59   |
| 2   | B     | 292 | GLU  | N-CA-C | 6.75  | 120.74      | 112.23   |
| 1   | A     | 568 | GLU  | CA-C-N | 6.75  | 133.98      | 121.62   |
| 1   | A     | 568 | GLU  | C-N-CA | 6.75  | 133.98      | 121.62   |
| 2   | B     | 165 | PRO  | CA-C-N | 6.75  | 130.45      | 120.87   |
| 2   | B     | 165 | PRO  | C-N-CA | 6.75  | 130.45      | 120.87   |
| 2   | B     | 597 | TYR  | O-C-N  | 6.75  | 130.12      | 122.22   |
| 3   | M     | 363 | ASN  | CA-C-N | -6.75 | 113.34      | 122.72   |
| 3   | M     | 363 | ASN  | C-N-CA | -6.75 | 113.34      | 122.72   |
| 4   | S     | 124 | ASN  | CA-C-O | -6.75 | 112.39      | 120.55   |
| 2   | B     | 153 | ILE  | CA-C-O | -6.75 | 112.35      | 120.78   |
| 2   | B     | 34  | SER  | N-CA-C | -6.75 | 103.93      | 111.28   |
| 1   | A     | 439 | ASP  | CA-C-O | 6.74  | 129.85      | 119.80   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 275 | ARG  | CA-C-N | 6.74  | 133.02      | 121.29   |
| 2   | B     | 275 | ARG  | C-N-CA | 6.74  | 133.02      | 121.29   |
| 1   | A     | 143 | VAL  | CA-C-O | -6.74 | 113.94      | 120.95   |
| 2   | B     | 36  | THR  | O-C-N  | 6.74  | 131.46      | 122.43   |
| 1   | A     | 374 | LEU  | CA-C-N | 6.74  | 130.03      | 120.53   |
| 1   | A     | 374 | LEU  | C-N-CA | 6.74  | 130.03      | 120.53   |
| 1   | A     | 501 | ASN  | N-CA-C | -6.73 | 98.27       | 108.96   |
| 3   | M     | 400 | ASP  | O-C-N  | 6.73  | 130.56      | 122.96   |
| 2   | B     | 45  | GLN  | CA-C-O | -6.71 | 113.43      | 120.55   |
| 2   | B     | 287 | GLU  | CA-C-O | 6.71  | 128.34      | 120.69   |
| 3   | M     | 277 | GLU  | CA-C-O | 6.71  | 127.70      | 120.38   |
| 4   | S     | 124 | ASN  | CA-C-N | 6.71  | 129.60      | 120.54   |
| 4   | S     | 124 | ASN  | C-N-CA | 6.71  | 129.60      | 120.54   |
| 2   | B     | 214 | ALA  | CA-C-O | -6.70 | 110.93      | 120.51   |
| 2   | B     | 577 | ASN  | O-C-N  | -6.70 | 115.26      | 121.36   |
| 4   | S     | 6   | LEU  | CA-C-O | 6.70  | 127.59      | 120.36   |
| 2   | B     | 254 | LYS  | CA-C-O | -6.70 | 113.39      | 120.55   |
| 1   | A     | 409 | VAL  | N-CA-C | 6.69  | 117.66      | 109.30   |
| 4   | S     | 53  | THR  | C-N-CD | 6.69  | 152.41      | 125.00   |
| 1   | A     | 170 | LEU  | CA-C-N | -6.68 | 111.96      | 122.65   |
| 1   | A     | 170 | LEU  | C-N-CA | -6.68 | 111.96      | 122.65   |
| 1   | A     | 566 | PHE  | O-C-N  | 6.68  | 131.32      | 122.43   |
| 1   | A     | 267 | GLU  | CA-C-O | -6.68 | 111.00      | 120.16   |
| 2   | B     | 517 | GLU  | CA-C-N | -6.68 | 110.07      | 121.09   |
| 2   | B     | 517 | GLU  | C-N-CA | -6.68 | 110.07      | 121.09   |
| 1   | A     | 494 | ASN  | CA-C-O | -6.67 | 112.30      | 119.97   |
| 2   | B     | 245 | GLN  | O-C-N  | 6.67  | 132.08      | 122.28   |
| 1   | A     | 445 | ASN  | CA-C-N | -6.67 | 114.17      | 122.84   |
| 1   | A     | 445 | ASN  | C-N-CA | -6.67 | 114.17      | 122.84   |
| 1   | A     | 469 | LEU  | N-CA-C | -6.66 | 104.10      | 111.82   |
| 2   | B     | 481 | LYS  | CA-C-N | 6.65  | 131.92      | 123.34   |
| 2   | B     | 481 | LYS  | C-N-CA | 6.65  | 131.92      | 123.34   |
| 2   | B     | 156 | HIS  | O-C-N  | 6.65  | 131.43      | 122.59   |
| 1   | A     | 630 | PRO  | CA-C-O | -6.65 | 109.69      | 119.00   |
| 4   | S     | 104 | THR  | CA-C-N | 6.63  | 131.92      | 120.58   |
| 4   | S     | 104 | THR  | C-N-CA | 6.63  | 131.92      | 120.58   |
| 2   | B     | 584 | SER  | CA-C-O | 6.63  | 127.45      | 120.42   |
| 2   | B     | 231 | ARG  | CA-C-O | -6.63 | 111.03      | 120.51   |
| 2   | B     | 384 | PHE  | CA-C-O | -6.63 | 114.23      | 119.66   |
| 1   | A     | 314 | ALA  | CA-C-O | -6.62 | 113.53      | 120.55   |
| 1   | A     | 631 | SER  | CA-C-N | 6.62  | 129.04      | 120.44   |
| 1   | A     | 631 | SER  | C-N-CA | 6.62  | 129.04      | 120.44   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 34  | SER  | CA-C-O  | -6.62 | 113.53      | 120.55   |
| 2   | B     | 384 | PHE  | N-CA-C  | -6.62 | 101.45      | 109.72   |
| 1   | A     | 80  | TYR  | CB-CA-C | 6.61  | 121.47      | 109.37   |
| 2   | B     | 94  | ASP  | CA-C-O  | -6.61 | 113.07      | 120.54   |
| 2   | B     | 432 | ALA  | CA-C-O  | -6.61 | 111.06      | 120.51   |
| 1   | A     | 352 | PHE  | CA-C-O  | -6.60 | 111.96      | 119.95   |
| 3   | M     | 421 | GLY  | CA-C-O  | 6.60  | 130.96      | 121.52   |
| 2   | B     | 118 | LEU  | CA-C-O  | -6.59 | 113.90      | 120.82   |
| 1   | A     | 218 | ALA  | CB-CA-C | 6.59  | 121.73      | 110.79   |
| 3   | M     | 103 | TYR  | N-CA-CB | 6.59  | 120.67      | 110.46   |
| 1   | A     | 418 | ILE  | N-CA-CB | -6.59 | 103.16      | 111.46   |
| 3   | M     | 59  | ASP  | O-C-N   | -6.59 | 113.50      | 122.33   |
| 2   | B     | 271 | GLU  | CA-C-N  | -6.58 | 107.77      | 120.80   |
| 2   | B     | 271 | GLU  | C-N-CA  | -6.58 | 107.77      | 120.80   |
| 1   | A     | 202 | LYS  | CA-C-O  | -6.57 | 113.46      | 120.42   |
| 4   | S     | 47  | GLN  | CA-C-O  | 6.57  | 128.36      | 120.81   |
| 3   | M     | 243 | ILE  | CA-C-N  | -6.56 | 114.34      | 123.13   |
| 3   | M     | 243 | ILE  | C-N-CA  | -6.56 | 114.34      | 123.13   |
| 3   | M     | 103 | TYR  | CB-CA-C | 6.56  | 121.79      | 110.45   |
| 2   | B     | 404 | ASN  | N-CA-C  | -6.56 | 99.45       | 109.41   |
| 2   | B     | 280 | PRO  | CA-C-N  | 6.55  | 131.78      | 120.58   |
| 2   | B     | 280 | PRO  | C-N-CA  | 6.55  | 131.78      | 120.58   |
| 1   | A     | 268 | PRO  | O-C-N   | 6.55  | 131.48      | 122.64   |
| 1   | A     | 195 | ALA  | CA-C-N  | 6.54  | 130.26      | 120.31   |
| 1   | A     | 195 | ALA  | C-N-CA  | 6.54  | 130.26      | 120.31   |
| 3   | M     | 402 | SER  | N-CA-C  | -6.54 | 104.34      | 113.37   |
| 3   | M     | 386 | PHE  | O-C-N   | -6.54 | 115.52      | 123.30   |
| 4   | S     | 117 | ASN  | O-C-N   | 6.54  | 132.06      | 122.97   |
| 2   | B     | 557 | SER  | CA-C-O  | 6.54  | 129.86      | 120.51   |
| 3   | M     | 281 | GLY  | CA-C-N  | 6.53  | 130.08      | 120.74   |
| 3   | M     | 281 | GLY  | C-N-CA  | 6.53  | 130.08      | 120.74   |
| 1   | A     | 239 | LEU  | O-C-N   | 6.53  | 130.72      | 122.23   |
| 1   | A     | 374 | LEU  | O-C-N   | 6.53  | 130.07      | 122.17   |
| 1   | A     | 459 | MET  | CA-C-O  | -6.53 | 113.98      | 120.70   |
| 1   | A     | 276 | PRO  | O-C-N   | -6.53 | 113.31      | 122.38   |
| 3   | M     | 384 | GLY  | CA-C-O  | -6.52 | 115.22      | 121.41   |
| 2   | B     | 556 | LEU  | O-C-N   | 6.51  | 129.57      | 122.15   |
| 2   | B     | 74  | ASP  | N-CA-C  | -6.51 | 98.58       | 108.67   |
| 3   | M     | 58  | ARG  | CA-C-N  | -6.51 | 109.61      | 120.68   |
| 3   | M     | 58  | ARG  | C-N-CA  | -6.51 | 109.61      | 120.68   |
| 1   | A     | 637 | GLU  | N-CA-C  | -6.51 | 105.20      | 113.01   |
| 1   | A     | 321 | THR  | CA-C-N  | 6.51  | 133.49      | 121.52   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 321 | THR  | C-N-CA  | 6.51  | 133.49      | 121.52   |
| 4   | S     | 1   | MET  | O-C-N   | -6.50 | 112.59      | 123.00   |
| 4   | S     | 60  | SER  | CA-C-N  | 6.50  | 134.37      | 122.79   |
| 4   | S     | 60  | SER  | C-N-CA  | 6.50  | 134.37      | 122.79   |
| 2   | B     | 46  | GLN  | CA-C-O  | -6.50 | 112.50      | 119.97   |
| 3   | M     | 278 | ILE  | CA-C-N  | -6.50 | 109.13      | 121.54   |
| 3   | M     | 278 | ILE  | C-N-CA  | -6.50 | 109.13      | 121.54   |
| 2   | B     | 82  | TYR  | O-C-N   | -6.50 | 112.95      | 122.43   |
| 2   | B     | 211 | ALA  | CA-C-N  | 6.50  | 128.81      | 120.88   |
| 2   | B     | 211 | ALA  | C-N-CA  | 6.50  | 128.81      | 120.88   |
| 3   | M     | 56  | VAL  | CB-CA-C | -6.49 | 103.57      | 111.88   |
| 3   | M     | 4   | SER  | O-C-N   | -6.49 | 115.74      | 123.27   |
| 3   | M     | 447 | ILE  | O-C-N   | -6.49 | 114.46      | 122.57   |
| 2   | B     | 274 | PRO  | N-CA-C  | -6.48 | 99.12       | 112.47   |
| 2   | B     | 510 | GLY  | CA-C-O  | -6.48 | 109.29      | 120.57   |
| 2   | B     | 33  | SER  | O-C-N   | 6.47  | 131.97      | 122.39   |
| 2   | B     | 518 | ILE  | N-CA-C  | 6.47  | 121.87      | 113.07   |
| 2   | B     | 145 | MET  | CA-C-O  | -6.47 | 113.60      | 121.36   |
| 3   | M     | 229 | LYS  | CA-C-O  | -6.47 | 111.47      | 120.21   |
| 2   | B     | 89  | ASN  | CA-C-O  | -6.46 | 111.67      | 119.49   |
| 2   | B     | 453 | TRP  | CA-C-O  | -6.46 | 112.54      | 119.97   |
| 4   | S     | 51  | LEU  | CA-C-O  | -6.46 | 113.61      | 120.40   |
| 1   | A     | 468 | SER  | CA-C-O  | -6.46 | 111.43      | 119.38   |
| 1   | A     | 80  | TYR  | CA-C-O  | -6.46 | 113.86      | 121.16   |
| 1   | A     | 502 | ASP  | O-C-N   | 6.45  | 130.78      | 122.39   |
| 3   | M     | 388 | ASN  | CA-C-N  | -6.45 | 113.29      | 123.23   |
| 3   | M     | 388 | ASN  | C-N-CA  | -6.45 | 113.29      | 123.23   |
| 3   | M     | 51  | LEU  | N-CA-CB | -6.45 | 99.59       | 110.49   |
| 3   | M     | 384 | GLY  | O-C-N   | 6.45  | 131.42      | 123.61   |
| 2   | B     | 69  | ILE  | CA-C-O  | 6.45  | 128.00      | 121.17   |
| 3   | M     | 69  | ILE  | CA-C-N  | -6.45 | 114.02      | 123.05   |
| 3   | M     | 69  | ILE  | C-N-CA  | -6.45 | 114.02      | 123.05   |
| 2   | B     | 112 | ASP  | CA-C-N  | 6.45  | 126.37      | 119.28   |
| 2   | B     | 112 | ASP  | C-N-CA  | 6.45  | 126.37      | 119.28   |
| 3   | M     | 400 | ASP  | CA-C-N  | 6.44  | 130.91      | 120.60   |
| 3   | M     | 400 | ASP  | C-N-CA  | 6.44  | 130.91      | 120.60   |
| 2   | B     | 165 | PRO  | N-CA-C  | 6.42  | 121.93      | 114.03   |
| 3   | M     | 316 | ARG  | CA-C-N  | -6.42 | 109.27      | 121.54   |
| 3   | M     | 316 | ARG  | C-N-CA  | -6.42 | 109.27      | 121.54   |
| 1   | A     | 214 | VAL  | CA-C-N  | 6.42  | 129.54      | 120.42   |
| 1   | A     | 214 | VAL  | C-N-CA  | 6.42  | 129.54      | 120.42   |
| 1   | A     | 220 | SER  | CA-C-O  | -6.41 | 113.70      | 120.63   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | M     | 311 | LYS  | N-CA-C  | -6.41 | 104.37      | 111.36   |
| 1   | A     | 405 | THR  | CB-CA-C | -6.41 | 98.95       | 110.23   |
| 1   | A     | 503 | ASN  | N-CA-C  | -6.41 | 104.29      | 111.28   |
| 3   | M     | 264 | GLY  | CA-C-N  | 6.41  | 131.44      | 122.41   |
| 3   | M     | 264 | GLY  | C-N-CA  | 6.41  | 131.44      | 122.41   |
| 2   | B     | 502 | SER  | CA-C-N  | -6.40 | 109.31      | 121.54   |
| 2   | B     | 502 | SER  | C-N-CA  | -6.40 | 109.31      | 121.54   |
| 4   | S     | 81  | ALA  | CA-C-N  | -6.40 | 112.57      | 122.49   |
| 4   | S     | 81  | ALA  | C-N-CA  | -6.40 | 112.57      | 122.49   |
| 1   | A     | 585 | PHE  | O-C-N   | 6.40  | 130.14      | 122.27   |
| 2   | B     | 472 | VAL  | N-CA-C  | -6.40 | 104.09      | 110.62   |
| 1   | A     | 378 | ILE  | CB-CA-C | -6.39 | 103.72      | 110.62   |
| 1   | A     | 92  | LEU  | O-C-N   | 6.39  | 128.89      | 122.12   |
| 1   | A     | 230 | PRO  | O-C-N   | 6.38  | 130.78      | 122.24   |
| 3   | M     | 55  | MET  | N-CA-C  | -6.38 | 103.05      | 111.02   |
| 1   | A     | 466 | ASP  | N-CA-C  | -6.37 | 96.52       | 107.61   |
| 3   | M     | 453 | ASP  | CA-C-N  | -6.37 | 114.88      | 123.10   |
| 3   | M     | 453 | ASP  | C-N-CA  | -6.37 | 114.88      | 123.10   |
| 1   | A     | 614 | LEU  | CA-C-N  | -6.37 | 111.24      | 120.29   |
| 1   | A     | 614 | LEU  | C-N-CA  | -6.37 | 111.24      | 120.29   |
| 2   | B     | 377 | TYR  | CA-C-O  | -6.37 | 111.74      | 119.32   |
| 1   | A     | 510 | THR  | O-C-N   | 6.37  | 128.97      | 122.09   |
| 3   | M     | 84  | LYS  | CA-C-N  | 6.37  | 131.87      | 121.87   |
| 3   | M     | 84  | LYS  | C-N-CA  | 6.37  | 131.87      | 121.87   |
| 2   | B     | 145 | MET  | O-C-N   | -6.36 | 115.93      | 123.06   |
| 3   | M     | 8   | THR  | N-CA-C  | -6.36 | 99.66       | 109.52   |
| 2   | B     | 336 | ASN  | O-C-N   | 6.36  | 131.05      | 122.59   |
| 2   | B     | 96  | LYS  | CA-C-O  | -6.36 | 113.68      | 120.42   |
| 1   | A     | 399 | ASP  | CA-C-O  | -6.36 | 112.36      | 120.31   |
| 2   | B     | 348 | THR  | CA-C-N  | -6.36 | 109.71      | 120.58   |
| 2   | B     | 348 | THR  | C-N-CA  | -6.36 | 109.71      | 120.58   |
| 2   | B     | 522 | GLU  | O-C-N   | 6.36  | 132.40      | 122.61   |
| 1   | A     | 188 | VAL  | CA-C-N  | 6.35  | 129.65      | 120.38   |
| 1   | A     | 188 | VAL  | C-N-CA  | 6.35  | 129.65      | 120.38   |
| 3   | M     | 103 | TYR  | CA-C-O  | 6.35  | 129.95      | 121.89   |
| 1   | A     | 416 | ILE  | C-N-CD  | 6.34  | 151.02      | 125.00   |
| 2   | B     | 244 | SER  | N-CA-C  | -6.34 | 105.39      | 113.01   |
| 1   | A     | 329 | ASN  | CA-C-O  | -6.34 | 113.20      | 120.24   |
| 1   | A     | 221 | VAL  | O-C-N   | 6.34  | 128.49      | 121.90   |
| 2   | B     | 23  | ALA  | N-CA-CB | 6.34  | 120.10      | 110.28   |
| 3   | M     | 234 | ARG  | CA-C-O  | 6.33  | 127.52      | 120.43   |
| 2   | B     | 572 | GLU  | CA-C-O  | -6.33 | 112.69      | 119.97   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 274 | LEU  | CA-C-N  | -6.32 | 106.37      | 121.80   |
| 1   | A     | 274 | LEU  | C-N-CA  | -6.32 | 106.37      | 121.80   |
| 2   | B     | 401 | THR  | CA-C-N  | 6.32  | 134.59      | 121.94   |
| 2   | B     | 401 | THR  | C-N-CA  | 6.32  | 134.59      | 121.94   |
| 3   | M     | 302 | TYR  | CA-C-N  | -6.32 | 114.08      | 122.99   |
| 3   | M     | 302 | TYR  | C-N-CA  | -6.32 | 114.08      | 122.99   |
| 4   | S     | 93  | GLU  | N-CA-C  | -6.32 | 100.00      | 110.17   |
| 3   | M     | 273 | HIS  | CA-C-O  | -6.32 | 114.54      | 121.87   |
| 2   | B     | 559 | ASP  | N-CA-C  | 6.32  | 120.99      | 113.16   |
| 2   | B     | 562 | ASN  | O-C-N   | 6.32  | 130.89      | 122.43   |
| 3   | M     | 388 | ASN  | N-CA-C  | 6.30  | 120.55      | 109.96   |
| 1   | A     | 500 | SER  | N-CA-C  | -6.30 | 105.55      | 113.18   |
| 2   | B     | 220 | ALA  | CB-CA-C | 6.30  | 120.89      | 110.81   |
| 2   | B     | 273 | SER  | O-C-N   | 6.30  | 127.58      | 121.28   |
| 2   | B     | 574 | ASN  | N-CA-C  | -6.30 | 104.86      | 113.30   |
| 3   | M     | 389 | SER  | O-C-N   | 6.30  | 133.01      | 122.93   |
| 2   | B     | 485 | LYS  | CA-C-O  | -6.30 | 111.83      | 119.32   |
| 2   | B     | 397 | GLN  | CA-C-O  | -6.29 | 113.75      | 120.42   |
| 1   | A     | 420 | ILE  | N-CA-C  | 6.29  | 122.47      | 108.88   |
| 2   | B     | 22  | ALA  | CA-C-N  | -6.29 | 110.76      | 120.31   |
| 2   | B     | 22  | ALA  | C-N-CA  | -6.29 | 110.76      | 120.31   |
| 3   | M     | 76  | CYS  | O-C-N   | -6.28 | 115.98      | 123.27   |
| 4   | S     | 76  | ILE  | CA-C-O  | 6.28  | 127.24      | 120.53   |
| 1   | A     | 544 | SER  | O-C-N   | 6.27  | 129.94      | 122.79   |
| 2   | B     | 524 | LYS  | CA-C-N  | -6.27 | 112.64      | 121.55   |
| 2   | B     | 524 | LYS  | C-N-CA  | -6.27 | 112.64      | 121.55   |
| 2   | B     | 239 | GLN  | N-CA-C  | 6.27  | 120.79      | 113.20   |
| 3   | M     | 80  | THR  | CB-CA-C | -6.26 | 98.85       | 109.38   |
| 4   | S     | 81  | ALA  | CB-CA-C | 6.26  | 122.89      | 110.42   |
| 2   | B     | 495 | ASP  | CA-C-O  | -6.26 | 112.77      | 119.97   |
| 2   | B     | 78  | ASP  | CA-C-O  | 6.26  | 129.46      | 120.51   |
| 2   | B     | 443 | SER  | CA-C-N  | 6.26  | 129.18      | 120.29   |
| 2   | B     | 443 | SER  | C-N-CA  | 6.26  | 129.18      | 120.29   |
| 1   | A     | 530 | ASN  | N-CA-C  | 6.25  | 119.75      | 111.75   |
| 1   | A     | 187 | LYS  | O-C-N   | 6.24  | 129.52      | 122.22   |
| 2   | B     | 518 | ILE  | O-C-N   | 6.24  | 130.56      | 122.26   |
| 3   | M     | 104 | PHE  | N-CA-C  | 6.22  | 124.05      | 110.80   |
| 4   | S     | 109 | LEU  | N-CA-C  | -6.21 | 104.51      | 111.28   |
| 4   | S     | 114 | THR  | N-CA-C  | 6.20  | 120.40      | 112.34   |
| 1   | A     | 194 | GLU  | O-C-N   | 6.20  | 128.69      | 122.12   |
| 1   | A     | 629 | LEU  | N-CA-C  | -6.19 | 105.20      | 113.25   |
| 1   | A     | 534 | LYS  | N-CA-CB | 6.19  | 119.18      | 109.83   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 438 | ALA  | CA-C-O  | -6.19 | 114.39      | 121.19   |
| 1   | A     | 116 | LYS  | CA-C-N  | -6.18 | 114.20      | 122.42   |
| 1   | A     | 116 | LYS  | C-N-CA  | -6.18 | 114.20      | 122.42   |
| 3   | M     | 95  | THR  | CA-C-O  | -6.18 | 113.12      | 120.10   |
| 3   | M     | 456 | SER  | CA-C-O  | -6.18 | 114.22      | 122.31   |
| 4   | S     | 13  | GLN  | CA-C-N  | -6.17 | 113.62      | 119.85   |
| 4   | S     | 13  | GLN  | C-N-CA  | -6.17 | 113.62      | 119.85   |
| 2   | B     | 232 | ARG  | CA-C-O  | -6.17 | 111.69      | 120.51   |
| 2   | B     | 484 | THR  | CA-C-N  | -6.17 | 112.93      | 122.49   |
| 2   | B     | 484 | THR  | C-N-CA  | -6.17 | 112.93      | 122.49   |
| 1   | A     | 168 | THR  | CA-C-N  | 6.16  | 129.68      | 120.31   |
| 1   | A     | 168 | THR  | C-N-CA  | 6.16  | 129.68      | 120.31   |
| 1   | A     | 447 | PHE  | CA-C-O  | -6.16 | 113.89      | 120.42   |
| 2   | B     | 375 | LEU  | CA-C-N  | -6.16 | 112.14      | 119.84   |
| 2   | B     | 375 | LEU  | C-N-CA  | -6.16 | 112.14      | 119.84   |
| 3   | M     | 326 | HIS  | CA-C-N  | -6.16 | 114.22      | 122.42   |
| 3   | M     | 326 | HIS  | C-N-CA  | -6.16 | 114.22      | 122.42   |
| 3   | M     | 44  | ASP  | N-CA-C  | -6.16 | 104.68      | 111.82   |
| 1   | A     | 541 | SER  | N-CA-C  | 6.16  | 120.26      | 112.87   |
| 2   | B     | 307 | ASN  | O-C-N   | 6.15  | 128.67      | 122.03   |
| 2   | B     | 570 | GLY  | CA-C-N  | -6.14 | 111.29      | 120.94   |
| 2   | B     | 570 | GLY  | C-N-CA  | -6.14 | 111.29      | 120.94   |
| 1   | A     | 449 | TRP  | CA-C-O  | -6.14 | 111.73      | 120.51   |
| 1   | A     | 586 | GLU  | N-CA-C  | -6.14 | 104.70      | 111.82   |
| 3   | M     | 293 | PRO  | CA-C-N  | -6.13 | 109.74      | 122.07   |
| 3   | M     | 293 | PRO  | C-N-CA  | -6.13 | 109.74      | 122.07   |
| 1   | A     | 572 | PHE  | N-CA-C  | 6.13  | 118.76      | 111.71   |
| 3   | M     | 331 | LEU  | N-CA-C  | -6.13 | 97.74       | 110.80   |
| 2   | B     | 571 | SER  | CA-C-N  | -6.13 | 110.99      | 120.31   |
| 2   | B     | 571 | SER  | C-N-CA  | -6.13 | 110.99      | 120.31   |
| 1   | A     | 277 | LYS  | O-C-N   | -6.13 | 115.17      | 122.46   |
| 1   | A     | 629 | LEU  | C-N-CD  | 6.13  | 150.13      | 125.00   |
| 2   | B     | 496 | LEU  | CA-C-O  | -6.13 | 112.92      | 119.97   |
| 3   | M     | 351 | SER  | N-CA-CB | -6.13 | 99.91       | 110.32   |
| 2   | B     | 585 | GLY  | CA-C-O  | -6.12 | 109.92      | 120.57   |
| 3   | M     | 226 | PHE  | CA-C-N  | -6.11 | 114.38      | 123.00   |
| 3   | M     | 226 | PHE  | C-N-CA  | -6.11 | 114.38      | 123.00   |
| 1   | A     | 490 | VAL  | CA-C-O  | -6.11 | 114.37      | 120.85   |
| 2   | B     | 184 | GLY  | CA-C-O  | 6.11  | 131.20      | 120.57   |
| 1   | A     | 527 | GLU  | O-C-N   | -6.10 | 115.65      | 122.12   |
| 3   | M     | 57  | GLY  | O-C-N   | -6.10 | 114.77      | 122.70   |
| 3   | M     | 79  | SER  | CA-C-O  | 6.10  | 128.13      | 121.06   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | M     | 395 | GLY  | CA-C-N  | -6.10 | 113.35      | 122.74   |
| 3   | M     | 395 | GLY  | C-N-CA  | -6.10 | 113.35      | 122.74   |
| 3   | M     | 339 | GLU  | CA-C-N  | -6.09 | 114.41      | 123.00   |
| 3   | M     | 339 | GLU  | C-N-CA  | -6.09 | 114.41      | 123.00   |
| 1   | A     | 259 | LEU  | O-C-N   | 6.09  | 128.42      | 122.09   |
| 2   | B     | 205 | PRO  | CA-C-O  | 6.09  | 127.88      | 119.18   |
| 2   | B     | 185 | LYS  | N-CA-C  | 6.08  | 117.91      | 111.28   |
| 1   | A     | 288 | THR  | CA-C-O  | -6.08 | 110.47      | 120.80   |
| 1   | A     | 589 | SER  | N-CA-C  | -6.08 | 105.72      | 113.01   |
| 3   | M     | 405 | THR  | N-CA-CB | -6.07 | 100.23      | 110.49   |
| 1   | A     | 192 | TYR  | N-CA-C  | 6.07  | 123.22      | 109.81   |
| 1   | A     | 304 | LEU  | N-CA-C  | 6.07  | 117.89      | 111.28   |
| 2   | B     | 166 | SER  | CA-C-O  | -6.06 | 114.37      | 121.16   |
| 1   | A     | 194 | GLU  | CA-C-O  | -6.06 | 114.12      | 120.55   |
| 3   | M     | 253 | ASN  | N-CA-C  | 6.06  | 123.21      | 109.81   |
| 3   | M     | 368 | ASP  | CA-C-N  | 6.06  | 127.42      | 119.84   |
| 3   | M     | 368 | ASP  | C-N-CA  | 6.06  | 127.42      | 119.84   |
| 3   | M     | 95  | THR  | N-CA-C  | -6.06 | 104.75      | 111.71   |
| 1   | A     | 320 | HIS  | N-CA-C  | -6.06 | 104.76      | 111.36   |
| 2   | B     | 384 | PHE  | CA-C-N  | 6.05  | 125.94      | 119.28   |
| 2   | B     | 384 | PHE  | C-N-CA  | 6.05  | 125.94      | 119.28   |
| 4   | S     | 84  | TYR  | CA-C-N  | -6.05 | 114.46      | 123.00   |
| 4   | S     | 84  | TYR  | C-N-CA  | -6.05 | 114.46      | 123.00   |
| 2   | B     | 88  | LYS  | CA-C-O  | -6.05 | 114.13      | 120.55   |
| 1   | A     | 442 | SER  | CA-C-N  | 6.05  | 134.04      | 121.94   |
| 1   | A     | 442 | SER  | C-N-CA  | 6.05  | 134.04      | 121.94   |
| 2   | B     | 354 | GLY  | CA-C-N  | 6.05  | 130.81      | 120.71   |
| 2   | B     | 354 | GLY  | C-N-CA  | 6.05  | 130.81      | 120.71   |
| 1   | A     | 505 | ASN  | O-C-N   | -6.05 | 114.22      | 122.33   |
| 1   | A     | 463 | ASP  | CA-C-N  | 6.05  | 132.85      | 121.97   |
| 1   | A     | 463 | ASP  | C-N-CA  | 6.05  | 132.85      | 121.97   |
| 2   | B     | 522 | GLU  | CB-CA-C | -6.05 | 102.96      | 111.85   |
| 1   | A     | 199 | ASN  | O-C-N   | 6.04  | 130.71      | 122.37   |
| 2   | B     | 279 | LEU  | CA-C-N  | -6.04 | 114.05      | 120.03   |
| 2   | B     | 279 | LEU  | C-N-CA  | -6.04 | 114.05      | 120.03   |
| 2   | B     | 407 | ASN  | CA-C-O  | -6.04 | 112.50      | 119.14   |
| 3   | M     | 471 | LYS  | CA-C-N  | -6.04 | 112.23      | 122.67   |
| 3   | M     | 471 | LYS  | C-N-CA  | -6.04 | 112.23      | 122.67   |
| 1   | A     | 505 | ASN  | CA-C-N  | -6.04 | 112.30      | 120.87   |
| 1   | A     | 505 | ASN  | C-N-CA  | -6.04 | 112.30      | 120.87   |
| 2   | B     | 424 | PHE  | N-CA-C  | 6.04  | 117.26      | 109.72   |
| 2   | B     | 577 | ASN  | N-CA-CB | -6.04 | 101.28      | 111.30   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 586 | GLU  | CA-C-O  | 6.03  | 126.91      | 119.97   |
| 1   | A     | 144 | GLY  | O-C-N   | 6.03  | 130.54      | 122.70   |
| 2   | B     | 397 | GLN  | O-C-N   | 6.03  | 129.02      | 122.15   |
| 1   | A     | 621 | LEU  | C-N-CD  | 6.03  | 149.71      | 125.00   |
| 4   | S     | 67  | GLU  | N-CA-C  | -6.02 | 102.42      | 110.55   |
| 1   | A     | 83  | ASP  | CA-C-O  | 6.02  | 127.78      | 120.62   |
| 3   | M     | 450 | GLU  | O-C-N   | -6.01 | 114.16      | 122.46   |
| 2   | B     | 462 | ASN  | N-CA-C  | -6.01 | 103.09      | 111.39   |
| 3   | M     | 453 | ASP  | O-C-N   | -6.01 | 115.38      | 123.19   |
| 1   | A     | 139 | ASP  | N-CA-C  | 6.00  | 117.90      | 111.36   |
| 4   | S     | 86  | THR  | CA-C-N  | -6.00 | 114.53      | 122.99   |
| 4   | S     | 86  | THR  | C-N-CA  | -6.00 | 114.53      | 122.99   |
| 1   | A     | 259 | LEU  | CA-C-O  | -6.00 | 114.48      | 120.90   |
| 1   | A     | 345 | ASN  | O-C-N   | 5.99  | 131.21      | 123.06   |
| 3   | M     | 477 | GLY  | N-CA-C  | 5.99  | 122.23      | 111.03   |
| 1   | A     | 136 | GLY  | O-C-N   | -5.99 | 114.91      | 122.70   |
| 3   | M     | 354 | ASP  | CB-CA-C | 5.99  | 120.81      | 109.37   |
| 3   | M     | 132 | GLY  | O-C-N   | 5.99  | 130.48      | 122.70   |
| 2   | B     | 200 | MET  | CA-C-N  | -5.99 | 110.11      | 121.54   |
| 2   | B     | 200 | MET  | C-N-CA  | -5.99 | 110.11      | 121.54   |
| 1   | A     | 393 | LYS  | O-C-N   | 5.98  | 128.97      | 122.15   |
| 2   | B     | 33  | SER  | CA-C-O  | -5.98 | 111.28      | 119.12   |
| 3   | M     | 375 | LYS  | CA-C-N  | -5.98 | 115.09      | 122.93   |
| 3   | M     | 375 | LYS  | C-N-CA  | -5.98 | 115.09      | 122.93   |
| 1   | A     | 173 | THR  | N-CA-C  | -5.98 | 102.63      | 110.53   |
| 4   | S     | 42  | ARG  | N-CA-C  | -5.98 | 100.75      | 110.20   |
| 1   | A     | 435 | ILE  | CA-C-N  | -5.98 | 111.22      | 120.31   |
| 1   | A     | 435 | ILE  | C-N-CA  | -5.98 | 111.22      | 120.31   |
| 3   | M     | 106 | LYS  | CA-C-O  | 5.98  | 129.06      | 120.51   |
| 1   | A     | 354 | GLN  | CA-C-O  | -5.97 | 114.18      | 120.63   |
| 2   | B     | 76  | SER  | N-CA-C  | -5.97 | 105.99      | 113.28   |
| 2   | B     | 507 | ALA  | CA-C-N  | 5.97  | 128.88      | 120.28   |
| 2   | B     | 507 | ALA  | C-N-CA  | 5.97  | 128.88      | 120.28   |
| 2   | B     | 292 | GLU  | CA-C-O  | 5.96  | 126.83      | 119.79   |
| 3   | M     | 266 | ASP  | CA-C-O  | 5.95  | 127.23      | 120.80   |
| 3   | M     | 274 | ASP  | O-C-N   | -5.95 | 114.95      | 122.27   |
| 3   | M     | 309 | GLN  | CA-C-O  | -5.95 | 114.58      | 120.70   |
| 4   | S     | 56  | SER  | CA-C-N  | 5.95  | 132.48      | 122.79   |
| 4   | S     | 56  | SER  | C-N-CA  | 5.95  | 132.48      | 122.79   |
| 1   | A     | 482 | ILE  | N-CA-C  | -5.94 | 104.94      | 110.53   |
| 2   | B     | 53  | SER  | N-CA-C  | -5.94 | 101.05      | 109.96   |
| 2   | B     | 146 | LYS  | O-C-N   | -5.94 | 115.39      | 122.46   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 273 | SER  | CA-C-O  | 5.94  | 125.74      | 119.80   |
| 2   | B     | 471 | TYR  | CA-C-N  | 5.94  | 128.60      | 120.46   |
| 2   | B     | 471 | TYR  | C-N-CA  | 5.94  | 128.60      | 120.46   |
| 4   | S     | 147 | ASN  | CA-C-O  | -5.93 | 113.15      | 119.97   |
| 2   | B     | 584 | SER  | CB-CA-C | -5.93 | 100.77      | 110.85   |
| 4   | S     | 15  | ARG  | N-CA-C  | -5.93 | 105.30      | 113.18   |
| 2   | B     | 149 | SER  | CA-C-N  | -5.92 | 112.37      | 122.56   |
| 2   | B     | 149 | SER  | C-N-CA  | -5.92 | 112.37      | 122.56   |
| 2   | B     | 197 | LYS  | O-C-N   | 5.92  | 130.47      | 122.59   |
| 1   | A     | 627 | GLU  | CA-C-O  | -5.92 | 112.91      | 120.31   |
| 3   | M     | 227 | GLU  | CA-C-N  | -5.92 | 112.46      | 120.87   |
| 3   | M     | 227 | GLU  | C-N-CA  | -5.92 | 112.46      | 120.87   |
| 3   | M     | 341 | SER  | CA-C-N  | -5.92 | 113.66      | 123.37   |
| 3   | M     | 341 | SER  | C-N-CA  | -5.92 | 113.66      | 123.37   |
| 3   | M     | 238 | GLY  | CA-C-N  | -5.92 | 113.86      | 122.44   |
| 3   | M     | 238 | GLY  | C-N-CA  | -5.92 | 113.86      | 122.44   |
| 3   | M     | 265 | ASN  | CA-C-N  | -5.92 | 111.85      | 121.26   |
| 3   | M     | 265 | ASN  | C-N-CA  | -5.92 | 111.85      | 121.26   |
| 1   | A     | 323 | CYS  | O-C-N   | -5.92 | 114.56      | 122.43   |
| 4   | S     | 121 | LEU  | CA-C-N  | -5.90 | 113.00      | 120.56   |
| 4   | S     | 121 | LEU  | C-N-CA  | -5.90 | 113.00      | 120.56   |
| 1   | A     | 98  | ASN  | N-CA-CB | 5.90  | 119.26      | 110.29   |
| 3   | M     | 414 | CYS  | CA-C-N  | -5.90 | 115.45      | 123.12   |
| 3   | M     | 414 | CYS  | C-N-CA  | -5.90 | 115.45      | 123.12   |
| 2   | B     | 478 | LEU  | CA-C-N  | -5.89 | 110.95      | 120.62   |
| 2   | B     | 478 | LEU  | C-N-CA  | -5.89 | 110.95      | 120.62   |
| 3   | M     | 41  | LEU  | CA-C-N  | -5.89 | 112.39      | 120.28   |
| 3   | M     | 41  | LEU  | C-N-CA  | -5.89 | 112.39      | 120.28   |
| 4   | S     | 89  | VAL  | CA-C-N  | -5.89 | 108.95      | 121.32   |
| 4   | S     | 89  | VAL  | C-N-CA  | -5.89 | 108.95      | 121.32   |
| 2   | B     | 466 | SER  | CA-C-O  | -5.89 | 114.18      | 120.42   |
| 1   | A     | 351 | ARG  | CA-C-N  | -5.88 | 113.25      | 122.49   |
| 1   | A     | 351 | ARG  | C-N-CA  | -5.88 | 113.25      | 122.49   |
| 2   | B     | 313 | SER  | N-CA-C  | 5.88  | 123.33      | 110.80   |
| 3   | M     | 61  | GLU  | N-CA-CB | 5.88  | 120.00      | 110.42   |
| 3   | M     | 372 | ILE  | CB-CA-C | -5.88 | 106.64      | 113.22   |
| 2   | B     | 255 | TYR  | CA-C-N  | 5.87  | 128.15      | 120.28   |
| 2   | B     | 255 | TYR  | C-N-CA  | 5.87  | 128.15      | 120.28   |
| 1   | A     | 65  | ASN  | CA-C-N  | 5.87  | 128.62      | 120.29   |
| 1   | A     | 65  | ASN  | C-N-CA  | 5.87  | 128.62      | 120.29   |
| 1   | A     | 138 | ASN  | CA-C-O  | -5.87 | 115.62      | 122.37   |
| 2   | B     | 383 | VAL  | O-C-N   | 5.87  | 129.03      | 122.75   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 510 | THR  | CA-C-N  | 5.86  | 128.49      | 120.46   |
| 1   | A     | 510 | THR  | C-N-CA  | 5.86  | 128.49      | 120.46   |
| 1   | A     | 234 | ILE  | N-CA-C  | -5.86 | 103.45      | 111.89   |
| 2   | B     | 262 | LYS  | C-N-CD  | 5.86  | 149.03      | 125.00   |
| 1   | A     | 89  | PHE  | N-CA-C  | 5.86  | 117.66      | 111.28   |
| 2   | B     | 433 | VAL  | O-C-N   | 5.86  | 132.56      | 121.84   |
| 3   | M     | 432 | THR  | CA-C-N  | -5.86 | 115.15      | 123.11   |
| 3   | M     | 432 | THR  | C-N-CA  | -5.86 | 115.15      | 123.11   |
| 1   | A     | 322 | PHE  | CA-C-N  | 5.85  | 131.88      | 120.99   |
| 1   | A     | 322 | PHE  | C-N-CA  | 5.85  | 131.88      | 120.99   |
| 3   | M     | 415 | ILE  | CA-C-N  | -5.85 | 114.93      | 123.00   |
| 3   | M     | 415 | ILE  | C-N-CA  | -5.85 | 114.93      | 123.00   |
| 3   | M     | 466 | LEU  | CA-C-N  | 5.85  | 132.99      | 122.64   |
| 3   | M     | 466 | LEU  | C-N-CA  | 5.85  | 132.99      | 122.64   |
| 1   | A     | 472 | LYS  | CA-C-O  | -5.85 | 113.24      | 119.97   |
| 2   | B     | 298 | ASP  | O-C-N   | 5.85  | 130.19      | 122.30   |
| 1   | A     | 192 | TYR  | O-C-N   | 5.84  | 128.04      | 121.32   |
| 2   | B     | 265 | VAL  | CA-C-N  | 5.84  | 130.38      | 122.90   |
| 2   | B     | 265 | VAL  | C-N-CA  | 5.84  | 130.38      | 122.90   |
| 1   | A     | 323 | CYS  | CA-C-O  | -5.83 | 111.75      | 119.10   |
| 2   | B     | 330 | SER  | CB-CA-C | 5.83  | 118.66      | 109.27   |
| 2   | B     | 114 | ASN  | O-C-N   | 5.83  | 128.79      | 122.15   |
| 3   | M     | 227 | GLU  | O-C-N   | -5.83 | 116.51      | 123.27   |
| 3   | M     | 8   | THR  | CA-C-O  | -5.83 | 114.62      | 121.44   |
| 2   | B     | 506 | ASN  | O-C-N   | 5.83  | 130.14      | 122.33   |
| 2   | B     | 577 | ASN  | CA-C-O  | -5.83 | 112.66      | 120.64   |
| 3   | M     | 73  | ASN  | CA-C-N  | -5.83 | 113.49      | 122.87   |
| 3   | M     | 73  | ASN  | C-N-CA  | -5.83 | 113.49      | 122.87   |
| 1   | A     | 468 | SER  | O-C-N   | 5.82  | 130.23      | 122.43   |
| 2   | B     | 265 | VAL  | O-C-N   | 5.82  | 128.61      | 122.67   |
| 2   | B     | 269 | SER  | N-CA-C  | 5.82  | 120.12      | 113.19   |
| 1   | A     | 595 | GLU  | O-C-N   | 5.82  | 128.37      | 122.09   |
| 2   | B     | 21  | GLU  | N-CA-C  | 5.82  | 120.65      | 113.50   |
| 3   | M     | 134 | PRO  | N-CA-CB | 5.82  | 108.75      | 103.34   |
| 4   | S     | 55  | PRO  | N-CA-C  | 5.82  | 121.40      | 113.84   |
| 2   | B     | 229 | HIS  | O-C-N   | 5.81  | 130.68      | 122.20   |
| 2   | B     | 325 | LEU  | N-CA-C  | -5.80 | 105.46      | 112.54   |
| 2   | B     | 518 | ILE  | CA-C-O  | -5.80 | 112.23      | 119.43   |
| 3   | M     | 3   | LEU  | CA-C-N  | -5.80 | 112.71      | 122.29   |
| 3   | M     | 3   | LEU  | C-N-CA  | -5.80 | 112.71      | 122.29   |
| 1   | A     | 533 | ILE  | N-CA-C  | 5.80  | 115.98      | 110.53   |
| 1   | A     | 224 | GLU  | N-CA-C  | -5.80 | 104.96      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 473 | ILE  | CA-C-N | -5.80 | 113.54      | 119.98   |
| 1   | A     | 473 | ILE  | C-N-CA | -5.80 | 113.54      | 119.98   |
| 3   | M     | 120 | ARG  | CA-C-O | -5.80 | 112.47      | 119.49   |
| 1   | A     | 244 | LEU  | CA-C-N | -5.79 | 111.53      | 121.09   |
| 1   | A     | 244 | LEU  | C-N-CA | -5.79 | 111.53      | 121.09   |
| 2   | B     | 242 | SER  | N-CA-C | 5.79  | 123.13      | 110.80   |
| 2   | B     | 335 | LYS  | O-C-N  | -5.79 | 115.98      | 122.12   |
| 2   | B     | 583 | PHE  | O-C-N  | 5.79  | 130.02      | 122.38   |
| 1   | A     | 411 | GLU  | N-CA-C | 5.79  | 120.49      | 112.45   |
| 1   | A     | 510 | THR  | CA-C-O | -5.78 | 114.74      | 120.70   |
| 4   | S     | 66  | ASP  | CA-C-O | 5.78  | 127.20      | 120.49   |
| 3   | M     | 361 | GLN  | CA-C-N | -5.78 | 114.16      | 123.23   |
| 3   | M     | 361 | GLN  | C-N-CA | -5.78 | 114.16      | 123.23   |
| 4   | S     | 101 | LEU  | CA-C-N | 5.78  | 129.79      | 120.55   |
| 4   | S     | 101 | LEU  | C-N-CA | 5.78  | 129.79      | 120.55   |
| 2   | B     | 465 | ALA  | N-CA-C | 5.78  | 117.58      | 111.28   |
| 2   | B     | 191 | GLU  | CA-C-O | -5.77 | 113.83      | 120.24   |
| 2   | B     | 80  | GLN  | O-C-N  | 5.77  | 128.23      | 122.12   |
| 2   | B     | 356 | LYS  | N-CA-C | -5.77 | 104.19      | 111.11   |
| 2   | B     | 577 | ASN  | C-N-CD | 5.76  | 148.62      | 125.00   |
| 2   | B     | 456 | ASP  | CA-C-N | 5.76  | 128.47      | 120.29   |
| 2   | B     | 456 | ASP  | C-N-CA | 5.76  | 128.47      | 120.29   |
| 3   | M     | 358 | ILE  | CA-C-N | -5.76 | 114.85      | 122.85   |
| 3   | M     | 358 | ILE  | C-N-CA | -5.76 | 114.85      | 122.85   |
| 1   | A     | 176 | TYR  | O-C-N  | 5.76  | 129.71      | 122.23   |
| 2   | B     | 541 | GLY  | CA-C-N | 5.76  | 127.04      | 119.84   |
| 2   | B     | 541 | GLY  | C-N-CA | 5.76  | 127.04      | 119.84   |
| 2   | B     | 222 | HIS  | O-C-N  | 5.75  | 130.10      | 122.56   |
| 2   | B     | 297 | PRO  | CA-C-O | -5.75 | 110.14      | 120.60   |
| 2   | B     | 406 | SER  | CA-C-N | -5.75 | 111.98      | 121.92   |
| 2   | B     | 406 | SER  | C-N-CA | -5.75 | 111.98      | 121.92   |
| 2   | B     | 488 | ARG  | CA-C-O | -5.74 | 113.86      | 120.24   |
| 2   | B     | 523 | PHE  | CA-C-O | 5.74  | 128.72      | 120.51   |
| 1   | A     | 173 | THR  | CA-C-N | 5.74  | 135.80      | 121.80   |
| 1   | A     | 173 | THR  | C-N-CA | 5.74  | 135.80      | 121.80   |
| 3   | M     | 428 | VAL  | CA-C-N | -5.74 | 110.59      | 121.54   |
| 3   | M     | 428 | VAL  | C-N-CA | -5.74 | 110.59      | 121.54   |
| 1   | A     | 355 | LEU  | CA-C-O | -5.73 | 113.38      | 119.97   |
| 1   | A     | 535 | ILE  | CA-C-O | -5.73 | 111.06      | 120.80   |
| 1   | A     | 328 | PRO  | N-CA-C | -5.73 | 106.39      | 113.84   |
| 1   | A     | 207 | LEU  | CA-C-N | -5.73 | 113.61      | 122.49   |
| 1   | A     | 207 | LEU  | C-N-CA | -5.73 | 113.61      | 122.49   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 190 | GLU  | CA-C-O  | -5.73 | 114.48      | 120.55   |
| 1   | A     | 210 | ASP  | N-CA-C  | 5.72  | 118.46      | 111.82   |
| 1   | A     | 228 | LYS  | N-CA-C  | 5.72  | 118.72      | 111.69   |
| 3   | M     | 294 | ASP  | CB-CA-C | 5.72  | 119.84      | 109.83   |
| 2   | B     | 298 | ASP  | CA-C-O  | -5.72 | 113.16      | 120.31   |
| 1   | A     | 149 | GLY  | O-C-N   | 5.71  | 130.12      | 122.70   |
| 1   | A     | 525 | LEU  | CA-C-N  | -5.71 | 115.59      | 122.90   |
| 1   | A     | 525 | LEU  | C-N-CA  | -5.71 | 115.59      | 122.90   |
| 2   | B     | 286 | ILE  | N-CA-CB | 5.71  | 119.33      | 110.14   |
| 1   | A     | 114 | PHE  | CA-C-N  | -5.71 | 112.43      | 120.82   |
| 1   | A     | 114 | PHE  | C-N-CA  | -5.71 | 112.43      | 120.82   |
| 4   | S     | 125 | TRP  | N-CA-C  | -5.71 | 104.26      | 111.11   |
| 2   | B     | 212 | VAL  | N-CA-C  | -5.70 | 105.55      | 110.74   |
| 2   | B     | 171 | GLY  | O-C-N   | 5.70  | 130.11      | 122.70   |
| 2   | B     | 106 | LEU  | O-C-N   | 5.70  | 128.89      | 122.22   |
| 4   | S     | 143 | GLU  | O-C-N   | 5.70  | 130.45      | 123.44   |
| 4   | S     | 63  | ASN  | N-CA-CB | 5.70  | 119.54      | 110.65   |
| 1   | A     | 620 | GLY  | O-C-N   | 5.69  | 130.74      | 122.26   |
| 3   | M     | 398 | ILE  | CA-C-N  | -5.69 | 114.17      | 122.19   |
| 3   | M     | 398 | ILE  | C-N-CA  | -5.69 | 114.17      | 122.19   |
| 2   | B     | 353 | GLN  | O-C-N   | 5.68  | 128.15      | 122.12   |
| 1   | A     | 358 | ARG  | CA-C-O  | -5.68 | 113.68      | 120.10   |
| 1   | A     | 528 | ASN  | O-C-N   | -5.68 | 113.09      | 121.89   |
| 2   | B     | 124 | GLN  | O-C-N   | 5.68  | 128.62      | 122.15   |
| 3   | M     | 457 | GLY  | CA-C-O  | 5.68  | 125.09      | 118.96   |
| 2   | B     | 44  | PRO  | CA-C-O  | -5.67 | 111.01      | 119.86   |
| 1   | A     | 199 | ASN  | CA-C-O  | -5.67 | 112.42      | 119.28   |
| 1   | A     | 419 | ILE  | CA-C-N  | 5.67  | 132.62      | 122.13   |
| 1   | A     | 419 | ILE  | C-N-CA  | 5.67  | 132.62      | 122.13   |
| 2   | B     | 156 | HIS  | CA-C-O  | -5.67 | 112.40      | 120.51   |
| 1   | A     | 118 | SER  | N-CA-C  | 5.66  | 118.39      | 111.82   |
| 1   | A     | 277 | LYS  | N-CA-C  | 5.66  | 118.41      | 108.56   |
| 3   | M     | 341 | SER  | CA-C-O  | 5.66  | 126.47      | 120.36   |
| 2   | B     | 446 | TRP  | CA-C-O  | -5.66 | 112.73      | 119.35   |
| 2   | B     | 420 | ALA  | N-CA-C  | 5.65  | 118.17      | 111.33   |
| 3   | M     | 83  | SER  | N-CA-C  | -5.65 | 99.23       | 108.67   |
| 2   | B     | 326 | TYR  | CA-C-N  | -5.65 | 111.28      | 120.71   |
| 2   | B     | 326 | TYR  | C-N-CA  | -5.65 | 111.28      | 120.71   |
| 2   | B     | 537 | PHE  | N-CA-C  | 5.65  | 118.17      | 111.33   |
| 1   | A     | 345 | ASN  | N-CA-C  | 5.65  | 119.06      | 107.37   |
| 2   | B     | 538 | SER  | CA-C-N  | -5.65 | 113.79      | 122.60   |
| 2   | B     | 538 | SER  | C-N-CA  | -5.65 | 113.79      | 122.60   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | S     | 137 | GLN  | CA-C-N  | 5.64  | 132.65      | 121.53   |
| 4   | S     | 137 | GLN  | C-N-CA  | 5.64  | 132.65      | 121.53   |
| 3   | M     | 237 | THR  | CA-C-O  | 5.64  | 127.83      | 121.51   |
| 1   | A     | 248 | ASP  | CA-C-N  | 5.63  | 129.56      | 121.50   |
| 1   | A     | 248 | ASP  | C-N-CA  | 5.63  | 129.56      | 121.50   |
| 1   | A     | 544 | SER  | CA-C-N  | 5.63  | 127.83      | 120.28   |
| 1   | A     | 544 | SER  | C-N-CA  | 5.63  | 127.83      | 120.28   |
| 2   | B     | 218 | CYS  | CA-C-N  | 5.63  | 132.33      | 121.18   |
| 2   | B     | 218 | CYS  | C-N-CA  | 5.63  | 132.33      | 121.18   |
| 3   | M     | 18  | TYR  | CA-C-N  | -5.63 | 115.23      | 123.00   |
| 3   | M     | 18  | TYR  | C-N-CA  | -5.63 | 115.23      | 123.00   |
| 3   | M     | 220 | GLU  | CA-C-N  | -5.63 | 115.17      | 123.05   |
| 3   | M     | 220 | GLU  | C-N-CA  | -5.63 | 115.17      | 123.05   |
| 1   | A     | 497 | LYS  | O-C-N   | 5.62  | 128.08      | 122.12   |
| 2   | B     | 315 | PRO  | O-C-N   | 5.62  | 128.97      | 122.17   |
| 1   | A     | 505 | ASN  | CA-C-O  | 5.62  | 126.42      | 119.79   |
| 2   | B     | 222 | HIS  | CA-C-O  | -5.62 | 115.62      | 122.64   |
| 4   | S     | 2   | ILE  | CA-C-N  | -5.62 | 111.78      | 121.66   |
| 4   | S     | 2   | ILE  | C-N-CA  | -5.62 | 111.78      | 121.66   |
| 2   | B     | 167 | ALA  | O-C-N   | 5.61  | 129.53      | 122.23   |
| 1   | A     | 193 | PRO  | CA-C-N  | -5.61 | 112.76      | 120.28   |
| 1   | A     | 193 | PRO  | C-N-CA  | -5.61 | 112.76      | 120.28   |
| 2   | B     | 275 | ARG  | O-C-N   | 5.61  | 129.55      | 122.65   |
| 3   | M     | 93  | LEU  | O-C-N   | 5.61  | 128.54      | 122.15   |
| 2   | B     | 274 | PRO  | CA-N-CD | -5.61 | 104.15      | 112.00   |
| 1   | A     | 176 | TYR  | CA-C-N  | 5.60  | 127.73      | 120.56   |
| 1   | A     | 176 | TYR  | C-N-CA  | 5.60  | 127.73      | 120.56   |
| 4   | S     | 89  | VAL  | O-C-N   | -5.60 | 116.98      | 122.97   |
| 1   | A     | 269 | LYS  | O-C-N   | 5.59  | 129.15      | 122.27   |
| 2   | B     | 561 | ASP  | O-C-N   | 5.59  | 130.03      | 122.59   |
| 3   | M     | 223 | HIS  | CA-C-N  | -5.59 | 114.65      | 122.71   |
| 3   | M     | 223 | HIS  | C-N-CA  | -5.59 | 114.65      | 122.71   |
| 3   | M     | 397 | TRP  | CA-C-N  | -5.59 | 115.50      | 123.11   |
| 3   | M     | 397 | TRP  | C-N-CA  | -5.59 | 115.50      | 123.11   |
| 3   | M     | 383 | HIS  | N-CA-C  | 5.59  | 122.71      | 110.80   |
| 1   | A     | 306 | GLU  | N-CA-C  | 5.59  | 122.71      | 110.80   |
| 4   | S     | 34  | GLN  | CA-C-O  | -5.59 | 113.54      | 119.97   |
| 2   | B     | 522 | GLU  | CA-C-N  | 5.58  | 132.21      | 121.54   |
| 2   | B     | 522 | GLU  | C-N-CA  | 5.58  | 132.21      | 121.54   |
| 1   | A     | 488 | ARG  | CA-C-O  | -5.58 | 114.50      | 120.42   |
| 3   | M     | 420 | THR  | N-CA-C  | -5.58 | 106.31      | 113.23   |
| 4   | S     | 85  | PHE  | CA-C-N  | -5.58 | 115.31      | 123.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | S     | 85  | PHE  | C-N-CA  | -5.58 | 115.31      | 123.00   |
| 1   | A     | 521 | GLU  | CA-C-N  | -5.57 | 113.73      | 122.65   |
| 1   | A     | 521 | GLU  | C-N-CA  | -5.57 | 113.73      | 122.65   |
| 1   | A     | 623 | MET  | CA-C-O  | -5.57 | 113.22      | 119.79   |
| 2   | B     | 90  | ILE  | N-CA-C  | -5.57 | 103.87      | 111.89   |
| 2   | B     | 225 | LEU  | O-C-N   | 5.57  | 129.82      | 122.30   |
| 3   | M     | 325 | LEU  | CA-C-N  | -5.57 | 115.20      | 123.11   |
| 3   | M     | 325 | LEU  | C-N-CA  | -5.57 | 115.20      | 123.11   |
| 1   | A     | 191 | GLN  | CA-C-N  | 5.57  | 135.38      | 121.80   |
| 1   | A     | 191 | GLN  | C-N-CA  | 5.57  | 135.38      | 121.80   |
| 2   | B     | 299 | LEU  | N-CA-C  | -5.56 | 105.13      | 111.14   |
| 2   | B     | 536 | ASN  | CA-C-N  | 5.56  | 128.00      | 120.38   |
| 2   | B     | 536 | ASN  | C-N-CA  | 5.56  | 128.00      | 120.38   |
| 4   | S     | 59  | LEU  | CA-C-O  | 5.56  | 127.20      | 120.81   |
| 2   | B     | 556 | LEU  | CA-C-O  | -5.56 | 114.53      | 120.42   |
| 3   | M     | 327 | PHE  | CA-C-N  | -5.56 | 115.03      | 122.42   |
| 3   | M     | 327 | PHE  | C-N-CA  | -5.56 | 115.03      | 122.42   |
| 1   | A     | 521 | GLU  | N-CA-C  | 5.56  | 117.42      | 111.36   |
| 1   | A     | 262 | ASN  | CA-C-N  | -5.55 | 111.71      | 120.60   |
| 1   | A     | 262 | ASN  | C-N-CA  | -5.55 | 111.71      | 120.60   |
| 2   | B     | 505 | ASP  | N-CA-C  | -5.55 | 105.23      | 111.28   |
| 2   | B     | 506 | ASN  | CA-C-O  | -5.55 | 113.25      | 119.79   |
| 2   | B     | 579 | PRO  | O-C-N   | -5.55 | 115.15      | 122.64   |
| 3   | M     | 79  | SER  | N-CA-C  | -5.54 | 100.64      | 109.23   |
| 1   | A     | 66  | SER  | CA-C-N  | 5.54  | 127.70      | 120.28   |
| 1   | A     | 66  | SER  | C-N-CA  | 5.54  | 127.70      | 120.28   |
| 2   | B     | 304 | GLN  | CA-C-O  | -5.53 | 113.85      | 120.10   |
| 3   | M     | 25  | PRO  | N-CA-C  | -5.53 | 98.28       | 112.10   |
| 1   | A     | 138 | ASN  | N-CA-CB | 5.53  | 118.03      | 110.57   |
| 2   | B     | 316 | THR  | CA-C-O  | -5.53 | 115.01      | 120.70   |
| 4   | S     | 58  | LEU  | CB-CA-C | 5.52  | 119.48      | 109.37   |
| 1   | A     | 291 | ILE  | O-C-N   | 5.51  | 129.07      | 121.90   |
| 2   | B     | 542 | PRO  | O-C-N   | 5.51  | 130.09      | 122.64   |
| 4   | S     | 97  | ALA  | O-C-N   | 5.51  | 128.48      | 122.20   |
| 3   | M     | 20  | LEU  | O-C-N   | -5.51 | 116.88      | 123.27   |
| 1   | A     | 275 | LEU  | C-N-CD  | 5.51  | 147.57      | 125.00   |
| 2   | B     | 90  | ILE  | CA-C-N  | -5.51 | 112.41      | 122.38   |
| 2   | B     | 90  | ILE  | C-N-CA  | -5.51 | 112.41      | 122.38   |
| 1   | A     | 102 | GLN  | CA-C-N  | 5.50  | 128.21      | 120.28   |
| 1   | A     | 102 | GLN  | C-N-CA  | 5.50  | 128.21      | 120.28   |
| 2   | B     | 377 | TYR  | O-C-N   | 5.50  | 128.90      | 122.24   |
| 1   | A     | 310 | GLU  | O-C-N   | 5.50  | 127.95      | 122.12   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 279 | LEU  | N-CA-C  | 5.50  | 116.91      | 110.31   |
| 3   | M     | 52  | ASP  | N-CA-CB | -5.50 | 101.84      | 110.30   |
| 1   | A     | 217 | ALA  | CA-C-N  | 5.49  | 127.64      | 120.28   |
| 1   | A     | 217 | ALA  | C-N-CA  | 5.49  | 127.64      | 120.28   |
| 3   | M     | 328 | GLN  | CA-C-O  | 5.49  | 126.45      | 120.58   |
| 1   | A     | 95  | MET  | CA-C-N  | -5.49 | 110.97      | 121.94   |
| 1   | A     | 95  | MET  | C-N-CA  | -5.49 | 110.97      | 121.94   |
| 3   | M     | 310 | VAL  | N-CA-C  | -5.48 | 105.03      | 110.62   |
| 3   | M     | 84  | LYS  | N-CA-C  | 5.48  | 122.47      | 110.80   |
| 1   | A     | 231 | GLN  | CA-C-O  | -5.48 | 112.66      | 120.16   |
| 3   | M     | 266 | ASP  | O-C-N   | 5.48  | 130.57      | 123.07   |
| 1   | A     | 633 | PHE  | N-CA-C  | -5.48 | 105.31      | 111.28   |
| 3   | M     | 354 | ASP  | N-CA-CB | 5.48  | 120.36      | 110.83   |
| 3   | M     | 353 | VAL  | N-CA-C  | -5.47 | 100.59      | 108.53   |
| 3   | M     | 384 | GLY  | N-CA-C  | -5.47 | 103.26      | 111.19   |
| 4   | S     | 24  | ASP  | CA-C-N  | 5.47  | 126.93      | 120.09   |
| 4   | S     | 24  | ASP  | C-N-CA  | 5.47  | 126.93      | 120.09   |
| 4   | S     | 119 | LEU  | O-C-N   | 5.47  | 129.66      | 122.33   |
| 1   | A     | 375 | VAL  | N-CA-C  | -5.47 | 104.39      | 110.62   |
| 3   | M     | 5   | PHE  | CA-C-N  | -5.47 | 114.01      | 122.59   |
| 3   | M     | 5   | PHE  | C-N-CA  | -5.47 | 114.01      | 122.59   |
| 2   | B     | 336 | ASN  | CA-C-O  | 5.46  | 128.32      | 120.51   |
| 2   | B     | 352 | ASN  | CA-C-N  | 5.46  | 127.60      | 120.28   |
| 2   | B     | 352 | ASN  | C-N-CA  | 5.46  | 127.60      | 120.28   |
| 1   | A     | 350 | SER  | N-CA-C  | -5.46 | 105.33      | 111.28   |
| 3   | M     | 239 | SER  | CA-C-N  | -5.46 | 116.06      | 122.93   |
| 3   | M     | 239 | SER  | C-N-CA  | -5.46 | 116.06      | 122.93   |
| 4   | S     | 79  | ASN  | CA-C-O  | -5.45 | 114.53      | 120.36   |
| 1   | A     | 308 | ASP  | CA-C-O  | -5.45 | 110.83      | 119.23   |
| 1   | A     | 396 | VAL  | CA-C-N  | -5.45 | 113.17      | 122.11   |
| 1   | A     | 396 | VAL  | C-N-CA  | -5.45 | 113.17      | 122.11   |
| 2   | B     | 141 | ALA  | CA-C-N  | -5.45 | 111.86      | 120.63   |
| 2   | B     | 141 | ALA  | C-N-CA  | -5.45 | 111.86      | 120.63   |
| 4   | S     | 91  | ASP  | CA-C-N  | -5.45 | 113.55      | 122.54   |
| 4   | S     | 91  | ASP  | C-N-CA  | -5.45 | 113.55      | 122.54   |
| 1   | A     | 302 | ASN  | N-CA-CB | 5.44  | 119.69      | 110.49   |
| 2   | B     | 511 | ILE  | CA-C-N  | -5.44 | 113.59      | 120.56   |
| 2   | B     | 511 | ILE  | C-N-CA  | -5.44 | 113.59      | 120.56   |
| 2   | B     | 75  | ASP  | CA-C-N  | 5.44  | 132.18      | 122.06   |
| 2   | B     | 75  | ASP  | C-N-CA  | 5.44  | 132.18      | 122.06   |
| 2   | B     | 32  | GLU  | O-C-N   | 5.43  | 130.36      | 122.43   |
| 2   | B     | 374 | PHE  | CA-C-N  | -5.43 | 112.98      | 120.26   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 374 | PHE  | C-N-CA  | -5.43 | 112.98      | 120.26   |
| 2   | B     | 438 | ARG  | CA-C-N  | -5.43 | 113.06      | 120.44   |
| 2   | B     | 438 | ARG  | C-N-CA  | -5.43 | 113.06      | 120.44   |
| 2   | B     | 57  | ARG  | O-C-N   | 5.42  | 130.25      | 122.28   |
| 2   | B     | 207 | VAL  | O-C-N   | 5.42  | 132.22      | 121.91   |
| 2   | B     | 464 | SER  | N-CA-C  | -5.42 | 103.32      | 110.43   |
| 1   | A     | 278 | ILE  | O-C-N   | -5.42 | 114.33      | 123.00   |
| 1   | A     | 528 | ASN  | CA-C-N  | -5.42 | 111.14      | 120.79   |
| 1   | A     | 528 | ASN  | C-N-CA  | -5.42 | 111.14      | 120.79   |
| 4   | S     | 82  | THR  | N-CA-C  | 5.42  | 120.56      | 113.30   |
| 2   | B     | 473 | ASN  | O-C-N   | 5.41  | 128.32      | 122.15   |
| 3   | M     | 267 | ILE  | N-CA-C  | -5.41 | 101.69      | 108.84   |
| 1   | A     | 627 | GLU  | O-C-N   | 5.41  | 129.60      | 122.30   |
| 4   | S     | 143 | GLU  | CA-C-O  | 5.41  | 127.51      | 120.21   |
| 3   | M     | 267 | ILE  | CA-C-N  | -5.40 | 110.82      | 121.41   |
| 3   | M     | 267 | ILE  | C-N-CA  | -5.40 | 110.82      | 121.41   |
| 1   | A     | 201 | ASP  | O-C-N   | 5.40  | 128.31      | 122.15   |
| 3   | M     | 119 | ASP  | CA-C-O  | -5.40 | 114.70      | 120.42   |
| 1   | A     | 242 | GLU  | N-CA-CB | 5.40  | 117.98      | 109.83   |
| 2   | B     | 125 | LYS  | CA-C-N  | 5.40  | 128.05      | 120.28   |
| 2   | B     | 125 | LYS  | C-N-CA  | 5.40  | 128.05      | 120.28   |
| 1   | A     | 111 | SER  | CA-C-N  | -5.39 | 111.72      | 120.72   |
| 1   | A     | 111 | SER  | C-N-CA  | -5.39 | 111.72      | 120.72   |
| 4   | S     | 23  | VAL  | CA-C-N  | -5.39 | 113.71      | 121.42   |
| 4   | S     | 23  | VAL  | C-N-CA  | -5.39 | 113.71      | 121.42   |
| 4   | S     | 138 | GLY  | N-CA-C  | -5.39 | 107.81      | 115.30   |
| 1   | A     | 230 | PRO  | CA-N-CD | 5.38  | 119.53      | 112.00   |
| 1   | A     | 366 | SER  | CA-C-N  | 5.38  | 129.16      | 120.55   |
| 1   | A     | 366 | SER  | C-N-CA  | 5.38  | 129.16      | 120.55   |
| 3   | M     | 287 | ASN  | N-CA-C  | 5.38  | 118.05      | 110.14   |
| 3   | M     | 46  | SER  | O-C-N   | -5.38 | 113.81      | 122.41   |
| 2   | B     | 539 | ASN  | CA-C-N  | 5.37  | 132.83      | 122.03   |
| 2   | B     | 539 | ASN  | C-N-CA  | 5.37  | 132.83      | 122.03   |
| 1   | A     | 404 | GLN  | CA-C-N  | 5.37  | 137.35      | 122.15   |
| 1   | A     | 404 | GLN  | C-N-CA  | 5.37  | 137.35      | 122.15   |
| 3   | M     | 279 | ASN  | O-C-N   | -5.37 | 115.44      | 122.59   |
| 1   | A     | 270 | LEU  | N-CA-C  | -5.37 | 105.09      | 111.69   |
| 2   | B     | 358 | MET  | CA-C-N  | 5.37  | 127.74      | 120.44   |
| 2   | B     | 358 | MET  | C-N-CA  | 5.37  | 127.74      | 120.44   |
| 3   | M     | 215 | TYR  | CA-C-N  | -5.37 | 115.96      | 123.10   |
| 3   | M     | 215 | TYR  | C-N-CA  | -5.37 | 115.96      | 123.10   |
| 3   | M     | 438 | SER  | CA-C-N  | -5.37 | 114.17      | 122.59   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | M     | 438 | SER  | C-N-CA  | -5.37 | 114.17      | 122.59   |
| 3   | M     | 299 | LEU  | CA-C-O  | 5.36  | 125.87      | 119.60   |
| 1   | A     | 530 | ASN  | CA-C-O  | -5.36 | 114.19      | 120.20   |
| 2   | B     | 264 | THR  | N-CA-C  | -5.36 | 101.26      | 109.41   |
| 3   | M     | 395 | GLY  | N-CA-C  | 5.36  | 120.05      | 111.64   |
| 2   | B     | 151 | ALA  | CA-C-N  | 5.35  | 125.07      | 119.82   |
| 2   | B     | 151 | ALA  | C-N-CA  | 5.35  | 125.07      | 119.82   |
| 3   | M     | 392 | MET  | N-CA-C  | -5.34 | 106.71      | 113.18   |
| 4   | S     | 100 | ASP  | N-CA-C  | 5.34  | 119.05      | 112.54   |
| 2   | B     | 79  | VAL  | N-CA-C  | 5.34  | 119.58      | 111.89   |
| 2   | B     | 22  | ALA  | CA-C-O  | -5.34 | 114.76      | 120.42   |
| 3   | M     | 388 | ASN  | CA-C-O  | -5.33 | 114.79      | 120.92   |
| 3   | M     | 357 | LYS  | CA-C-N  | -5.33 | 115.86      | 123.11   |
| 3   | M     | 357 | LYS  | C-N-CA  | -5.33 | 115.86      | 123.11   |
| 2   | B     | 338 | LYS  | O-C-N   | 5.33  | 127.77      | 122.12   |
| 3   | M     | 444 | ALA  | N-CA-CB | -5.33 | 102.28      | 110.01   |
| 2   | B     | 557 | SER  | CA-C-N  | -5.33 | 111.36      | 121.54   |
| 2   | B     | 557 | SER  | C-N-CA  | -5.33 | 111.36      | 121.54   |
| 1   | A     | 98  | ASN  | CB-CA-C | 5.33  | 119.26      | 109.46   |
| 4   | S     | 160 | ALA  | CA-C-N  | -5.32 | 111.83      | 121.14   |
| 4   | S     | 160 | ALA  | C-N-CA  | -5.32 | 111.83      | 121.14   |
| 2   | B     | 133 | GLU  | CA-C-O  | -5.31 | 113.52      | 119.79   |
| 3   | M     | 388 | ASN  | O-C-N   | -5.31 | 117.00      | 123.16   |
| 3   | M     | 280 | ASP  | N-CA-CB | -5.31 | 101.52      | 110.49   |
| 1   | A     | 63  | ASP  | N-CA-C  | 5.31  | 125.86      | 111.00   |
| 2   | B     | 562 | ASN  | CA-C-O  | -5.31 | 112.85      | 119.38   |
| 2   | B     | 519 | ALA  | N-CA-CB | -5.30 | 101.30      | 110.32   |
| 2   | B     | 227 | HIS  | CA-C-O  | -5.29 | 112.94      | 120.51   |
| 4   | S     | 113 | PHE  | CA-C-N  | -5.29 | 112.11      | 120.63   |
| 4   | S     | 113 | PHE  | C-N-CA  | -5.29 | 112.11      | 120.63   |
| 3   | M     | 367 | ALA  | N-CA-CB | -5.29 | 101.81      | 110.43   |
| 2   | B     | 597 | TYR  | CA-C-O  | -5.28 | 114.13      | 120.10   |
| 2   | B     | 576 | GLN  | N-CA-CB | 5.28  | 117.91      | 110.36   |
| 4   | S     | 94  | SER  | O-C-N   | 5.28  | 128.87      | 122.85   |
| 4   | S     | 123 | PHE  | CA-C-N  | -5.28 | 114.78      | 122.86   |
| 4   | S     | 123 | PHE  | C-N-CA  | -5.28 | 114.78      | 122.86   |
| 1   | A     | 251 | TRP  | CA-C-N  | 5.28  | 127.92      | 120.42   |
| 1   | A     | 251 | TRP  | C-N-CA  | 5.28  | 127.92      | 120.42   |
| 2   | B     | 309 | LEU  | N-CA-C  | -5.28 | 105.61      | 111.36   |
| 3   | M     | 127 | CYS  | CA-C-N  | -5.28 | 112.29      | 120.31   |
| 3   | M     | 127 | CYS  | C-N-CA  | -5.28 | 112.29      | 120.31   |
| 1   | A     | 247 | ILE  | N-CA-C  | 5.28  | 116.89      | 108.87   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 197 | ARG  | CA-C-N  | -5.27 | 113.16      | 120.38   |
| 1   | A     | 197 | ARG  | C-N-CA  | -5.27 | 113.16      | 120.38   |
| 2   | B     | 162 | VAL  | N-CA-C  | -5.27 | 104.50      | 111.09   |
| 2   | B     | 562 | ASN  | CA-C-N  | 5.27  | 130.59      | 122.42   |
| 2   | B     | 562 | ASN  | C-N-CA  | 5.27  | 130.59      | 122.42   |
| 1   | A     | 326 | GLN  | N-CA-C  | 5.27  | 119.33      | 113.01   |
| 3   | M     | 480 | GLN  | CA-C-N  | -5.26 | 116.28      | 123.12   |
| 3   | M     | 480 | GLN  | C-N-CA  | -5.26 | 116.28      | 123.12   |
| 2   | B     | 405 | GLU  | N-CA-C  | 5.26  | 117.92      | 111.82   |
| 2   | B     | 256 | CYS  | CA-C-N  | -5.26 | 110.77      | 121.18   |
| 2   | B     | 256 | CYS  | C-N-CA  | -5.26 | 110.77      | 121.18   |
| 3   | M     | 326 | HIS  | O-C-N   | -5.26 | 116.51      | 123.13   |
| 3   | M     | 131 | ALA  | CA-C-O  | 5.25  | 127.63      | 121.54   |
| 2   | B     | 495 | ASP  | CA-C-N  | -5.25 | 112.33      | 120.31   |
| 2   | B     | 495 | ASP  | C-N-CA  | -5.25 | 112.33      | 120.31   |
| 1   | A     | 444 | VAL  | CB-CA-C | 5.25  | 119.23      | 111.26   |
| 1   | A     | 296 | ASN  | CA-C-N  | 5.24  | 127.31      | 120.28   |
| 1   | A     | 296 | ASN  | C-N-CA  | 5.24  | 127.31      | 120.28   |
| 3   | M     | 212 | ASN  | CA-C-N  | -5.24 | 114.24      | 122.73   |
| 3   | M     | 212 | ASN  | C-N-CA  | -5.24 | 114.24      | 122.73   |
| 3   | M     | 45  | SER  | N-CA-C  | -5.24 | 99.64       | 110.80   |
| 4   | S     | 147 | ASN  | O-C-N   | 5.24  | 128.71      | 122.27   |
| 1   | A     | 584 | PHE  | CA-C-O  | -5.24 | 115.00      | 120.55   |
| 2   | B     | 80  | GLN  | CA-C-N  | -5.24 | 112.35      | 120.31   |
| 2   | B     | 80  | GLN  | C-N-CA  | -5.24 | 112.35      | 120.31   |
| 3   | M     | 324 | SER  | O-C-N   | -5.23 | 116.82      | 123.05   |
| 1   | A     | 321 | THR  | N-CA-C  | 5.23  | 118.44      | 111.75   |
| 3   | M     | 462 | LYS  | N-CA-CB | 5.23  | 117.84      | 110.36   |
| 3   | M     | 320 | ILE  | N-CA-C  | -5.23 | 98.47       | 109.34   |
| 1   | A     | 135 | ASP  | CA-C-O  | -5.22 | 115.01      | 120.55   |
| 1   | A     | 488 | ARG  | CA-C-N  | 5.22  | 127.80      | 120.28   |
| 1   | A     | 488 | ARG  | C-N-CA  | 5.22  | 127.80      | 120.28   |
| 3   | M     | 352 | GLN  | N-CA-C  | -5.22 | 99.69       | 110.80   |
| 2   | B     | 331 | PRO  | O-C-N   | 5.22  | 128.48      | 122.17   |
| 2   | B     | 561 | ASP  | CA-C-O  | -5.22 | 113.05      | 120.51   |
| 1   | A     | 360 | LEU  | CA-C-N  | -5.21 | 111.41      | 121.58   |
| 1   | A     | 360 | LEU  | C-N-CA  | -5.21 | 111.41      | 121.58   |
| 1   | A     | 399 | ASP  | N-CA-C  | 5.21  | 119.55      | 112.04   |
| 3   | M     | 216 | VAL  | CA-C-N  | -5.21 | 115.06      | 122.77   |
| 3   | M     | 216 | VAL  | C-N-CA  | -5.21 | 115.06      | 122.77   |
| 1   | A     | 251 | TRP  | CA-C-O  | -5.21 | 113.98      | 119.97   |
| 1   | A     | 349 | ILE  | CA-C-N  | -5.21 | 113.30      | 120.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 349 | ILE  | C-N-CA  | -5.21 | 113.30      | 120.28   |
| 2   | B     | 517 | GLU  | N-CA-C  | 5.21  | 116.95      | 111.28   |
| 4   | S     | 105 | PHE  | N-CA-C  | -5.21 | 105.29      | 111.69   |
| 2   | B     | 145 | MET  | N-CA-C  | -5.21 | 102.04      | 110.32   |
| 3   | M     | 339 | GLU  | O-C-N   | -5.20 | 117.19      | 123.27   |
| 1   | A     | 401 | VAL  | CA-C-O  | -5.20 | 114.28      | 120.78   |
| 1   | A     | 625 | LEU  | N-CA-C  | -5.19 | 105.51      | 111.07   |
| 2   | B     | 566 | ALA  | N-CA-CB | -5.19 | 102.87      | 110.40   |
| 2   | B     | 257 | LYS  | N-CA-C  | -5.19 | 106.78      | 113.01   |
| 2   | B     | 487 | LEU  | O-C-N   | 5.19  | 128.29      | 122.22   |
| 1   | A     | 344 | ILE  | N-CA-C  | 5.18  | 118.39      | 111.44   |
| 3   | M     | 254 | PRO  | CA-C-N  | 5.18  | 132.17      | 122.74   |
| 3   | M     | 254 | PRO  | C-N-CA  | 5.18  | 132.17      | 122.74   |
| 3   | M     | 368 | ASP  | N-CA-C  | -5.18 | 100.52      | 109.58   |
| 2   | B     | 147 | MET  | CA-C-O  | 5.18  | 127.07      | 121.06   |
| 2   | B     | 280 | PRO  | CA-C-O  | -5.17 | 115.46      | 122.08   |
| 2   | B     | 286 | ILE  | O-C-N   | 5.17  | 128.28      | 122.75   |
| 2   | B     | 316 | THR  | CA-C-N  | 5.17  | 129.22      | 120.64   |
| 2   | B     | 316 | THR  | C-N-CA  | 5.17  | 129.22      | 120.64   |
| 2   | B     | 582 | ASP  | CA-C-N  | 5.17  | 130.53      | 122.26   |
| 2   | B     | 582 | ASP  | C-N-CA  | 5.17  | 130.53      | 122.26   |
| 3   | M     | 358 | ILE  | N-CA-C  | 5.17  | 115.02      | 107.37   |
| 4   | S     | 55  | PRO  | CB-CA-C | -5.17 | 104.51      | 111.85   |
| 4   | S     | 139 | GLY  | CA-C-O  | 5.17  | 125.50      | 119.19   |
| 2   | B     | 89  | ASN  | O-C-N   | 5.17  | 129.11      | 122.39   |
| 3   | M     | 285 | PRO  | N-CA-C  | 5.17  | 120.56      | 113.84   |
| 1   | A     | 241 | TYR  | CA-C-N  | 5.16  | 128.04      | 120.71   |
| 1   | A     | 241 | TYR  | C-N-CA  | 5.16  | 128.04      | 120.71   |
| 3   | M     | 223 | HIS  | CA-C-O  | 5.16  | 126.63      | 120.28   |
| 4   | S     | 11  | LYS  | CA-C-N  | 5.16  | 130.16      | 122.74   |
| 4   | S     | 11  | LYS  | C-N-CA  | 5.16  | 130.16      | 122.74   |
| 1   | A     | 546 | SER  | O-C-N   | 5.15  | 128.02      | 122.15   |
| 2   | B     | 109 | ALA  | N-CA-C  | -5.15 | 105.78      | 111.71   |
| 3   | M     | 434 | SER  | CA-C-N  | -5.15 | 115.72      | 122.99   |
| 3   | M     | 434 | SER  | C-N-CA  | -5.15 | 115.72      | 122.99   |
| 2   | B     | 569 | THR  | CB-CA-C | -5.15 | 102.17      | 110.77   |
| 2   | B     | 598 | LEU  | O-C-N   | 5.15  | 129.23      | 122.33   |
| 3   | M     | 241 | HIS  | CA-C-N  | -5.15 | 117.80      | 122.80   |
| 3   | M     | 241 | HIS  | C-N-CA  | -5.15 | 117.80      | 122.80   |
| 4   | S     | 70  | ASN  | O-C-N   | -5.15 | 115.74      | 122.59   |
| 2   | B     | 535 | GLN  | N-CA-C  | -5.15 | 105.16      | 111.75   |
| 1   | A     | 530 | ASN  | CA-C-N  | -5.15 | 111.93      | 120.68   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 530 | ASN  | C-N-CA  | -5.15 | 111.93      | 120.68   |
| 3   | M     | 377 | LYS  | O-C-N   | -5.14 | 116.14      | 122.11   |
| 3   | M     | 287 | ASN  | CA-C-O  | -5.14 | 115.20      | 121.78   |
| 3   | M     | 360 | LEU  | N-CA-C  | 5.14  | 116.64      | 108.67   |
| 3   | M     | 446 | GLY  | CA-C-N  | 5.14  | 131.22      | 121.97   |
| 3   | M     | 446 | GLY  | C-N-CA  | 5.14  | 131.22      | 121.97   |
| 4   | S     | 16  | LEU  | CA-C-N  | -5.14 | 115.69      | 122.98   |
| 4   | S     | 16  | LEU  | C-N-CA  | -5.14 | 115.69      | 122.98   |
| 1   | A     | 78  | GLU  | N-CA-C  | -5.13 | 105.77      | 111.36   |
| 3   | M     | 443 | SER  | CA-C-O  | -5.13 | 114.79      | 120.38   |
| 1   | A     | 203 | PHE  | CA-C-O  | -5.13 | 115.11      | 120.55   |
| 3   | M     | 334 | ASP  | N-CA-C  | -5.12 | 108.30      | 114.75   |
| 3   | M     | 442 | GLN  | N-CA-C  | 5.12  | 115.81      | 108.74   |
| 3   | M     | 456 | SER  | N-CA-C  | 5.12  | 118.92      | 109.24   |
| 1   | A     | 65  | ASN  | CA-C-O  | -5.12 | 114.08      | 119.97   |
| 2   | B     | 120 | ILE  | N-CA-C  | -5.12 | 105.42      | 111.00   |
| 2   | B     | 335 | LYS  | N-CA-CB | 5.12  | 117.64      | 110.12   |
| 2   | B     | 278 | PRO  | CA-C-N  | -5.12 | 113.98      | 123.55   |
| 2   | B     | 278 | PRO  | C-N-CA  | -5.12 | 113.98      | 123.55   |
| 4   | S     | 77  | TYR  | CA-C-N  | -5.11 | 114.87      | 122.74   |
| 4   | S     | 77  | TYR  | C-N-CA  | -5.11 | 114.87      | 122.74   |
| 4   | S     | 7   | ILE  | CA-C-O  | -5.11 | 115.07      | 120.53   |
| 4   | S     | 102 | ILE  | N-CA-C  | -5.11 | 105.44      | 111.00   |
| 3   | M     | 337 | GLU  | CA-C-N  | -5.10 | 114.66      | 122.62   |
| 3   | M     | 337 | GLU  | C-N-CA  | -5.10 | 114.66      | 122.62   |
| 3   | M     | 406 | GLY  | O-C-N   | -5.10 | 116.06      | 122.70   |
| 1   | A     | 270 | LEU  | CA-C-N  | -5.10 | 113.39      | 120.38   |
| 1   | A     | 270 | LEU  | C-N-CA  | -5.10 | 113.39      | 120.38   |
| 1   | A     | 352 | PHE  | N-CA-C  | 5.10  | 119.04      | 112.41   |
| 4   | S     | 8   | PHE  | CA-C-N  | -5.10 | 111.78      | 122.03   |
| 4   | S     | 8   | PHE  | C-N-CA  | -5.10 | 111.78      | 122.03   |
| 1   | A     | 445 | ASN  | CA-C-O  | 5.09  | 126.22      | 120.00   |
| 4   | S     | 65  | ASN  | CA-C-N  | -5.09 | 114.33      | 121.72   |
| 4   | S     | 65  | ASN  | C-N-CA  | -5.09 | 114.33      | 121.72   |
| 4   | S     | 106 | VAL  | N-CA-C  | -5.09 | 105.58      | 110.72   |
| 3   | M     | 294 | ASP  | N-CA-CB | 5.09  | 118.60      | 110.46   |
| 1   | A     | 154 | ILE  | N-CA-CB | -5.09 | 104.67      | 112.15   |
| 2   | B     | 542 | PRO  | CA-C-O  | -5.08 | 111.35      | 120.60   |
| 1   | A     | 290 | VAL  | N-CA-C  | -5.08 | 104.75      | 111.09   |
| 3   | M     | 79  | SER  | CA-C-N  | -5.07 | 114.27      | 122.23   |
| 3   | M     | 79  | SER  | C-N-CA  | -5.07 | 114.27      | 122.23   |
| 4   | S     | 140 | MET  | CA-C-O  | 5.07  | 126.17      | 120.70   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 339 | PHE  | CA-C-O  | -5.07 | 115.05      | 120.42   |
| 3   | M     | 247 | ARG  | CA-C-N  | -5.06 | 114.32      | 122.82   |
| 3   | M     | 247 | ARG  | C-N-CA  | -5.06 | 114.32      | 122.82   |
| 3   | M     | 69  | ILE  | O-C-N   | -5.06 | 117.80      | 123.26   |
| 2   | B     | 21  | GLU  | CA-C-N  | 5.05  | 127.47      | 120.29   |
| 2   | B     | 21  | GLU  | C-N-CA  | 5.05  | 127.47      | 120.29   |
| 3   | M     | 131 | ALA  | N-CA-CB | -5.05 | 104.31      | 111.84   |
| 3   | M     | 461 | GLY  | CA-C-N  | -5.05 | 111.77      | 120.97   |
| 3   | M     | 461 | GLY  | C-N-CA  | -5.05 | 111.77      | 120.97   |
| 1   | A     | 150 | LEU  | CA-C-N  | -5.05 | 112.28      | 120.72   |
| 1   | A     | 150 | LEU  | C-N-CA  | -5.05 | 112.28      | 120.72   |
| 4   | S     | 126 | GLN  | O-C-N   | 5.05  | 127.47      | 122.12   |
| 3   | M     | 42  | LEU  | CA-C-O  | -5.04 | 115.20      | 120.55   |
| 3   | M     | 54  | SER  | N-CA-CB | -5.04 | 104.32      | 110.98   |
| 3   | M     | 62  | VAL  | CA-C-O  | -5.04 | 115.18      | 120.27   |
| 3   | M     | 295 | GLY  | CA-C-N  | 5.04  | 128.50      | 121.24   |
| 3   | M     | 295 | GLY  | C-N-CA  | 5.04  | 128.50      | 121.24   |
| 1   | A     | 211 | ASP  | CA-C-O  | -5.04 | 114.64      | 120.49   |
| 4   | S     | 143 | GLU  | CA-C-N  | 5.04  | 130.27      | 122.26   |
| 4   | S     | 143 | GLU  | C-N-CA  | 5.04  | 130.27      | 122.26   |
| 1   | A     | 620 | GLY  | CA-C-O  | -5.04 | 109.77      | 119.54   |
| 1   | A     | 343 | LYS  | N-CA-C  | -5.03 | 105.24      | 111.33   |
| 1   | A     | 403 | LEU  | N-CA-C  | -5.03 | 105.31      | 111.75   |
| 2   | B     | 57  | ARG  | CA-C-O  | -5.03 | 113.86      | 120.00   |
| 1   | A     | 546 | SER  | CA-C-O  | -5.03 | 115.09      | 120.42   |
| 2   | B     | 241 | ASP  | N-CA-C  | -5.03 | 103.04      | 110.48   |
| 2   | B     | 406 | SER  | N-CA-C  | 5.02  | 119.03      | 113.01   |
| 4   | S     | 90  | ASP  | O-C-N   | 5.02  | 128.57      | 122.85   |
| 1   | A     | 164 | ASP  | CA-C-O  | -5.02 | 114.20      | 119.97   |
| 2   | B     | 273 | SER  | N-CA-CB | -5.02 | 100.50      | 109.68   |
| 4   | S     | 21  | THR  | C-N-CD  | 5.01  | 145.56      | 125.00   |
| 2   | B     | 104 | TYR  | CA-C-N  | 5.01  | 127.30      | 120.54   |
| 2   | B     | 104 | TYR  | C-N-CA  | 5.01  | 127.30      | 120.54   |
| 2   | B     | 399 | LEU  | N-CA-C  | -5.01 | 105.27      | 111.33   |
| 3   | M     | 355 | ASP  | CA-C-O  | -5.00 | 113.36      | 120.51   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | M     | 22  | ALA  | CA   |
| 4   | S     | 69  | ASN  | CA   |

All (125) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 117 | ASP  | Mainchain |
| 1   | A     | 174 | ARG  | Mainchain |
| 1   | A     | 192 | TYR  | Mainchain |
| 1   | A     | 199 | ASN  | Mainchain |
| 1   | A     | 204 | VAL  | Mainchain |
| 1   | A     | 219 | VAL  | Mainchain |
| 1   | A     | 233 | PHE  | Mainchain |
| 1   | A     | 240 | LEU  | Mainchain |
| 1   | A     | 244 | LEU  | Mainchain |
| 1   | A     | 260 | PHE  | Mainchain |
| 1   | A     | 275 | LEU  | Mainchain |
| 1   | A     | 277 | LYS  | Mainchain |
| 1   | A     | 278 | ILE  | Mainchain |
| 1   | A     | 282 | MET  | Mainchain |
| 1   | A     | 288 | THR  | Mainchain |
| 1   | A     | 289 | SER  | Mainchain |
| 1   | A     | 290 | VAL  | Mainchain |
| 1   | A     | 298 | ILE  | Mainchain |
| 1   | A     | 302 | ASN  | Mainchain |
| 1   | A     | 306 | GLU  | Mainchain |
| 1   | A     | 319 | LEU  | Mainchain |
| 1   | A     | 320 | HIS  | Mainchain |
| 1   | A     | 323 | CYS  | Mainchain |
| 1   | A     | 325 | SER  | Mainchain |
| 1   | A     | 328 | PRO  | Mainchain |
| 1   | A     | 350 | SER  | Mainchain |
| 1   | A     | 399 | ASP  | Peptide   |
| 1   | A     | 400 | VAL  | Peptide   |
| 1   | A     | 441 | TYR  | Mainchain |
| 1   | A     | 462 | GLN  | Mainchain |
| 1   | A     | 487 | MET  | Mainchain |
| 1   | A     | 500 | SER  | Mainchain |
| 1   | A     | 501 | ASN  | Mainchain |
| 1   | A     | 505 | ASN  | Mainchain |
| 1   | A     | 506 | LYS  | Mainchain |
| 1   | A     | 527 | GLU  | Mainchain |
| 1   | A     | 528 | ASN  | Mainchain |
| 1   | A     | 529 | GLY  | Mainchain |
| 1   | A     | 531 | ASP  | Mainchain |
| 1   | A     | 535 | ILE  | Mainchain |
| 1   | A     | 536 | MET  | Mainchain |
| 1   | A     | 538 | GLU  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 539 | ASN  | Mainchain |
| 1   | A     | 565 | ASN  | Mainchain |
| 1   | A     | 569 | ASP  | Mainchain |
| 1   | A     | 571 | ARG  | Mainchain |
| 1   | A     | 586 | GLU  | Mainchain |
| 1   | A     | 588 | LEU  | Mainchain |
| 1   | A     | 64  | LEU  | Mainchain |
| 1   | A     | 80  | TYR  | Mainchain |
| 1   | A     | 84  | MET  | Mainchain |
| 1   | A     | 94  | VAL  | Mainchain |
| 2   | B     | 126 | SER  | Mainchain |
| 2   | B     | 142 | LEU  | Mainchain |
| 2   | B     | 147 | MET  | Mainchain |
| 2   | B     | 181 | TYR  | Mainchain |
| 2   | B     | 186 | ASN  | Mainchain |
| 2   | B     | 237 | ILE  | Mainchain |
| 2   | B     | 267 | ASP  | Mainchain |
| 2   | B     | 278 | PRO  | Peptide   |
| 2   | B     | 288 | TYR  | Mainchain |
| 2   | B     | 293 | VAL  | Mainchain |
| 2   | B     | 310 | ILE  | Mainchain |
| 2   | B     | 326 | TYR  | Mainchain |
| 2   | B     | 375 | LEU  | Mainchain |
| 2   | B     | 377 | TYR  | Mainchain |
| 2   | B     | 381 | PHE  | Mainchain |
| 2   | B     | 384 | PHE  | Mainchain |
| 2   | B     | 404 | ASN  | Mainchain |
| 2   | B     | 41  | ASN  | Peptide   |
| 2   | B     | 444 | THR  | Mainchain |
| 2   | B     | 459 | GLU  | Mainchain |
| 2   | B     | 485 | LYS  | Mainchain |
| 2   | B     | 497 | LEU  | Mainchain |
| 2   | B     | 523 | PHE  | Mainchain |
| 2   | B     | 536 | ASN  | Mainchain |
| 2   | B     | 557 | SER  | Mainchain |
| 2   | B     | 56  | SER  | Mainchain |
| 2   | B     | 569 | THR  | Mainchain |
| 2   | B     | 573 | GLU  | Mainchain |
| 2   | B     | 581 | TYR  | Mainchain |
| 2   | B     | 584 | SER  | Mainchain |
| 2   | B     | 78  | ASP  | Mainchain |
| 2   | B     | 82  | TYR  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | M     | 102 | GLU  | Mainchain |
| 3   | M     | 103 | TYR  | Mainchain |
| 3   | M     | 104 | PHE  | Mainchain |
| 3   | M     | 105 | ASP  | Peptide   |
| 3   | M     | 131 | ALA  | Mainchain |
| 3   | M     | 134 | PRO  | Mainchain |
| 3   | M     | 265 | ASN  | Mainchain |
| 3   | M     | 284 | SER  | Mainchain |
| 3   | M     | 292 | PRO  | Peptide   |
| 3   | M     | 40  | GLN  | Mainchain |
| 3   | M     | 405 | THR  | Mainchain |
| 3   | M     | 421 | GLY  | Mainchain |
| 3   | M     | 426 | LYS  | Peptide   |
| 3   | M     | 445 | SER  | Peptide   |
| 3   | M     | 45  | SER  | Peptide   |
| 3   | M     | 456 | SER  | Mainchain |
| 3   | M     | 462 | LYS  | Peptide   |
| 3   | M     | 477 | GLY  | Peptide   |
| 3   | M     | 51  | LEU  | Peptide   |
| 3   | M     | 57  | GLY  | Mainchain |
| 3   | M     | 79  | SER  | Mainchain |
| 3   | M     | 8   | THR  | Mainchain |
| 3   | M     | 85  | GLY  | Mainchain |
| 4   | S     | 101 | LEU  | Mainchain |
| 4   | S     | 102 | ILE  | Mainchain |
| 4   | S     | 135 | ILE  | Mainchain |
| 4   | S     | 161 | GLU  | Mainchain |
| 4   | S     | 163 | THR  | Peptide   |
| 4   | S     | 167 | ILE  | Peptide   |
| 4   | S     | 22  | PRO  | Mainchain |
| 4   | S     | 43  | ASN  | Mainchain |
| 4   | S     | 46  | PHE  | Mainchain |
| 4   | S     | 50  | PHE  | Mainchain |
| 4   | S     | 53  | THR  | Mainchain |
| 4   | S     | 56  | SER  | Mainchain |
| 4   | S     | 57  | LEU  | Mainchain |
| 4   | S     | 58  | LEU  | Peptide   |
| 4   | S     | 64  | ASN  | Mainchain |
| 4   | S     | 66  | ASP  | Mainchain |
| 4   | S     | 69  | ASN  | Mainchain |
| 4   | S     | 71  | GLU  | 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     | 4625  | 0        | 4710     | 1276    | 0            |
| 2   | B     | 4961  | 0        | 4991     | 2505    | 0            |
| 3   | M     | 3158  | 0        | 3121     | 1006    | 0            |
| 4   | S     | 1358  | 0        | 1341     | 369     | 0            |
| All | All   | 14102 | 0        | 14163    | 4741    | 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 168.

All (4741) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:316:THR:HG23 | 3:M:90:PHE:CE2   | 1.28                     | 1.66              |
| 2:B:162:VAL:HG21 | 2:B:195:ILE:CG2  | 1.27                     | 1.65              |
| 1:A:638:LEU:HB2  | 2:B:558:TYR:CD1  | 1.25                     | 1.63              |
| 2:B:193:LEU:HD22 | 2:B:225:LEU:CB   | 1.19                     | 1.62              |
| 2:B:193:LEU:CG   | 2:B:225:LEU:HG   | 1.30                     | 1.62              |
| 1:A:638:LEU:CD2  | 2:B:558:TYR:HB3  | 1.26                     | 1.61              |
| 3:M:131:ALA:CA   | 3:M:131:ALA:CB   | 1.79                     | 1.60              |
| 2:B:523:PHE:CZ   | 2:B:580:TYR:CD1  | 1.86                     | 1.60              |
| 2:B:479:VAL:CG1  | 2:B:486:HIS:CE1  | 1.79                     | 1.60              |
| 2:B:24:ALA:HB3   | 2:B:35:TYR:CE2   | 1.33                     | 1.59              |
| 1:A:638:LEU:HG   | 2:B:520:SER:CB   | 1.32                     | 1.58              |
| 2:B:70:MET:HE3   | 2:B:107:ARG:CB   | 1.33                     | 1.58              |
| 2:B:127:LEU:HD13 | 2:B:157:THR:CG2  | 1.31                     | 1.58              |
| 2:B:139:LEU:CD2  | 2:B:173:VAL:HA   | 1.35                     | 1.56              |
| 2:B:252:LEU:HD13 | 2:B:302:PHE:CD1  | 1.40                     | 1.56              |
| 1:A:630:PRO:CG   | 2:B:617:LEU:CD1  | 1.84                     | 1.56              |
| 2:B:24:ALA:HB3   | 2:B:35:TYR:CZ    | 1.40                     | 1.55              |
| 2:B:523:PHE:HZ   | 2:B:580:TYR:CD1  | 1.12                     | 1.55              |
| 1:A:630:PRO:CG   | 2:B:617:LEU:HD13 | 1.08                     | 1.55              |
| 4:S:64:ASN:CA    | 4:S:64:ASN:C     | 1.80                     | 1.55              |
| 2:B:193:LEU:HD13 | 2:B:225:LEU:CG   | 1.24                     | 1.54              |
| 1:A:404:GLN:HA   | 2:B:3:ASP:CG     | 1.30                     | 1.54              |
| 2:B:193:LEU:CD1  | 2:B:225:LEU:HG   | 1.23                     | 1.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:16:LEU:CD1   | 4:S:125:TRP:HE1  | 1.16                     | 1.53              |
| 2:B:70:MET:CE    | 2:B:107:ARG:HB2  | 1.33                     | 1.52              |
| 3:M:282:VAL:N    | 3:M:282:VAL:CA   | 1.68                     | 1.52              |
| 3:M:281:GLY:CA   | 3:M:281:GLY:C    | 1.78                     | 1.51              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:HD13 | 1.46                     | 1.50              |
| 2:B:102:HIS:CE1  | 2:B:138:ALA:N    | 1.78                     | 1.50              |
| 2:B:216:LYS:CB   | 2:B:251:LEU:HD13 | 1.38                     | 1.49              |
| 2:B:158:VAL:HG11 | 2:B:177:ILE:CG1  | 1.40                     | 1.49              |
| 1:A:595:GLU:CD   | 2:B:476:ARG:NH1  | 1.71                     | 1.49              |
| 1:A:638:LEU:CD1  | 2:B:558:TYR:CD2  | 1.94                     | 1.48              |
| 2:B:127:LEU:CD1  | 2:B:157:THR:HG21 | 1.41                     | 1.48              |
| 1:A:638:LEU:HD22 | 2:B:558:TYR:CB   | 1.40                     | 1.48              |
| 4:S:163:THR:CA   | 4:S:163:THR:C    | 1.81                     | 1.47              |
| 2:B:25:VAL:HG21  | 2:B:36:THR:CA    | 1.43                     | 1.47              |
| 2:B:316:THR:CG2  | 3:M:90:PHE:CE2   | 1.92                     | 1.47              |
| 1:A:200:PHE:CZ   | 1:A:236:LEU:HD21 | 1.49                     | 1.46              |
| 1:A:630:PRO:HG3  | 2:B:617:LEU:CD1  | 1.37                     | 1.46              |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:C    | 1.41                     | 1.45              |
| 1:A:638:LEU:CB   | 2:B:558:TYR:CG   | 1.78                     | 1.45              |
| 2:B:25:VAL:CG2   | 2:B:36:THR:N     | 1.79                     | 1.44              |
| 2:B:549:LEU:HD21 | 2:B:611:ALA:N    | 1.12                     | 1.44              |
| 2:B:193:LEU:HD13 | 2:B:225:LEU:CD2  | 1.47                     | 1.44              |
| 2:B:208:ILE:HD13 | 2:B:236:ILE:CG2  | 1.47                     | 1.44              |
| 1:A:404:GLN:C    | 2:B:3:ASP:HB3    | 1.37                     | 1.43              |
| 2:B:546:CYS:CB   | 2:B:607:ILE:HG12 | 1.44                     | 1.43              |
| 1:A:65:ASN:HA    | 4:S:166:LYS:CA   | 1.39                     | 1.43              |
| 1:A:179:LYS:HB3  | 4:S:142:ILE:CD1  | 1.34                     | 1.43              |
| 1:A:638:LEU:CG   | 2:B:520:SER:HB3  | 1.48                     | 1.43              |
| 1:A:403:LEU:O    | 2:B:3:ASP:CB     | 1.65                     | 1.43              |
| 2:B:534:ILE:HG21 | 2:B:594:ALA:CB   | 1.44                     | 1.43              |
| 2:B:102:HIS:CE1  | 2:B:138:ALA:HA   | 1.54                     | 1.42              |
| 2:B:102:HIS:NE2  | 2:B:138:ALA:HA   | 1.25                     | 1.42              |
| 2:B:513:TRP:N    | 2:B:551:LEU:HD13 | 1.33                     | 1.42              |
| 2:B:25:VAL:HG22  | 2:B:36:THR:N     | 1.14                     | 1.42              |
| 2:B:215:TYR:CD1  | 2:B:233:TYR:HE1  | 1.37                     | 1.42              |
| 2:B:486:HIS:ND1  | 2:B:518:ILE:HD13 | 1.34                     | 1.42              |
| 2:B:29:LYS:HE2   | 2:B:30:LEU:N     | 1.26                     | 1.41              |
| 2:B:102:HIS:CE1  | 2:B:138:ALA:CA   | 2.00                     | 1.41              |
| 2:B:226:LEU:HD23 | 2:B:255:TYR:CD1  | 1.52                     | 1.41              |
| 2:B:316:THR:CG2  | 3:M:90:PHE:HE2   | 1.29                     | 1.41              |
| 2:B:316:THR:HG23 | 3:M:90:PHE:CD2   | 1.55                     | 1.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:479:VAL:HG13 | 2:B:486:HIS:ND1  | 1.31                     | 1.40              |
| 4:S:16:LEU:HD13  | 4:S:125:TRP:NE1  | 1.10                     | 1.40              |
| 2:B:24:ALA:CB    | 2:B:35:TYR:CE1   | 2.04                     | 1.40              |
| 1:A:638:LEU:HD13 | 2:B:558:TYR:CB   | 1.50                     | 1.39              |
| 2:B:24:ALA:CB    | 2:B:35:TYR:CZ    | 2.05                     | 1.39              |
| 2:B:155:LEU:HD23 | 2:B:192:LEU:CD1  | 1.51                     | 1.39              |
| 2:B:243:TRP:CZ3  | 3:M:94:GLU:HB3   | 1.57                     | 1.38              |
| 2:B:193:LEU:CD2  | 2:B:225:LEU:CB   | 2.01                     | 1.38              |
| 2:B:278:PRO:HD2  | 2:B:292:GLU:CB   | 1.50                     | 1.38              |
| 3:M:41:LEU:CD1   | 3:M:52:ASP:H     | 1.37                     | 1.38              |
| 1:A:638:LEU:HD22 | 2:B:558:TYR:CA   | 1.54                     | 1.35              |
| 2:B:29:LYS:CE    | 2:B:30:LEU:H     | 1.35                     | 1.35              |
| 2:B:513:TRP:HA   | 2:B:551:LEU:CD2  | 1.55                     | 1.35              |
| 1:A:404:GLN:O    | 2:B:3:ASP:HB3    | 1.17                     | 1.34              |
| 1:A:638:LEU:CG   | 2:B:558:TYR:HB3  | 1.57                     | 1.34              |
| 2:B:24:ALA:HB3   | 2:B:35:TYR:CD2   | 1.62                     | 1.34              |
| 2:B:479:VAL:HG11 | 2:B:486:HIS:CE1  | 1.47                     | 1.33              |
| 2:B:181:TYR:O    | 2:B:183:ALA:N    | 1.61                     | 1.33              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:CD1  | 2.11                     | 1.33              |
| 2:B:21:GLU:OE1   | 2:B:39:SER:CB    | 1.75                     | 1.32              |
| 2:B:513:TRP:N    | 2:B:551:LEU:CD1  | 1.90                     | 1.32              |
| 1:A:111:SER:HB2  | 1:A:152:THR:OG1  | 1.29                     | 1.32              |
| 2:B:193:LEU:CD1  | 2:B:225:LEU:CG   | 1.90                     | 1.32              |
| 2:B:243:TRP:CH2  | 3:M:94:GLU:HG2   | 1.63                     | 1.32              |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:CA   | 1.58                     | 1.31              |
| 2:B:243:TRP:HH2  | 3:M:94:GLU:C     | 1.35                     | 1.31              |
| 2:B:83:PHE:CZ    | 2:B:119:SER:HB3  | 1.64                     | 1.31              |
| 1:A:599:ARG:NH1  | 2:B:513:TRP:HZ3  | 1.24                     | 1.31              |
| 2:B:178:ILE:CG2  | 2:B:217:GLU:HB2  | 1.59                     | 1.31              |
| 1:A:257:LEU:HD22 | 1:A:278:ILE:CG2  | 1.60                     | 1.31              |
| 2:B:162:VAL:CG2  | 2:B:195:ILE:CG2  | 2.09                     | 1.31              |
| 1:A:404:GLN:HA   | 2:B:3:ASP:CB     | 1.60                     | 1.30              |
| 1:A:638:LEU:HB2  | 2:B:558:TYR:CG   | 1.14                     | 1.30              |
| 1:A:258:LYS:NZ   | 4:S:94:SER:HB3   | 1.47                     | 1.30              |
| 1:A:125:THR:OG1  | 1:A:158:LEU:HD13 | 1.13                     | 1.30              |
| 2:B:230:PHE:CE2  | 2:B:298:ASP:O    | 1.84                     | 1.30              |
| 2:B:230:PHE:CZ   | 2:B:252:LEU:HD22 | 1.66                     | 1.30              |
| 2:B:252:LEU:HB2  | 2:B:302:PHE:CZ   | 1.66                     | 1.29              |
| 2:B:556:LEU:CA   | 2:B:588:ILE:HD11 | 1.61                     | 1.29              |
| 3:M:221:THR:N    | 3:M:474:THR:OG1  | 1.64                     | 1.29              |
| 2:B:193:LEU:HD22 | 2:B:225:LEU:CG   | 1.60                     | 1.29              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:534:ILE:CD1  | 2:B:591:MET:O    | 1.80                     | 1.29              |
| 2:B:223:LEU:CB   | 2:B:259:TYR:CD1  | 1.78                     | 1.29              |
| 1:A:179:LYS:CB   | 4:S:142:ILE:CD1  | 2.03                     | 1.28              |
| 2:B:223:LEU:HD13 | 2:B:259:TYR:N    | 1.48                     | 1.28              |
| 2:B:247:TYR:OH   | 3:M:137:SER:HB3  | 1.33                     | 1.28              |
| 2:B:546:CYS:HB2  | 2:B:607:ILE:CG1  | 1.64                     | 1.28              |
| 2:B:243:TRP:HE1  | 3:M:98:ARG:CD    | 1.45                     | 1.28              |
| 2:B:278:PRO:HA   | 2:B:288:TYR:C    | 1.59                     | 1.28              |
| 2:B:584:SER:O    | 2:B:588:ILE:HG22 | 1.30                     | 1.28              |
| 2:B:278:PRO:CD   | 2:B:292:GLU:HB2  | 1.62                     | 1.27              |
| 1:A:369:SER:HB2  | 1:A:424:TYR:CE2  | 1.68                     | 1.27              |
| 1:A:404:GLN:HA   | 2:B:3:ASP:OD2    | 1.19                     | 1.27              |
| 2:B:193:LEU:CD2  | 2:B:225:LEU:HG   | 1.63                     | 1.27              |
| 2:B:512:VAL:C    | 2:B:551:LEU:HD13 | 1.56                     | 1.27              |
| 1:A:186:PHE:CE1  | 1:A:224:GLU:CB   | 2.17                     | 1.27              |
| 2:B:245:GLN:CD   | 2:B:309:LEU:CD1  | 2.08                     | 1.27              |
| 2:B:102:HIS:HE1  | 2:B:138:ALA:N    | 1.17                     | 1.27              |
| 2:B:479:VAL:HG11 | 2:B:486:HIS:NE2  | 1.49                     | 1.27              |
| 2:B:184:GLY:O    | 2:B:188:TYR:HD1  | 1.14                     | 1.26              |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:CB   | 1.63                     | 1.26              |
| 2:B:316:THR:CB   | 3:M:90:PHE:HE2   | 1.46                     | 1.26              |
| 1:A:638:LEU:CD1  | 2:B:558:TYR:CB   | 2.12                     | 1.26              |
| 2:B:279:LEU:N    | 2:B:288:TYR:HB2  | 1.47                     | 1.26              |
| 1:A:88:ASN:ND2   | 1:A:120:ILE:HG21 | 1.48                     | 1.26              |
| 2:B:231:ARG:HG3  | 2:B:298:ASP:OD1  | 1.35                     | 1.26              |
| 1:A:65:ASN:HA    | 4:S:166:LYS:CB   | 1.49                     | 1.25              |
| 2:B:98:LYS:NZ    | 2:B:134:LEU:HB3  | 1.50                     | 1.25              |
| 2:B:162:VAL:CG2  | 2:B:195:ILE:HG23 | 1.65                     | 1.25              |
| 3:M:432:THR:OG1  | 3:M:480:GLN:HG3  | 1.33                     | 1.25              |
| 1:A:88:ASN:CG    | 1:A:120:ILE:HG21 | 1.61                     | 1.25              |
| 1:A:275:LEU:O    | 1:A:276:PRO:C    | 1.73                     | 1.25              |
| 2:B:20:ARG:HD2   | 2:B:35:TYR:OH    | 1.35                     | 1.25              |
| 2:B:239:GLN:OE1  | 3:M:279:ASN:HA   | 1.26                     | 1.25              |
| 2:B:353:GLN:CB   | 3:M:50:TYR:HD1   | 1.46                     | 1.25              |
| 2:B:230:PHE:HE2  | 2:B:298:ASP:O    | 1.04                     | 1.25              |
| 2:B:136:CYS:SG   | 2:B:169:VAL:HA   | 1.77                     | 1.25              |
| 2:B:167:ALA:HA   | 2:B:202:ASP:OD1  | 1.33                     | 1.25              |
| 2:B:230:PHE:CE1  | 2:B:252:LEU:HD23 | 1.71                     | 1.25              |
| 2:B:472:VAL:CG1  | 2:B:510:GLY:HA3  | 1.65                     | 1.25              |
| 2:B:245:GLN:CD   | 2:B:309:LEU:HD11 | 1.61                     | 1.25              |
| 2:B:215:TYR:CD1  | 2:B:233:TYR:CE1  | 2.24                     | 1.24              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:65:ASN:CA    | 4:S:166:LYS:HA   | 1.46                     | 1.24              |
| 1:A:84:MET:SD    | 1:A:113:SER:HA   | 1.78                     | 1.24              |
| 2:B:216:LYS:HA   | 2:B:251:LEU:CD1  | 1.64                     | 1.24              |
| 2:B:219:TYR:CZ   | 2:B:226:LEU:CA   | 2.19                     | 1.24              |
| 2:B:422:ALA:HB3  | 2:B:424:PHE:CD1  | 1.71                     | 1.24              |
| 2:B:241:ASP:CB   | 3:M:274:ASP:OD1  | 1.84                     | 1.24              |
| 3:M:16:PHE:HA    | 3:M:118:TYR:CE1  | 1.73                     | 1.24              |
| 2:B:24:ALA:HB1   | 2:B:35:TYR:CD1   | 1.71                     | 1.24              |
| 2:B:181:TYR:O    | 2:B:182:ARG:C    | 1.75                     | 1.24              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:HB2  | 1.73                     | 1.24              |
| 2:B:231:ARG:CG   | 2:B:298:ASP:OD1  | 1.85                     | 1.24              |
| 1:A:200:PHE:CZ   | 1:A:236:LEU:CD2  | 2.20                     | 1.23              |
| 1:A:289:SER:CB   | 4:S:96:LEU:HD13  | 1.66                     | 1.23              |
| 2:B:345:ARG:NH1  | 3:M:305:ASP:OD2  | 1.68                     | 1.23              |
| 1:A:404:GLN:CA   | 2:B:3:ASP:HB3    | 1.67                     | 1.23              |
| 2:B:21:GLU:OE2   | 2:B:35:TYR:CG    | 1.91                     | 1.23              |
| 2:B:422:ALA:HB3  | 2:B:424:PHE:CE1  | 1.71                     | 1.23              |
| 2:B:523:PHE:CZ   | 2:B:580:TYR:CG   | 2.25                     | 1.23              |
| 2:B:70:MET:CE    | 2:B:107:ARG:CB   | 1.98                     | 1.23              |
| 2:B:519:ALA:O    | 2:B:523:PHE:HB3  | 1.30                     | 1.23              |
| 3:M:222:PHE:O    | 3:M:479:PHE:CE2  | 1.92                     | 1.23              |
| 2:B:252:LEU:CD1  | 2:B:302:PHE:CD1  | 2.21                     | 1.23              |
| 2:B:278:PRO:HA   | 2:B:288:TYR:CB   | 1.68                     | 1.23              |
| 2:B:21:GLU:OE2   | 2:B:35:TYR:CD1   | 1.92                     | 1.23              |
| 2:B:24:ALA:CB    | 2:B:35:TYR:CD1   | 2.22                     | 1.23              |
| 2:B:223:LEU:HB3  | 2:B:259:TYR:CD1  | 1.06                     | 1.23              |
| 1:A:638:LEU:HD13 | 2:B:558:TYR:CG   | 1.73                     | 1.22              |
| 2:B:25:VAL:HG11  | 2:B:36:THR:OG1   | 1.39                     | 1.22              |
| 2:B:243:TRP:CH2  | 3:M:94:GLU:C     | 2.17                     | 1.22              |
| 1:A:408:ILE:HG22 | 4:S:64:ASN:C     | 1.56                     | 1.22              |
| 1:A:638:LEU:CG   | 2:B:520:SER:CB   | 2.07                     | 1.22              |
| 2:B:290:SER:O    | 2:B:292:GLU:N    | 1.71                     | 1.22              |
| 1:A:563:CYS:HB3  | 1:A:621:LEU:CD1  | 1.70                     | 1.22              |
| 2:B:241:ASP:HB2  | 3:M:274:ASP:CG   | 1.64                     | 1.22              |
| 2:B:352:ASN:ND2  | 3:M:70:ASN:HB3   | 1.54                     | 1.22              |
| 2:B:479:VAL:HG13 | 2:B:486:HIS:CE1  | 1.55                     | 1.22              |
| 2:B:546:CYS:CA   | 2:B:607:ILE:HG12 | 1.69                     | 1.22              |
| 2:B:280:PRO:HG2  | 2:B:283:TYR:CD1  | 1.74                     | 1.21              |
| 2:B:337:THR:CA   | 2:B:373:LEU:HD21 | 1.69                     | 1.21              |
| 2:B:219:TYR:CD1  | 2:B:226:LEU:HD13 | 1.75                     | 1.21              |
| 2:B:353:GLN:HB3  | 3:M:50:TYR:CD1   | 1.75                     | 1.21              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:486:HIS:CE1  | 2:B:518:ILE:HD13 | 1.75                     | 1.21              |
| 1:A:638:LEU:CD1  | 2:B:558:TYR:HD2  | 1.39                     | 1.21              |
| 2:B:158:VAL:CG1  | 2:B:177:ILE:CG1  | 2.19                     | 1.21              |
| 3:M:244:VAL:HA   | 3:M:472:TYR:CD2  | 1.75                     | 1.21              |
| 2:B:193:LEU:CD1  | 2:B:225:LEU:CD2  | 2.12                     | 1.20              |
| 2:B:243:TRP:NE1  | 3:M:98:ARG:HD2   | 1.54                     | 1.20              |
| 2:B:513:TRP:CA   | 2:B:551:LEU:CD1  | 2.18                     | 1.20              |
| 1:A:404:GLN:CA   | 2:B:3:ASP:OD2    | 1.90                     | 1.20              |
| 2:B:42:ILE:O     | 2:B:46:GLN:OE1   | 1.60                     | 1.20              |
| 2:B:102:HIS:CE1  | 2:B:137:PHE:C    | 2.17                     | 1.20              |
| 1:A:275:LEU:HD21 | 1:A:311:THR:OG1  | 1.39                     | 1.20              |
| 3:M:344:ILE:CG2  | 3:M:347:PHE:HB3  | 1.73                     | 1.20              |
| 2:B:193:LEU:CD2  | 2:B:225:LEU:CG   | 2.15                     | 1.19              |
| 2:B:293:VAL:O    | 2:B:299:LEU:CG   | 1.89                     | 1.19              |
| 2:B:374:PHE:CE2  | 2:B:402:LEU:HD11 | 1.76                     | 1.19              |
| 2:B:567:GLN:O    | 2:B:569:THR:N    | 1.75                     | 1.19              |
| 1:A:186:PHE:CE1  | 1:A:224:GLU:HB2  | 1.72                     | 1.19              |
| 2:B:16:LYS:HD2   | 3:M:118:TYR:CE2  | 1.76                     | 1.19              |
| 2:B:277:CYS:O    | 2:B:288:TYR:CB   | 1.88                     | 1.19              |
| 1:A:595:GLU:OE2  | 2:B:476:ARG:NH1  | 1.76                     | 1.19              |
| 2:B:219:TYR:CZ   | 2:B:226:LEU:HB2  | 1.76                     | 1.19              |
| 2:B:309:LEU:HB3  | 2:B:317:VAL:CG1  | 1.71                     | 1.19              |
| 2:B:556:LEU:HA   | 2:B:588:ILE:CD1  | 1.72                     | 1.19              |
| 2:B:243:TRP:CH2  | 3:M:94:GLU:CG    | 2.24                     | 1.18              |
| 2:B:567:GLN:O    | 2:B:569:THR:OG1  | 1.61                     | 1.18              |
| 2:B:140:SER:HB2  | 2:B:172:GLU:OE1  | 1.42                     | 1.18              |
| 2:B:155:LEU:CD2  | 2:B:192:LEU:CD1  | 2.19                     | 1.18              |
| 1:A:638:LEU:CG   | 2:B:558:TYR:CG   | 2.26                     | 1.18              |
| 2:B:16:LYS:HD3   | 3:M:119:ASP:OD1  | 1.37                     | 1.18              |
| 2:B:219:TYR:CD1  | 2:B:226:LEU:HB2  | 1.77                     | 1.18              |
| 2:B:549:LEU:HD21 | 2:B:611:ALA:CA   | 1.74                     | 1.18              |
| 2:B:83:PHE:CE2   | 2:B:119:SER:HB3  | 1.78                     | 1.18              |
| 2:B:226:LEU:CD2  | 2:B:255:TYR:CD1  | 2.25                     | 1.18              |
| 2:B:567:GLN:O    | 2:B:569:THR:CB   | 1.92                     | 1.18              |
| 1:A:464:ILE:HA   | 2:B:1:MET:SD     | 1.84                     | 1.18              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:CB   | 2.26                     | 1.18              |
| 2:B:337:THR:HA   | 2:B:373:LEU:HD21 | 1.25                     | 1.18              |
| 1:A:599:ARG:NH1  | 2:B:513:TRP:CZ3  | 2.12                     | 1.17              |
| 2:B:549:LEU:CD2  | 2:B:611:ALA:N    | 2.07                     | 1.17              |
| 1:A:260:PHE:O    | 1:A:261:THR:C    | 1.77                     | 1.17              |
| 2:B:513:TRP:HA   | 2:B:551:LEU:CD1  | 1.74                     | 1.17              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:563:CYS:HB3  | 1:A:621:LEU:HD11 | 1.26                     | 1.17              |
| 2:B:139:LEU:HD23 | 2:B:173:VAL:CA   | 1.73                     | 1.17              |
| 1:A:404:GLN:CA   | 2:B:3:ASP:CB     | 2.21                     | 1.17              |
| 2:B:197:LYS:HB2  | 2:B:229:HIS:NE2  | 1.58                     | 1.17              |
| 2:B:247:TYR:OH   | 3:M:137:SER:CB   | 1.92                     | 1.17              |
| 1:A:404:GLN:O    | 2:B:3:ASP:CB     | 1.93                     | 1.17              |
| 1:A:595:GLU:OE2  | 2:B:476:ARG:CZ   | 1.92                     | 1.17              |
| 2:B:216:LYS:CA   | 2:B:251:LEU:HD13 | 1.72                     | 1.17              |
| 1:A:403:LEU:O    | 2:B:3:ASP:HB2    | 1.00                     | 1.16              |
| 2:B:25:VAL:CB    | 2:B:36:THR:OG1   | 1.91                     | 1.16              |
| 3:M:435:LEU:O    | 3:M:479:PHE:CD2  | 1.97                     | 1.16              |
| 1:A:225:LEU:HB3  | 1:A:233:PHE:CE1  | 1.81                     | 1.16              |
| 1:A:630:PRO:HG3  | 2:B:617:LEU:HD11 | 1.25                     | 1.16              |
| 2:B:143:SER:CB   | 2:B:179:LYS:HD2  | 1.74                     | 1.16              |
| 2:B:534:ILE:CG2  | 2:B:594:ALA:HB1  | 1.73                     | 1.16              |
| 3:M:355:ASP:OD2  | 3:M:357:LYS:NZ   | 1.77                     | 1.16              |
| 2:B:87:VAL:HG13  | 2:B:122:SER:CB   | 1.75                     | 1.16              |
| 2:B:534:ILE:HD13 | 2:B:591:MET:O    | 1.40                     | 1.16              |
| 2:B:24:ALA:HB3   | 2:B:35:TYR:CE1   | 1.74                     | 1.16              |
| 2:B:219:TYR:CD1  | 2:B:226:LEU:HD22 | 1.81                     | 1.16              |
| 1:A:638:LEU:CD1  | 2:B:558:TYR:HB3  | 1.72                     | 1.16              |
| 2:B:472:VAL:HG11 | 2:B:510:GLY:CA   | 1.76                     | 1.16              |
| 2:B:25:VAL:CG1   | 2:B:36:THR:OG1   | 1.93                     | 1.15              |
| 1:A:595:GLU:CA   | 2:B:476:ARG:HH22 | 1.58                     | 1.15              |
| 2:B:245:GLN:CG   | 2:B:309:LEU:HD11 | 1.75                     | 1.15              |
| 2:B:534:ILE:HG21 | 2:B:594:ALA:HB3  | 1.23                     | 1.15              |
| 2:B:278:PRO:HD2  | 2:B:292:GLU:CG   | 1.75                     | 1.15              |
| 3:M:219:LEU:HD13 | 3:M:472:TYR:O    | 1.42                     | 1.15              |
| 1:A:404:GLN:HB3  | 2:B:7:ARG:NH2    | 1.60                     | 1.15              |
| 2:B:519:ALA:O    | 2:B:523:PHE:CB   | 1.95                     | 1.15              |
| 3:M:379:LEU:HA   | 3:M:412:ARG:O    | 1.44                     | 1.15              |
| 1:A:594:PHE:CD2  | 2:B:477:MET:HG3  | 1.81                     | 1.15              |
| 2:B:136:CYS:C    | 2:B:172:GLU:HG3  | 1.72                     | 1.15              |
| 1:A:179:LYS:HZ1  | 4:S:141:VAL:HA   | 1.12                     | 1.14              |
| 2:B:243:TRP:CH2  | 3:M:94:GLU:CB    | 2.30                     | 1.14              |
| 1:A:179:LYS:HB3  | 4:S:142:ILE:HD12 | 1.29                     | 1.14              |
| 1:A:595:GLU:OE1  | 2:B:476:ARG:NH1  | 1.79                     | 1.14              |
| 2:B:25:VAL:HG21  | 2:B:36:THR:CB    | 1.76                     | 1.14              |
| 2:B:70:MET:HE1   | 2:B:107:ARG:HB2  | 1.16                     | 1.14              |
| 2:B:230:PHE:CZ   | 2:B:252:LEU:CD2  | 2.31                     | 1.14              |
| 1:A:114:PHE:CZ   | 1:A:152:THR:O    | 2.01                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:25:VAL:CG2   | 2:B:36:THR:CA    | 2.16                     | 1.14              |
| 2:B:293:VAL:O    | 2:B:299:LEU:HG   | 1.43                     | 1.14              |
| 2:B:178:ILE:CG1  | 2:B:214:ALA:HB1  | 1.76                     | 1.14              |
| 2:B:208:ILE:CD1  | 2:B:236:ILE:HG21 | 1.78                     | 1.14              |
| 2:B:534:ILE:HG21 | 2:B:594:ALA:HB1  | 1.15                     | 1.14              |
| 1:A:638:LEU:HG   | 2:B:520:SER:HB2  | 1.21                     | 1.13              |
| 1:A:638:LEU:CG   | 2:B:558:TYR:CB   | 2.23                     | 1.13              |
| 2:B:234:CYS:O    | 2:B:237:ILE:HG22 | 1.43                     | 1.13              |
| 3:M:268:GLY:N    | 3:M:302:TYR:OH   | 1.77                     | 1.13              |
| 1:A:225:LEU:HD13 | 1:A:233:PHE:HZ   | 1.04                     | 1.13              |
| 1:A:332:TYR:CZ   | 1:A:336:ILE:HD11 | 1.83                     | 1.13              |
| 2:B:353:GLN:CG   | 3:M:50:TYR:HD1   | 1.60                     | 1.13              |
| 3:M:59:ASP:O     | 3:M:61:GLU:N     | 1.81                     | 1.13              |
| 1:A:638:LEU:CD1  | 2:B:558:TYR:CG   | 2.25                     | 1.13              |
| 1:A:102:GLN:HE22 | 4:S:166:LYS:NZ   | 1.47                     | 1.12              |
| 2:B:18:ILE:HB    | 2:B:23:ALA:HB2   | 1.24                     | 1.12              |
| 2:B:21:GLU:OE1   | 2:B:39:SER:HB2   | 1.39                     | 1.12              |
| 2:B:80:GLN:HG2   | 2:B:115:LEU:HD21 | 1.25                     | 1.12              |
| 2:B:87:VAL:CG1   | 2:B:122:SER:HB3  | 1.79                     | 1.12              |
| 2:B:151:ALA:HA   | 2:B:180:LEU:HD11 | 1.29                     | 1.13              |
| 2:B:123:LEU:HD13 | 2:B:142:LEU:HG   | 1.15                     | 1.12              |
| 2:B:230:PHE:CE1  | 2:B:252:LEU:CD2  | 2.31                     | 1.12              |
| 2:B:523:PHE:HZ   | 2:B:580:TYR:CE1  | 1.67                     | 1.12              |
| 2:B:553:ALA:HB2  | 2:B:614:ILE:CD1  | 1.79                     | 1.12              |
| 1:A:295:VAL:HG22 | 1:A:315:CYS:HB3  | 1.27                     | 1.12              |
| 2:B:280:PRO:CG   | 2:B:283:TYR:CD1  | 2.33                     | 1.12              |
| 1:A:179:LYS:CB   | 4:S:142:ILE:HD13 | 1.66                     | 1.12              |
| 2:B:374:PHE:HD2  | 2:B:402:LEU:CD2  | 1.62                     | 1.12              |
| 2:B:545:ARG:HD3  | 2:B:602:ASP:HB2  | 1.25                     | 1.12              |
| 2:B:559:ASP:CB   | 2:B:563:PHE:CD1  | 2.32                     | 1.12              |
| 1:A:408:ILE:CG2  | 4:S:64:ASN:C     | 2.21                     | 1.12              |
| 1:A:594:PHE:CE2  | 2:B:477:MET:HG3  | 1.84                     | 1.11              |
| 2:B:486:HIS:NE2  | 2:B:518:ILE:HB   | 1.65                     | 1.11              |
| 2:B:139:LEU:HG   | 2:B:176:ALA:HB2  | 1.28                     | 1.11              |
| 2:B:437:SER:HB2  | 2:B:474:VAL:HG13 | 1.18                     | 1.11              |
| 4:S:135:ILE:O    | 4:S:141:VAL:HA   | 1.49                     | 1.11              |
| 1:A:121:LEU:HD21 | 1:A:158:LEU:HB2  | 1.11                     | 1.11              |
| 1:A:630:PRO:HG2  | 2:B:617:LEU:CD1  | 1.64                     | 1.11              |
| 2:B:38:TYR:HA    | 2:B:42:ILE:N     | 1.65                     | 1.11              |
| 2:B:78:ASP:O     | 2:B:79:VAL:C     | 1.72                     | 1.11              |
| 2:B:143:SER:HB2  | 2:B:179:LYS:HB2  | 1.33                     | 1.11              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:559:ASP:O    | 2:B:563:PHE:N    | 1.82                     | 1.11              |
| 1:A:179:LYS:HE2  | 4:S:140:MET:O    | 1.48                     | 1.11              |
| 2:B:181:TYR:CE1  | 2:B:222:HIS:CD2  | 2.37                     | 1.11              |
| 2:B:216:LYS:HB2  | 2:B:251:LEU:HD13 | 1.19                     | 1.11              |
| 2:B:219:TYR:CZ   | 2:B:226:LEU:CB   | 2.32                     | 1.11              |
| 2:B:252:LEU:CD1  | 2:B:302:PHE:CE1  | 2.32                     | 1.11              |
| 3:M:347:PHE:CE1  | 3:M:350:VAL:CG1  | 2.33                     | 1.11              |
| 1:A:156:PRO:HB3  | 1:A:192:TYR:CE1  | 1.86                     | 1.10              |
| 2:B:25:VAL:HG22  | 2:B:35:TYR:C     | 1.74                     | 1.10              |
| 2:B:155:LEU:CD2  | 2:B:192:LEU:HD12 | 1.79                     | 1.10              |
| 2:B:243:TRP:NE1  | 3:M:98:ARG:CD    | 2.09                     | 1.10              |
| 3:M:41:LEU:HD13  | 3:M:52:ASP:N     | 1.63                     | 1.10              |
| 3:M:222:PHE:O    | 3:M:479:PHE:CZ   | 2.04                     | 1.10              |
| 2:B:24:ALA:CB    | 2:B:35:TYR:CE2   | 2.26                     | 1.10              |
| 2:B:219:TYR:CE2  | 2:B:226:LEU:HB2  | 1.86                     | 1.10              |
| 2:B:433:VAL:HG12 | 2:B:474:VAL:CG2  | 1.81                     | 1.10              |
| 1:A:257:LEU:HD22 | 1:A:278:ILE:HG22 | 1.16                     | 1.10              |
| 1:A:464:ILE:C    | 2:B:1:MET:SD     | 2.35                     | 1.10              |
| 1:A:589:SER:O    | 1:A:597:GLN:HG3  | 1.49                     | 1.10              |
| 2:B:559:ASP:HB2  | 2:B:563:PHE:CD1  | 1.86                     | 1.10              |
| 2:B:44:PRO:HB3   | 2:B:82:TYR:OH    | 1.49                     | 1.10              |
| 2:B:479:VAL:HG13 | 2:B:486:HIS:CG   | 1.84                     | 1.10              |
| 1:A:289:SER:HB3  | 4:S:96:LEU:CD1   | 1.67                     | 1.10              |
| 2:B:219:TYR:CG   | 2:B:226:LEU:HB2  | 1.86                     | 1.10              |
| 2:B:243:TRP:CE2  | 3:M:98:ARG:HD2   | 1.87                     | 1.10              |
| 1:A:101:GLN:OE1  | 4:S:167:ILE:HD11 | 1.51                     | 1.09              |
| 1:A:638:LEU:HD12 | 2:B:558:TYR:HD2  | 0.95                     | 1.09              |
| 2:B:277:CYS:O    | 2:B:288:TYR:HB3  | 0.93                     | 1.09              |
| 1:A:609:LEU:CD2  | 1:A:628:VAL:HG11 | 1.81                     | 1.09              |
| 2:B:374:PHE:CD2  | 2:B:402:LEU:HD21 | 1.87                     | 1.09              |
| 1:A:65:ASN:CA    | 4:S:166:LYS:CA   | 2.15                     | 1.09              |
| 1:A:114:PHE:CD1  | 1:A:153:ILE:HG23 | 1.88                     | 1.09              |
| 1:A:225:LEU:CD1  | 1:A:233:PHE:CZ   | 2.35                     | 1.09              |
| 1:A:638:LEU:CB   | 2:B:558:TYR:CD1  | 2.17                     | 1.09              |
| 2:B:86:VAL:HG12  | 2:B:101:ILE:HG23 | 1.35                     | 1.09              |
| 2:B:178:ILE:CG1  | 2:B:214:ALA:C    | 2.25                     | 1.09              |
| 2:B:216:LYS:CA   | 2:B:251:LEU:CD1  | 2.28                     | 1.09              |
| 2:B:239:GLN:OE1  | 3:M:279:ASN:CA   | 1.89                     | 1.09              |
| 2:B:241:ASP:HB2  | 3:M:274:ASP:OD1  | 0.93                     | 1.09              |
| 2:B:243:TRP:CH2  | 3:M:95:THR:N     | 2.20                     | 1.09              |
| 2:B:513:TRP:HA   | 2:B:551:LEU:HD22 | 1.35                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:549:LEU:HD11 | 2:B:611:ALA:HA   | 1.19                     | 1.09              |
| 2:B:578:PRO:HD2  | 2:B:581:TYR:CE1  | 1.87                     | 1.09              |
| 1:A:151:SER:HB2  | 1:A:187:LYS:HB2  | 1.34                     | 1.09              |
| 1:A:429:VAL:CB   | 1:A:469:LEU:HD11 | 1.82                     | 1.09              |
| 1:A:586:GLU:O    | 1:A:587:ASN:C    | 1.77                     | 1.09              |
| 2:B:136:CYS:SG   | 2:B:169:VAL:CA   | 2.40                     | 1.09              |
| 2:B:371:GLN:CD   | 2:B:401:THR:O    | 1.95                     | 1.09              |
| 3:M:106:LYS:HB3  | 3:M:296:LYS:HZ3  | 1.11                     | 1.09              |
| 3:M:265:ASN:OD1  | 3:M:313:SER:OG   | 1.67                     | 1.09              |
| 1:A:638:LEU:HD12 | 2:B:558:TYR:CD2  | 1.72                     | 1.09              |
| 2:B:151:ALA:CA   | 2:B:180:LEU:HD11 | 1.83                     | 1.09              |
| 2:B:337:THR:HA   | 2:B:373:LEU:CD2  | 1.82                     | 1.09              |
| 2:B:353:GLN:CG   | 3:M:50:TYR:CD1   | 2.35                     | 1.09              |
| 2:B:537:PHE:CD2  | 2:B:598:LEU:HB3  | 1.87                     | 1.09              |
| 1:A:429:VAL:HB   | 1:A:469:LEU:HD11 | 1.32                     | 1.08              |
| 2:B:25:VAL:HG23  | 2:B:35:TYR:HD2   | 1.14                     | 1.08              |
| 2:B:461:HIS:O    | 2:B:462:ASN:C    | 1.84                     | 1.08              |
| 2:B:178:ILE:HG12 | 2:B:214:ALA:HB1  | 1.25                     | 1.08              |
| 2:B:223:LEU:HD13 | 2:B:258:GLN:C    | 1.77                     | 1.08              |
| 2:B:527:PRO:HB3  | 2:B:587:ARG:HG3  | 1.22                     | 1.08              |
| 2:B:70:MET:HE3   | 2:B:107:ARG:HB3  | 1.30                     | 1.08              |
| 2:B:87:VAL:HG13  | 2:B:122:SER:HB3  | 1.27                     | 1.08              |
| 2:B:139:LEU:CD2  | 2:B:173:VAL:CA   | 2.31                     | 1.08              |
| 2:B:215:TYR:HD1  | 2:B:233:TYR:CE1  | 1.65                     | 1.08              |
| 2:B:278:PRO:HG2  | 2:B:292:GLU:OE1  | 1.52                     | 1.08              |
| 2:B:184:GLY:O    | 2:B:188:TYR:CD1  | 2.07                     | 1.08              |
| 2:B:226:LEU:HD23 | 2:B:255:TYR:CE1  | 1.89                     | 1.08              |
| 2:B:261:PRO:HB2  | 2:B:290:SER:HB3  | 1.32                     | 1.08              |
| 3:M:41:LEU:CD1   | 3:M:52:ASP:N     | 2.14                     | 1.08              |
| 3:M:343:ASN:HA   | 3:M:408:VAL:HG13 | 1.18                     | 1.08              |
| 1:A:102:GLN:NE2  | 4:S:166:LYS:HD3  | 1.69                     | 1.07              |
| 1:A:189:PHE:HB2  | 1:A:225:LEU:HD21 | 1.31                     | 1.07              |
| 2:B:120:ILE:HG13 | 2:B:150:LEU:HD22 | 1.23                     | 1.07              |
| 2:B:123:LEU:HD12 | 2:B:142:LEU:CD2  | 1.83                     | 1.07              |
| 2:B:162:VAL:CB   | 2:B:195:ILE:HG23 | 1.84                     | 1.07              |
| 2:B:216:LYS:HA   | 2:B:251:LEU:HD11 | 1.31                     | 1.07              |
| 2:B:549:LEU:CD2  | 2:B:607:ILE:O    | 2.02                     | 1.07              |
| 3:M:96:ILE:HG21  | 3:M:125:PHE:CZ   | 1.86                     | 1.07              |
| 1:A:258:LYS:NZ   | 4:S:94:SER:CB    | 2.18                     | 1.07              |
| 2:B:70:MET:HE3   | 2:B:107:ARG:CG   | 1.84                     | 1.07              |
| 2:B:278:PRO:HA   | 2:B:288:TYR:CA   | 1.84                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:537:PHE:HB3  | 2:B:598:LEU:HD13 | 1.07                     | 1.07              |
| 1:A:244:LEU:HD11 | 1:A:281:LEU:CD1  | 1.85                     | 1.07              |
| 1:A:404:GLN:CA   | 2:B:3:ASP:CG     | 2.26                     | 1.07              |
| 2:B:41:ASN:HB3   | 2:B:43:ASN:OD1   | 1.52                     | 1.07              |
| 2:B:196:LEU:O    | 2:B:215:TYR:OH   | 1.71                     | 1.07              |
| 2:B:212:VAL:HG21 | 2:B:248:LEU:HD21 | 1.30                     | 1.07              |
| 2:B:252:LEU:CB   | 2:B:302:PHE:CZ   | 2.37                     | 1.07              |
| 2:B:523:PHE:CZ   | 2:B:580:TYR:CE1  | 2.42                     | 1.07              |
| 1:A:638:LEU:CD1  | 2:B:520:SER:CA   | 2.31                     | 1.07              |
| 2:B:21:GLU:OE1   | 2:B:39:SER:HB3   | 1.49                     | 1.07              |
| 2:B:199:LEU:O    | 2:B:201:ALA:N    | 1.86                     | 1.07              |
| 2:B:38:TYR:HA    | 2:B:42:ILE:H     | 1.14                     | 1.07              |
| 1:A:125:THR:OG1  | 1:A:158:LEU:CD1  | 2.02                     | 1.06              |
| 2:B:354:GLY:O    | 2:B:358:MET:HG2  | 1.55                     | 1.06              |
| 2:B:523:PHE:CD1  | 2:B:582:ASP:OD2  | 2.07                     | 1.06              |
| 1:A:638:LEU:CD2  | 2:B:558:TYR:CB   | 2.04                     | 1.06              |
| 2:B:223:LEU:CD1  | 2:B:258:GLN:C    | 2.28                     | 1.06              |
| 2:B:247:TYR:CE1  | 3:M:137:SER:OG   | 2.07                     | 1.06              |
| 2:B:279:LEU:H    | 2:B:288:TYR:HB2  | 1.01                     | 1.06              |
| 2:B:523:PHE:CE1  | 2:B:580:TYR:CG   | 2.42                     | 1.06              |
| 2:B:534:ILE:CG2  | 2:B:594:ALA:CB   | 2.33                     | 1.06              |
| 3:M:245:ASP:HB3  | 3:M:472:TYR:CD1  | 1.89                     | 1.06              |
| 1:A:189:PHE:CB   | 1:A:225:LEU:HD21 | 1.86                     | 1.06              |
| 1:A:215:VAL:CG1  | 1:A:243:ILE:CG2  | 2.34                     | 1.06              |
| 2:B:208:ILE:HG12 | 2:B:236:ILE:HD13 | 1.33                     | 1.06              |
| 2:B:219:TYR:HB3  | 2:B:223:LEU:HD23 | 1.32                     | 1.06              |
| 2:B:236:ILE:HG22 | 2:B:240:LEU:HD11 | 1.33                     | 1.06              |
| 2:B:523:PHE:CE1  | 2:B:580:TYR:CB   | 2.36                     | 1.06              |
| 2:B:567:GLN:C    | 2:B:569:THR:N    | 2.12                     | 1.06              |
| 2:B:25:VAL:HG21  | 2:B:36:THR:HA    | 1.30                     | 1.06              |
| 2:B:105:LEU:HB3  | 2:B:145:MET:HE1  | 1.14                     | 1.06              |
| 2:B:549:LEU:HD22 | 2:B:611:ALA:HB2  | 1.35                     | 1.06              |
| 4:S:17:VAL:HG21  | 4:S:19:PHE:CZ    | 1.90                     | 1.06              |
| 1:A:464:ILE:CA   | 2:B:1:MET:SD     | 2.43                     | 1.06              |
| 2:B:171:GLY:CA   | 2:B:207:VAL:HG13 | 1.85                     | 1.06              |
| 2:B:181:TYR:CE1  | 2:B:185:LYS:HG3  | 1.91                     | 1.06              |
| 2:B:243:TRP:CZ3  | 3:M:94:GLU:CB    | 2.38                     | 1.06              |
| 2:B:337:THR:HG23 | 2:B:373:LEU:HD11 | 1.28                     | 1.06              |
| 2:B:490:ILE:HG13 | 2:B:518:ILE:HG21 | 1.35                     | 1.06              |
| 3:M:245:ASP:O    | 3:M:472:TYR:CE1  | 2.07                     | 1.06              |
| 1:A:176:TYR:OH   | 4:S:148:ARG:HB3  | 1.54                     | 1.05              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:316:THR:CG2  | 3:M:90:PHE:CD2   | 2.25                     | 1.05              |
| 2:B:517:GLU:OE2  | 2:B:554:LYS:NZ   | 1.89                     | 1.05              |
| 1:A:207:LEU:O    | 1:A:243:ILE:HD11 | 1.55                     | 1.05              |
| 1:A:225:LEU:HD13 | 1:A:233:PHE:CZ   | 1.89                     | 1.05              |
| 2:B:167:ALA:CA   | 2:B:202:ASP:OD1  | 2.05                     | 1.05              |
| 2:B:553:ALA:HB2  | 2:B:614:ILE:HD13 | 1.30                     | 1.05              |
| 2:B:25:VAL:HG23  | 2:B:35:TYR:CD2   | 1.90                     | 1.05              |
| 2:B:193:LEU:CD2  | 2:B:225:LEU:HB2  | 1.85                     | 1.05              |
| 2:B:158:VAL:HG11 | 2:B:177:ILE:HG13 | 1.33                     | 1.05              |
| 2:B:193:LEU:HD13 | 2:B:225:LEU:HD21 | 1.36                     | 1.05              |
| 2:B:219:TYR:CZ   | 2:B:226:LEU:HA   | 1.87                     | 1.05              |
| 2:B:219:TYR:CD2  | 2:B:226:LEU:HB2  | 1.90                     | 1.05              |
| 3:M:105:ASP:O    | 3:M:106:LYS:CB   | 2.03                     | 1.05              |
| 1:A:186:PHE:HE1  | 1:A:224:GLU:HB2  | 0.96                     | 1.04              |
| 2:B:24:ALA:CB    | 2:B:35:TYR:CG    | 2.40                     | 1.04              |
| 2:B:170:ARG:HH12 | 2:B:198:GLU:HG2  | 1.15                     | 1.04              |
| 2:B:513:TRP:CA   | 2:B:551:LEU:HD13 | 1.83                     | 1.04              |
| 1:A:404:GLN:C    | 2:B:3:ASP:CB     | 2.30                     | 1.04              |
| 1:A:436:CYS:SG   | 1:A:450:TYR:CZ   | 2.50                     | 1.04              |
| 2:B:47:LEU:HD22  | 2:B:66:ILE:HG13  | 1.39                     | 1.04              |
| 2:B:216:LYS:CB   | 2:B:251:LEU:CD1  | 2.35                     | 1.04              |
| 2:B:374:PHE:CD2  | 2:B:402:LEU:CD2  | 2.40                     | 1.04              |
| 3:M:218:LEU:HA   | 3:M:472:TYR:CE2  | 1.93                     | 1.04              |
| 1:A:163:ALA:HB1  | 1:A:199:ASN:HD21 | 0.94                     | 1.04              |
| 1:A:180:LYS:NZ   | 4:S:137:GLN:HB3  | 1.72                     | 1.04              |
| 2:B:24:ALA:HB3   | 2:B:35:TYR:CG    | 1.92                     | 1.04              |
| 2:B:155:LEU:CD2  | 2:B:192:LEU:HD11 | 1.83                     | 1.04              |
| 2:B:178:ILE:HD12 | 2:B:218:CYS:H    | 1.16                     | 1.04              |
| 2:B:278:PRO:CA   | 2:B:288:TYR:C    | 2.30                     | 1.04              |
| 2:B:123:LEU:CD1  | 2:B:142:LEU:HG   | 1.88                     | 1.04              |
| 2:B:158:VAL:CG1  | 2:B:177:ILE:HG13 | 1.86                     | 1.04              |
| 1:A:200:PHE:CE2  | 1:A:236:LEU:HD21 | 1.91                     | 1.03              |
| 1:A:405:THR:N    | 2:B:7:ARG:CZ     | 2.10                     | 1.03              |
| 2:B:42:ILE:O     | 2:B:46:GLN:CD    | 2.00                     | 1.03              |
| 2:B:162:VAL:HG21 | 2:B:195:ILE:HG22 | 1.08                     | 1.03              |
| 2:B:162:VAL:HG21 | 2:B:195:ILE:HG23 | 1.13                     | 1.03              |
| 3:M:379:LEU:HD23 | 3:M:411:LEU:HG   | 1.38                     | 1.03              |
| 1:A:186:PHE:CZ   | 1:A:224:GLU:HG2  | 1.92                     | 1.03              |
| 1:A:215:VAL:CG1  | 1:A:243:ILE:HG21 | 1.88                     | 1.03              |
| 1:A:637:GLU:HA   | 2:B:517:GLU:OE1  | 1.57                     | 1.03              |
| 3:M:219:LEU:CD1  | 3:M:472:TYR:O    | 2.06                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:404:ASN:O    | 2:B:405:GLU:C    | 1.83                     | 1.03              |
| 2:B:542:PRO:HA   | 2:B:602:ASP:OD2  | 1.56                     | 1.03              |
| 3:M:350:VAL:HG22 | 3:M:442:GLN:HG2  | 1.40                     | 1.03              |
| 2:B:98:LYS:HZ1   | 2:B:134:LEU:HB3  | 1.03                     | 1.03              |
| 2:B:174:ALA:CB   | 2:B:211:ALA:HA   | 1.89                     | 1.03              |
| 2:B:197:LYS:HA   | 2:B:229:HIS:CD2  | 1.92                     | 1.03              |
| 2:B:278:PRO:CB   | 2:B:288:TYR:O    | 2.07                     | 1.03              |
| 2:B:556:LEU:HD22 | 2:B:588:ILE:HG12 | 1.38                     | 1.03              |
| 1:A:186:PHE:CE1  | 1:A:224:GLU:CG   | 2.42                     | 1.03              |
| 1:A:225:LEU:CB   | 1:A:233:PHE:CZ   | 2.41                     | 1.03              |
| 4:S:131:VAL:HG22 | 4:S:153:VAL:HG22 | 1.41                     | 1.03              |
| 1:A:180:LYS:NZ   | 4:S:137:GLN:CB   | 2.20                     | 1.02              |
| 1:A:222:ILE:HG21 | 1:A:240:LEU:HD11 | 1.41                     | 1.02              |
| 1:A:289:SER:O    | 1:A:290:VAL:C    | 1.87                     | 1.02              |
| 2:B:278:PRO:HD2  | 2:B:292:GLU:HB2  | 1.16                     | 1.02              |
| 1:A:176:TYR:CE2  | 4:S:143:GLU:OE2  | 2.11                     | 1.02              |
| 1:A:219:VAL:HG21 | 1:A:256:LEU:HD21 | 1.41                     | 1.02              |
| 1:A:638:LEU:CD1  | 2:B:520:SER:N    | 2.21                     | 1.02              |
| 2:B:105:LEU:O    | 2:B:106:LEU:C    | 1.96                     | 1.02              |
| 2:B:247:TYR:CZ   | 3:M:137:SER:OG   | 2.10                     | 1.02              |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:HB3  | 1.41                     | 1.02              |
| 2:B:437:SER:CB   | 2:B:474:VAL:HG13 | 1.89                     | 1.02              |
| 3:M:347:PHE:CD1  | 3:M:350:VAL:HB   | 1.95                     | 1.02              |
| 1:A:233:PHE:O    | 1:A:234:ILE:C    | 1.77                     | 1.02              |
| 2:B:230:PHE:CE2  | 2:B:234:CYS:SG   | 2.52                     | 1.02              |
| 2:B:278:PRO:HD3  | 2:B:289:PRO:O    | 1.59                     | 1.02              |
| 1:A:163:ALA:HB1  | 1:A:199:ASN:ND2  | 1.74                     | 1.02              |
| 1:A:605:GLU:HG3  | 1:A:632:PHE:CD2  | 1.95                     | 1.02              |
| 1:A:638:LEU:CB   | 2:B:520:SER:HB3  | 1.89                     | 1.02              |
| 2:B:260:LEU:HA   | 2:B:293:VAL:HG21 | 1.38                     | 1.02              |
| 1:A:114:PHE:CZ   | 1:A:153:ILE:HA   | 1.95                     | 1.02              |
| 2:B:102:HIS:NE2  | 2:B:138:ALA:CA   | 2.12                     | 1.02              |
| 2:B:143:SER:C    | 2:B:179:LYS:HD3  | 1.85                     | 1.02              |
| 2:B:212:VAL:O    | 2:B:213:LEU:C    | 1.91                     | 1.02              |
| 2:B:523:PHE:CD1  | 2:B:559:ASP:OD1  | 2.13                     | 1.02              |
| 2:B:546:CYS:CB   | 2:B:607:ILE:CG1  | 2.27                     | 1.02              |
| 4:S:53:THR:HG21  | 4:S:68:VAL:HA    | 1.39                     | 1.02              |
| 1:A:88:ASN:CG    | 1:A:120:ILE:CG2  | 2.33                     | 1.01              |
| 1:A:154:ILE:CG2  | 1:A:191:GLN:HG3  | 1.90                     | 1.01              |
| 2:B:25:VAL:CG2   | 2:B:36:THR:OG1   | 2.08                     | 1.01              |
| 2:B:566:ALA:O    | 2:B:574:ASN:CB   | 2.07                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:344:ILE:HG22 | 3:M:347:PHE:HB3  | 1.40                     | 1.01              |
| 1:A:349:ILE:HG21 | 1:A:378:ILE:HG22 | 1.40                     | 1.01              |
| 2:B:42:ILE:C     | 2:B:46:GLN:OE1   | 2.01                     | 1.01              |
| 2:B:252:LEU:HB2  | 2:B:302:PHE:CE1  | 1.94                     | 1.01              |
| 4:S:8:PHE:CZ     | 4:S:86:THR:OG1   | 2.11                     | 1.01              |
| 2:B:139:LEU:CG   | 2:B:176:ALA:HB2  | 1.90                     | 1.01              |
| 2:B:223:LEU:HB3  | 2:B:259:TYR:CG   | 1.96                     | 1.01              |
| 2:B:230:PHE:HZ   | 2:B:252:LEU:HD22 | 1.20                     | 1.01              |
| 2:B:497:LEU:HD23 | 2:B:533:LEU:HD21 | 1.40                     | 1.01              |
| 3:M:432:THR:OG1  | 3:M:480:GLN:CG   | 2.07                     | 1.01              |
| 3:M:443:SER:HB3  | 3:M:447:ILE:HG13 | 1.43                     | 1.01              |
| 1:A:154:ILE:HB   | 1:A:191:GLN:HG3  | 1.41                     | 1.01              |
| 1:A:258:LYS:HZ1  | 4:S:94:SER:CB    | 1.71                     | 1.01              |
| 1:A:638:LEU:HD13 | 2:B:558:TYR:CD2  | 1.72                     | 1.01              |
| 1:A:638:LEU:HD13 | 2:B:558:TYR:HB2  | 1.36                     | 1.01              |
| 3:M:95:THR:OG1   | 3:M:137:SER:HB2  | 1.59                     | 1.01              |
| 2:B:24:ALA:CB    | 2:B:35:TYR:CD2   | 2.42                     | 1.00              |
| 2:B:337:THR:CG2  | 2:B:373:LEU:HD11 | 1.91                     | 1.00              |
| 2:B:374:PHE:CD2  | 2:B:402:LEU:HD11 | 1.96                     | 1.00              |
| 2:B:433:VAL:HG12 | 2:B:474:VAL:HG21 | 1.02                     | 1.00              |
| 1:A:381:GLU:O    | 1:A:382:ASP:C    | 1.93                     | 1.00              |
| 2:B:458:MET:SD   | 2:B:471:TYR:HB3  | 2.02                     | 1.00              |
| 2:B:534:ILE:HD11 | 2:B:591:MET:O    | 1.60                     | 1.00              |
| 1:A:595:GLU:N    | 2:B:476:ARG:HH22 | 1.60                     | 1.00              |
| 2:B:143:SER:OG   | 2:B:179:LYS:HD2  | 1.61                     | 1.00              |
| 2:B:261:PRO:HB2  | 2:B:290:SER:CB   | 1.91                     | 1.00              |
| 2:B:309:LEU:HB3  | 2:B:317:VAL:HG11 | 1.40                     | 1.00              |
| 2:B:523:PHE:HB2  | 2:B:559:ASP:OD2  | 1.61                     | 1.00              |
| 1:A:533:ILE:HG12 | 1:A:562:TRP:CH2  | 1.97                     | 1.00              |
| 2:B:25:VAL:HG21  | 2:B:36:THR:OG1   | 1.59                     | 1.00              |
| 2:B:297:PRO:O    | 2:B:301:LEU:HG   | 1.61                     | 1.00              |
| 2:B:509:ALA:HB1  | 2:B:547:GLN:HG3  | 1.41                     | 1.00              |
| 2:B:578:PRO:HD2  | 2:B:581:TYR:CD1  | 1.95                     | 1.00              |
| 1:A:225:LEU:CD1  | 1:A:233:PHE:HZ   | 1.72                     | 1.00              |
| 1:A:239:LEU:O    | 1:A:242:GLU:O    | 1.78                     | 1.00              |
| 1:A:262:ASN:O    | 1:A:265:GLN:O    | 1.77                     | 1.00              |
| 2:B:136:CYS:SG   | 2:B:168:MET:C    | 2.45                     | 1.00              |
| 2:B:158:VAL:HG11 | 2:B:177:ILE:HG12 | 1.01                     | 1.00              |
| 2:B:178:ILE:HG23 | 2:B:217:GLU:CB   | 1.91                     | 1.00              |
| 2:B:252:LEU:HD13 | 2:B:302:PHE:HD1  | 1.20                     | 1.00              |
| 2:B:259:TYR:HD2  | 2:B:261:PRO:HG3  | 1.27                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:418:TYR:CD1  | 2:B:418:TYR:C    | 2.33                     | 1.00              |
| 2:B:259:TYR:CD2  | 2:B:261:PRO:HG3  | 1.97                     | 1.00              |
| 2:B:353:GLN:HB3  | 3:M:50:TYR:HD1   | 1.05                     | 1.00              |
| 2:B:374:PHE:HZ   | 2:B:381:PHE:CD1  | 1.80                     | 1.00              |
| 1:A:609:LEU:HG   | 1:A:628:VAL:CG1  | 1.92                     | 0.99              |
| 2:B:181:TYR:CE2  | 2:B:218:CYS:O    | 2.14                     | 0.99              |
| 2:B:212:VAL:O    | 2:B:214:ALA:N    | 1.95                     | 0.99              |
| 2:B:546:CYS:HB2  | 2:B:607:ILE:HG12 | 1.19                     | 0.99              |
| 2:B:278:PRO:C    | 2:B:288:TYR:HB2  | 1.85                     | 0.99              |
| 2:B:566:ALA:C    | 2:B:574:ASN:ND2  | 2.19                     | 0.99              |
| 2:B:549:LEU:CD2  | 2:B:611:ALA:HB2  | 1.91                     | 0.99              |
| 1:A:101:GLN:OE1  | 4:S:167:ILE:CD1  | 2.11                     | 0.99              |
| 1:A:450:TYR:OH   | 1:A:476:GLN:CG   | 2.10                     | 0.99              |
| 2:B:422:ALA:CB   | 2:B:424:PHE:CE1  | 2.46                     | 0.99              |
| 1:A:225:LEU:CB   | 1:A:233:PHE:CE1  | 2.46                     | 0.99              |
| 1:A:637:GLU:OE2  | 2:B:517:GLU:HG2  | 1.57                     | 0.99              |
| 2:B:243:TRP:HE1  | 3:M:98:ARG:HD2   | 1.15                     | 0.99              |
| 2:B:513:TRP:HA   | 2:B:551:LEU:CG   | 1.91                     | 0.99              |
| 1:A:260:PHE:CD2  | 1:A:274:LEU:HG   | 1.96                     | 0.99              |
| 2:B:337:THR:HA   | 2:B:373:LEU:HD11 | 1.42                     | 0.99              |
| 3:M:245:ASP:O    | 3:M:472:TYR:CZ   | 2.16                     | 0.99              |
| 4:S:35:VAL:HG12  | 4:S:75:ILE:HD13  | 1.41                     | 0.99              |
| 2:B:252:LEU:HD12 | 2:B:302:PHE:CE1  | 1.98                     | 0.99              |
| 3:M:245:ASP:CB   | 3:M:472:TYR:CD1  | 2.46                     | 0.99              |
| 1:A:65:ASN:CA    | 4:S:166:LYS:CB   | 2.39                     | 0.99              |
| 1:A:289:SER:HB3  | 4:S:96:LEU:HD13  | 1.00                     | 0.99              |
| 1:A:323:CYS:SG   | 1:A:334:SER:HB3  | 2.03                     | 0.99              |
| 2:B:193:LEU:HD22 | 2:B:225:LEU:HB3  | 0.99                     | 0.99              |
| 2:B:512:VAL:HG11 | 2:B:548:ILE:HA   | 1.41                     | 0.99              |
| 3:M:293:PRO:HD2  | 3:M:293:PRO:O    | 1.62                     | 0.99              |
| 2:B:200:MET:HG2  | 2:B:232:ARG:HB3  | 1.43                     | 0.99              |
| 2:B:155:LEU:HD21 | 2:B:192:LEU:HD12 | 1.40                     | 0.98              |
| 2:B:352:ASN:O    | 2:B:355:ASN:HB2  | 1.63                     | 0.98              |
| 2:B:479:VAL:CG2  | 2:B:486:HIS:CD2  | 2.45                     | 0.98              |
| 2:B:566:ALA:CA   | 2:B:574:ASN:CG   | 2.34                     | 0.98              |
| 2:B:106:LEU:HD22 | 2:B:144:ASP:CB   | 1.92                     | 0.98              |
| 2:B:374:PHE:CD2  | 2:B:402:LEU:CD1  | 2.47                     | 0.98              |
| 3:M:106:LYS:HB3  | 3:M:296:LYS:NZ   | 1.75                     | 0.98              |
| 2:B:433:VAL:CG1  | 2:B:474:VAL:HG21 | 1.93                     | 0.98              |
| 2:B:25:VAL:HG11  | 2:B:36:THR:CB    | 1.93                     | 0.98              |
| 2:B:197:LYS:CB   | 2:B:229:HIS:NE2  | 2.26                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:223:LEU:CD1  | 2:B:258:GLN:HB3  | 1.93                     | 0.98              |
| 2:B:353:GLN:CB   | 3:M:50:TYR:CD1   | 2.37                     | 0.98              |
| 3:M:350:VAL:HG13 | 3:M:442:GLN:CB   | 1.94                     | 0.98              |
| 1:A:258:LYS:CE   | 4:S:94:SER:HB3   | 1.92                     | 0.98              |
| 3:M:364:VAL:O    | 3:M:367:ALA:O    | 1.80                     | 0.98              |
| 3:M:380:ARG:O    | 3:M:410:VAL:O    | 1.82                     | 0.98              |
| 2:B:256:CYS:SG   | 2:B:328:LEU:CD2  | 2.52                     | 0.98              |
| 2:B:563:PHE:HD2  | 2:B:584:SER:CB   | 1.76                     | 0.98              |
| 3:M:223:HIS:CD2  | 3:M:478:ASN:HA   | 1.99                     | 0.98              |
| 2:B:227:HIS:O    | 2:B:229:HIS:N    | 1.97                     | 0.98              |
| 2:B:267:ASP:O    | 2:B:276:SER:HB2  | 1.63                     | 0.98              |
| 3:M:222:PHE:CD1  | 3:M:240:ILE:HG23 | 1.98                     | 0.98              |
| 3:M:244:VAL:O    | 3:M:299:LEU:N    | 1.96                     | 0.98              |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:CD1  | 1.94                     | 0.98              |
| 2:B:143:SER:C    | 2:B:179:LYS:CD   | 2.36                     | 0.98              |
| 2:B:588:ILE:HG23 | 2:B:618:PHE:CZ   | 1.97                     | 0.98              |
| 2:B:132:SER:HB2  | 2:B:169:VAL:HG23 | 1.45                     | 0.97              |
| 2:B:550:VAL:HG22 | 2:B:610:ARG:HD3  | 1.45                     | 0.97              |
| 3:M:223:HIS:HA   | 3:M:479:PHE:CD2  | 1.98                     | 0.97              |
| 2:B:181:TYR:CD2  | 2:B:218:CYS:O    | 2.17                     | 0.97              |
| 3:M:378:ILE:O    | 3:M:413:GLY:HA3  | 1.64                     | 0.97              |
| 2:B:219:TYR:OH   | 2:B:226:LEU:HA   | 1.62                     | 0.97              |
| 2:B:261:PRO:CD   | 2:B:293:VAL:HG23 | 1.94                     | 0.97              |
| 2:B:523:PHE:HD1  | 2:B:582:ASP:OD2  | 1.43                     | 0.97              |
| 3:M:350:VAL:HG13 | 3:M:442:GLN:HB3  | 1.46                     | 0.97              |
| 3:M:443:SER:HB3  | 3:M:447:ILE:CG1  | 1.93                     | 0.97              |
| 1:A:319:LEU:O    | 1:A:320:HIS:C    | 2.05                     | 0.97              |
| 1:A:323:CYS:SG   | 1:A:334:SER:CB   | 2.52                     | 0.97              |
| 1:A:638:LEU:HD12 | 2:B:520:SER:N    | 1.77                     | 0.97              |
| 1:A:594:PHE:CD2  | 2:B:477:MET:CG   | 2.47                     | 0.97              |
| 1:A:638:LEU:CD1  | 2:B:520:SER:HB3  | 1.94                     | 0.97              |
| 2:B:196:LEU:HB3  | 2:B:215:TYR:CE2  | 2.00                     | 0.97              |
| 2:B:501:THR:HA   | 2:B:508:ARG:HH22 | 1.29                     | 0.97              |
| 1:A:102:GLN:NE2  | 4:S:166:LYS:CD   | 2.27                     | 0.97              |
| 1:A:555:LEU:HD13 | 1:A:581:LEU:CD1  | 1.95                     | 0.97              |
| 2:B:230:PHE:CD2  | 2:B:298:ASP:HB3  | 1.99                     | 0.97              |
| 2:B:237:ILE:O    | 2:B:238:LYS:C    | 1.99                     | 0.97              |
| 2:B:559:ASP:HB2  | 2:B:563:PHE:CE1  | 1.99                     | 0.97              |
| 1:A:102:GLN:HE21 | 4:S:166:LYS:CD   | 1.78                     | 0.96              |
| 1:A:154:ILE:CB   | 1:A:191:GLN:HG3  | 1.95                     | 0.96              |
| 1:A:219:VAL:HG11 | 1:A:256:LEU:HD23 | 1.46                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:178:ILE:HG13 | 2:B:214:ALA:CB   | 1.94                     | 0.96              |
| 2:B:316:THR:OG1  | 3:M:90:PHE:CE2   | 2.16                     | 0.96              |
| 1:A:257:LEU:CD2  | 1:A:278:ILE:HG22 | 1.94                     | 0.96              |
| 1:A:260:PHE:CZ   | 1:A:274:LEU:HD11 | 2.00                     | 0.96              |
| 2:B:151:ALA:HA   | 2:B:180:LEU:CD1  | 1.95                     | 0.96              |
| 2:B:337:THR:HA   | 2:B:373:LEU:CD1  | 1.95                     | 0.96              |
| 1:A:461:CYS:O    | 1:A:462:GLN:C    | 1.94                     | 0.96              |
| 2:B:403:ILE:HB   | 2:B:408:VAL:HG22 | 1.45                     | 0.96              |
| 2:B:105:LEU:HB3  | 2:B:145:MET:CE   | 1.94                     | 0.96              |
| 2:B:139:LEU:HD11 | 2:B:176:ALA:CB   | 1.95                     | 0.96              |
| 1:A:179:LYS:HZ1  | 4:S:141:VAL:CA   | 1.70                     | 0.96              |
| 3:M:218:LEU:HA   | 3:M:472:TYR:CD2  | 1.99                     | 0.96              |
| 2:B:337:THR:N    | 2:B:373:LEU:HD21 | 1.80                     | 0.96              |
| 2:B:537:PHE:HB3  | 2:B:598:LEU:CD1  | 1.94                     | 0.96              |
| 3:M:351:SER:HB2  | 3:M:440:ILE:O    | 1.66                     | 0.96              |
| 2:B:508:ARG:O    | 2:B:512:VAL:HG23 | 1.66                     | 0.96              |
| 1:A:595:GLU:HA   | 2:B:476:ARG:NH2  | 1.79                     | 0.95              |
| 2:B:297:PRO:O    | 2:B:301:LEU:CG   | 2.14                     | 0.95              |
| 3:M:272:LEU:CD2  | 3:M:278:ILE:HB   | 1.96                     | 0.95              |
| 4:S:17:VAL:CG2   | 4:S:19:PHE:CZ    | 2.49                     | 0.95              |
| 2:B:133:GLU:HA   | 2:B:168:MET:SD   | 2.06                     | 0.95              |
| 2:B:239:GLN:OE1  | 3:M:279:ASN:C    | 2.08                     | 0.95              |
| 2:B:490:ILE:CG1  | 2:B:518:ILE:HG21 | 1.95                     | 0.95              |
| 3:M:105:ASP:O    | 3:M:106:LYS:HB3  | 1.65                     | 0.95              |
| 1:A:200:PHE:HZ   | 1:A:236:LEU:CD2  | 1.75                     | 0.95              |
| 1:A:488:ARG:O    | 1:A:491:THR:OG1  | 1.84                     | 0.95              |
| 2:B:106:LEU:CD2  | 2:B:144:ASP:HB3  | 1.96                     | 0.95              |
| 2:B:174:ALA:HB1  | 2:B:211:ALA:HA   | 1.46                     | 0.95              |
| 1:A:114:PHE:CE2  | 1:A:152:THR:O    | 2.19                     | 0.95              |
| 1:A:403:LEU:HD23 | 1:A:422:GLU:HG3  | 1.46                     | 0.95              |
| 2:B:189:HIS:NE2  | 2:B:193:LEU:HD11 | 1.80                     | 0.95              |
| 2:B:513:TRP:CA   | 2:B:551:LEU:CD2  | 2.44                     | 0.95              |
| 4:S:1:MET:N      | 4:S:93:GLU:OE1   | 1.99                     | 0.95              |
| 1:A:186:PHE:CE1  | 1:A:224:GLU:HG2  | 2.00                     | 0.95              |
| 2:B:374:PHE:CZ   | 2:B:381:PHE:CD1  | 2.54                     | 0.95              |
| 3:M:362:PHE:O    | 3:M:363:ASN:C    | 2.07                     | 0.95              |
| 2:B:155:LEU:HD23 | 2:B:192:LEU:HD11 | 0.97                     | 0.95              |
| 2:B:278:PRO:HB3  | 2:B:288:TYR:O    | 1.65                     | 0.95              |
| 2:B:479:VAL:HG22 | 2:B:486:HIS:CD2  | 2.01                     | 0.95              |
| 2:B:566:ALA:HA   | 2:B:574:ASN:CG   | 1.90                     | 0.95              |
| 1:A:559:PHE:CE1  | 1:A:581:LEU:HD22 | 2.02                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:278:PRO:CA   | 2:B:288:TYR:CB   | 2.44                     | 0.95              |
| 2:B:559:ASP:HB3  | 2:B:563:PHE:CD1  | 1.98                     | 0.95              |
| 3:M:223:HIS:HD1  | 3:M:476:THR:HG1  | 1.01                     | 0.95              |
| 1:A:404:GLN:O    | 2:B:3:ASP:C      | 2.10                     | 0.95              |
| 2:B:231:ARG:HG2  | 2:B:298:ASP:OD1  | 1.65                     | 0.95              |
| 3:M:339:GLU:HG3  | 3:M:412:ARG:HG2  | 1.45                     | 0.95              |
| 2:B:219:TYR:CD1  | 2:B:226:LEU:CD2  | 2.49                     | 0.95              |
| 3:M:59:ASP:O     | 3:M:60:LEU:C     | 1.83                     | 0.95              |
| 1:A:215:VAL:HG13 | 1:A:243:ILE:HG21 | 1.45                     | 0.95              |
| 2:B:566:ALA:HA   | 2:B:574:ASN:HB3  | 1.48                     | 0.95              |
| 3:M:265:ASN:OD1  | 3:M:313:SER:CB   | 2.15                     | 0.95              |
| 1:A:65:ASN:HA    | 4:S:166:LYS:HA   | 1.07                     | 0.94              |
| 2:B:136:CYS:SG   | 2:B:169:VAL:N    | 2.39                     | 0.94              |
| 2:B:178:ILE:CG1  | 2:B:214:ALA:CB   | 2.45                     | 0.94              |
| 2:B:486:HIS:CE1  | 2:B:518:ILE:HB   | 2.02                     | 0.94              |
| 2:B:278:PRO:CD   | 2:B:292:GLU:CB   | 2.30                     | 0.94              |
| 2:B:316:THR:CB   | 3:M:90:PHE:CE2   | 2.39                     | 0.94              |
| 1:A:179:LYS:CE   | 4:S:140:MET:O    | 2.15                     | 0.94              |
| 2:B:212:VAL:CG2  | 2:B:248:LEU:HD21 | 1.97                     | 0.94              |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:HB3  | 0.97                     | 0.94              |
| 2:B:25:VAL:HG13  | 2:B:33:SER:HA    | 1.50                     | 0.94              |
| 2:B:83:PHE:CZ    | 2:B:119:SER:CB   | 2.50                     | 0.94              |
| 2:B:143:SER:O    | 2:B:179:LYS:HD3  | 1.67                     | 0.94              |
| 2:B:219:TYR:CD1  | 2:B:226:LEU:CG   | 2.50                     | 0.94              |
| 2:B:343:LEU:HD23 | 2:B:363:ILE:HD13 | 1.48                     | 0.94              |
| 3:M:96:ILE:HG23  | 3:M:125:PHE:CE1  | 2.02                     | 0.94              |
| 1:A:595:GLU:CD   | 2:B:476:ARG:CZ   | 2.38                     | 0.94              |
| 4:S:80:TYR:O     | 4:S:81:ALA:C     | 2.07                     | 0.94              |
| 4:S:80:TYR:O     | 4:S:82:THR:N     | 2.00                     | 0.94              |
| 2:B:232:ARG:O    | 2:B:236:ILE:HG13 | 1.68                     | 0.94              |
| 2:B:245:GLN:OE1  | 2:B:309:LEU:CD1  | 2.14                     | 0.94              |
| 2:B:513:TRP:CA   | 2:B:551:LEU:HD11 | 1.95                     | 0.94              |
| 1:A:176:TYR:CZ   | 4:S:143:GLU:OE2  | 2.21                     | 0.94              |
| 1:A:225:LEU:HB3  | 1:A:233:PHE:CZ   | 2.03                     | 0.94              |
| 2:B:219:TYR:CD1  | 2:B:226:LEU:CB   | 2.47                     | 0.94              |
| 2:B:223:LEU:CD1  | 2:B:258:GLN:CB   | 2.46                     | 0.94              |
| 2:B:267:ASP:H    | 2:B:289:PRO:CB   | 1.80                     | 0.94              |
| 2:B:527:PRO:CB   | 2:B:587:ARG:HG3  | 1.98                     | 0.94              |
| 3:M:41:LEU:HD13  | 3:M:52:ASP:H     | 0.79                     | 0.94              |
| 2:B:139:LEU:HD21 | 2:B:173:VAL:HA   | 1.47                     | 0.94              |
| 2:B:208:ILE:CG1  | 2:B:236:ILE:HD13 | 1.98                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:158:VAL:HG13 | 2:B:173:VAL:HG12 | 1.48                     | 0.93              |
| 2:B:167:ALA:O    | 2:B:207:VAL:HG21 | 1.65                     | 0.93              |
| 2:B:216:LYS:CG   | 2:B:251:LEU:HD13 | 1.99                     | 0.93              |
| 2:B:215:TYR:HD2  | 2:B:219:TYR:CE1  | 1.86                     | 0.93              |
| 2:B:340:ILE:HG12 | 2:B:373:LEU:HD23 | 1.49                     | 0.93              |
| 3:M:347:PHE:O    | 3:M:348:LYS:C    | 2.11                     | 0.93              |
| 1:A:289:SER:CA   | 4:S:96:LEU:HD13  | 1.98                     | 0.93              |
| 2:B:549:LEU:HD21 | 2:B:611:ALA:H    | 1.17                     | 0.93              |
| 1:A:595:GLU:HA   | 2:B:476:ARG:HH22 | 1.30                     | 0.93              |
| 2:B:38:TYR:CA    | 2:B:42:ILE:H     | 1.80                     | 0.93              |
| 1:A:638:LEU:HD22 | 2:B:558:TYR:C    | 1.92                     | 0.93              |
| 2:B:90:ILE:O     | 2:B:98:LYS:HE2   | 1.67                     | 0.93              |
| 2:B:178:ILE:HG23 | 2:B:217:GLU:HB2  | 0.95                     | 0.93              |
| 2:B:476:ARG:HA   | 2:B:514:LEU:HD13 | 1.48                     | 0.93              |
| 2:B:564:LYS:HD2  | 2:B:621:GLY:O    | 1.67                     | 0.93              |
| 1:A:215:VAL:HG11 | 1:A:243:ILE:HG23 | 1.48                     | 0.93              |
| 2:B:230:PHE:HE1  | 2:B:252:LEU:HD23 | 1.24                     | 0.93              |
| 1:A:101:GLN:CD   | 4:S:167:ILE:HD11 | 1.93                     | 0.93              |
| 1:A:244:LEU:HG   | 1:A:281:LEU:HD11 | 1.49                     | 0.93              |
| 2:B:566:ALA:HA   | 2:B:574:ASN:CB   | 1.98                     | 0.93              |
| 3:M:220:GLU:CG   | 3:M:439:TYR:HD1  | 1.82                     | 0.93              |
| 3:M:222:PHE:C    | 3:M:479:PHE:CZ   | 2.47                     | 0.93              |
| 4:S:89:VAL:HG11  | 4:S:98:ILE:HG13  | 1.48                     | 0.93              |
| 1:A:637:GLU:OE1  | 2:B:554:LYS:NZ   | 2.02                     | 0.93              |
| 2:B:556:LEU:HA   | 2:B:588:ILE:HD11 | 0.93                     | 0.93              |
| 4:S:8:PHE:CD1    | 4:S:84:TYR:HB2   | 2.03                     | 0.92              |
| 1:A:179:LYS:HB3  | 4:S:142:ILE:HD13 | 0.93                     | 0.92              |
| 1:A:638:LEU:HG   | 2:B:520:SER:CA   | 2.00                     | 0.92              |
| 2:B:171:GLY:N    | 2:B:207:VAL:HG13 | 1.83                     | 0.92              |
| 2:B:241:ASP:CB   | 3:M:274:ASP:HA   | 2.00                     | 0.92              |
| 2:B:252:LEU:CB   | 2:B:302:PHE:CE1  | 2.52                     | 0.92              |
| 2:B:527:PRO:HB3  | 2:B:587:ARG:CG   | 1.99                     | 0.92              |
| 1:A:289:SER:C    | 4:S:96:LEU:HD13  | 1.94                     | 0.92              |
| 2:B:21:GLU:CD    | 2:B:35:TYR:CD2   | 2.46                     | 0.92              |
| 2:B:513:TRP:N    | 2:B:551:LEU:HD11 | 1.82                     | 0.92              |
| 3:M:336:ASP:OD1  | 3:M:415:ILE:O    | 1.86                     | 0.92              |
| 1:A:77:LEU:O     | 1:A:80:TYR:O     | 1.87                     | 0.92              |
| 1:A:513:ARG:HD2  | 1:A:550:VAL:HG21 | 1.52                     | 0.92              |
| 2:B:42:ILE:CA    | 2:B:46:GLN:OE1   | 2.17                     | 0.92              |
| 3:M:235:LEU:HD11 | 3:M:306:LEU:HB3  | 1.52                     | 0.92              |
| 2:B:219:TYR:CZ   | 2:B:226:LEU:N    | 2.37                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:568:VAL:O    | 2:B:571:SER:HB2  | 1.69                     | 0.92              |
| 2:B:248:LEU:O    | 2:B:252:LEU:HG   | 1.68                     | 0.92              |
| 2:B:497:LEU:O    | 2:B:498:THR:C    | 2.00                     | 0.92              |
| 1:A:573:GLU:O    | 1:A:574:ILE:C    | 2.01                     | 0.92              |
| 1:A:595:GLU:CA   | 2:B:476:ARG:NH2  | 2.33                     | 0.92              |
| 1:A:260:PHE:CG   | 1:A:274:LEU:HG   | 2.05                     | 0.92              |
| 2:B:143:SER:HB2  | 2:B:179:LYS:CB   | 2.00                     | 0.92              |
| 2:B:241:ASP:HB3  | 3:M:274:ASP:HA   | 1.50                     | 0.92              |
| 2:B:479:VAL:CG1  | 2:B:486:HIS:NE2  | 2.12                     | 0.92              |
| 3:M:96:ILE:CG2   | 3:M:125:PHE:CE1  | 2.53                     | 0.92              |
| 1:A:121:LEU:HD13 | 1:A:155:THR:HG23 | 1.52                     | 0.92              |
| 1:A:219:VAL:CG1  | 1:A:256:LEU:HD23 | 2.00                     | 0.92              |
| 2:B:290:SER:O    | 2:B:291:TYR:C    | 1.93                     | 0.92              |
| 1:A:102:GLN:HE21 | 4:S:166:LYS:HD3  | 1.27                     | 0.91              |
| 1:A:156:PRO:HB3  | 1:A:192:TYR:HE1  | 1.23                     | 0.91              |
| 1:A:180:LYS:HZ2  | 4:S:137:GLN:HB3  | 1.36                     | 0.91              |
| 2:B:41:ASN:CB    | 2:B:43:ASN:OD1   | 2.18                     | 0.91              |
| 1:A:289:SER:CB   | 4:S:96:LEU:CD1   | 2.36                     | 0.91              |
| 1:A:349:ILE:CG2  | 1:A:378:ILE:HG22 | 2.00                     | 0.91              |
| 2:B:393:ILE:HG23 | 2:B:431:MET:HG2  | 1.52                     | 0.91              |
| 2:B:518:ILE:O    | 2:B:518:ILE:HD12 | 1.70                     | 0.91              |
| 2:B:549:LEU:CD1  | 2:B:611:ALA:HA   | 1.98                     | 0.91              |
| 2:B:211:ALA:O    | 2:B:214:ALA:HB3  | 1.67                     | 0.91              |
| 1:A:502:ASP:OD2  | 1:A:506:LYS:NZ   | 2.03                     | 0.91              |
| 1:A:609:LEU:HD23 | 1:A:628:VAL:HG11 | 1.51                     | 0.91              |
| 2:B:105:LEU:CB   | 2:B:145:MET:HE1  | 1.99                     | 0.91              |
| 2:B:437:SER:HB2  | 2:B:474:VAL:CG1  | 2.00                     | 0.91              |
| 2:B:546:CYS:HA   | 2:B:607:ILE:HG12 | 1.48                     | 0.91              |
| 2:B:70:MET:HE1   | 2:B:104:TYR:O    | 1.71                     | 0.91              |
| 3:M:16:PHE:HA    | 3:M:118:TYR:CD1  | 2.05                     | 0.91              |
| 3:M:344:ILE:CG2  | 3:M:347:PHE:CB   | 2.48                     | 0.91              |
| 2:B:219:TYR:CE2  | 2:B:226:LEU:N    | 2.39                     | 0.91              |
| 3:M:220:GLU:HG3  | 3:M:439:TYR:HD1  | 1.36                     | 0.91              |
| 1:A:189:PHE:CB   | 1:A:225:LEU:CD2  | 2.48                     | 0.91              |
| 2:B:374:PHE:CE2  | 2:B:402:LEU:CD1  | 2.53                     | 0.91              |
| 1:A:244:LEU:CD1  | 1:A:281:LEU:CD1  | 2.47                     | 0.91              |
| 2:B:82:TYR:O     | 2:B:83:PHE:C     | 2.01                     | 0.91              |
| 2:B:307:ASN:OD1  | 2:B:339:PHE:CD2  | 2.22                     | 0.91              |
| 2:B:374:PHE:HE2  | 2:B:402:LEU:HD11 | 1.36                     | 0.91              |
| 2:B:567:GLN:HA   | 2:B:569:THR:OG1  | 1.70                     | 0.91              |
| 3:M:71:LYS:HB3   | 3:M:74:TYR:CZ    | 2.06                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:180:LYS:HZ2  | 4:S:137:GLN:CB   | 1.83                     | 0.91              |
| 1:A:204:VAL:HG13 | 1:A:239:LEU:CD1  | 2.00                     | 0.91              |
| 2:B:105:LEU:HG   | 2:B:119:SER:HB2  | 1.53                     | 0.91              |
| 2:B:124:GLN:HA   | 2:B:127:LEU:HD12 | 1.53                     | 0.91              |
| 2:B:252:LEU:HB3  | 2:B:302:PHE:CE2  | 2.06                     | 0.91              |
| 2:B:277:CYS:C    | 2:B:288:TYR:HB3  | 1.96                     | 0.91              |
| 1:A:220:SER:O    | 1:A:223:CYS:HB3  | 1.71                     | 0.90              |
| 1:A:630:PRO:CB   | 2:B:617:LEU:HD13 | 2.00                     | 0.90              |
| 1:A:638:LEU:HD11 | 2:B:520:SER:HA   | 1.53                     | 0.90              |
| 2:B:123:LEU:HD13 | 2:B:142:LEU:CG   | 2.01                     | 0.90              |
| 2:B:193:LEU:HD13 | 2:B:225:LEU:CD1  | 1.99                     | 0.90              |
| 2:B:219:TYR:CD1  | 2:B:226:LEU:CD1  | 2.44                     | 0.90              |
| 2:B:256:CYS:SG   | 2:B:328:LEU:HD22 | 2.11                     | 0.90              |
| 2:B:337:THR:HG23 | 2:B:373:LEU:CD1  | 2.01                     | 0.90              |
| 2:B:486:HIS:ND1  | 2:B:518:ILE:CD1  | 2.29                     | 0.90              |
| 2:B:584:SER:O    | 2:B:588:ILE:CG2  | 2.18                     | 0.90              |
| 3:M:347:PHE:CE1  | 3:M:350:VAL:HG12 | 2.04                     | 0.90              |
| 1:A:190:LEU:HD12 | 1:A:228:LYS:HG3  | 1.52                     | 0.90              |
| 2:B:189:HIS:CE1  | 2:B:193:LEU:HD11 | 2.06                     | 0.90              |
| 2:B:29:LYS:CE    | 2:B:30:LEU:N     | 2.07                     | 0.90              |
| 2:B:231:ARG:NH2  | 2:B:279:LEU:HD21 | 1.85                     | 0.90              |
| 2:B:566:ALA:O    | 2:B:574:ASN:HB3  | 1.72                     | 0.90              |
| 1:A:114:PHE:CG   | 1:A:153:ILE:HG23 | 2.05                     | 0.90              |
| 1:A:370:LYS:O    | 1:A:374:LEU:HD13 | 1.72                     | 0.90              |
| 1:A:563:CYS:HB3  | 1:A:621:LEU:HD12 | 1.51                     | 0.90              |
| 2:B:24:ALA:HB2   | 2:B:35:TYR:CZ    | 2.04                     | 0.90              |
| 2:B:219:TYR:CG   | 2:B:226:LEU:HD22 | 2.06                     | 0.90              |
| 1:A:516:ILE:HG22 | 1:A:554:ALA:CB   | 2.02                     | 0.90              |
| 1:A:638:LEU:HD11 | 2:B:520:SER:CA   | 2.00                     | 0.90              |
| 2:B:20:ARG:CD    | 2:B:21:GLU:HB2   | 2.00                     | 0.90              |
| 2:B:486:HIS:CE1  | 2:B:518:ILE:CD1  | 2.54                     | 0.90              |
| 1:A:599:ARG:CZ   | 2:B:513:TRP:CZ3  | 2.54                     | 0.90              |
| 2:B:181:TYR:CE1  | 2:B:222:HIS:HD2  | 1.88                     | 0.90              |
| 2:B:353:GLN:HG2  | 3:M:50:TYR:CD1   | 2.04                     | 0.90              |
| 2:B:523:PHE:CE1  | 2:B:580:TYR:CD1  | 2.56                     | 0.90              |
| 3:M:219:LEU:HD22 | 3:M:473:LYS:HA   | 1.53                     | 0.90              |
| 1:A:536:MET:O    | 1:A:537:THR:C    | 1.94                     | 0.90              |
| 2:B:174:ALA:O    | 2:B:175:LEU:C    | 2.05                     | 0.90              |
| 3:M:240:ILE:HG21 | 3:M:444:ALA:O    | 1.72                     | 0.90              |
| 2:B:102:HIS:ND1  | 2:B:137:PHE:C    | 2.30                     | 0.90              |
| 2:B:106:LEU:CD2  | 2:B:144:ASP:CB   | 2.50                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:208:ILE:CD1  | 2:B:236:ILE:CG2  | 2.42                     | 0.90              |
| 2:B:261:PRO:HD3  | 2:B:293:VAL:HG23 | 1.53                     | 0.90              |
| 2:B:299:LEU:O    | 2:B:302:PHE:HB3  | 1.72                     | 0.90              |
| 2:B:29:LYS:CD    | 2:B:30:LEU:H     | 1.84                     | 0.90              |
| 2:B:226:LEU:HD23 | 2:B:255:TYR:HD1  | 1.28                     | 0.90              |
| 2:B:545:ARG:HD2  | 2:B:602:ASP:CG   | 1.97                     | 0.90              |
| 1:A:176:TYR:CD2  | 4:S:143:GLU:OE2  | 2.25                     | 0.90              |
| 1:A:563:CYS:CB   | 1:A:621:LEU:HD11 | 2.02                     | 0.90              |
| 2:B:25:VAL:HG22  | 2:B:36:THR:H     | 1.25                     | 0.90              |
| 2:B:553:ALA:HB2  | 2:B:614:ILE:CG1  | 2.02                     | 0.90              |
| 2:B:170:ARG:HA   | 2:B:199:LEU:HD22 | 1.53                     | 0.89              |
| 2:B:418:TYR:O    | 2:B:419:VAL:C    | 2.00                     | 0.89              |
| 1:A:381:GLU:HA   | 1:A:384:LEU:HD23 | 1.51                     | 0.89              |
| 1:A:638:LEU:CA   | 2:B:520:SER:HB3  | 1.97                     | 0.89              |
| 2:B:374:PHE:HB3  | 2:B:402:LEU:CD2  | 2.01                     | 0.89              |
| 2:B:123:LEU:O    | 2:B:127:LEU:HG   | 1.70                     | 0.89              |
| 2:B:193:LEU:CD2  | 2:B:225:LEU:HB3  | 1.87                     | 0.89              |
| 2:B:375:LEU:HD21 | 2:B:402:LEU:O    | 1.71                     | 0.89              |
| 3:M:334:ASP:O    | 3:M:417:TYR:N    | 2.05                     | 0.89              |
| 2:B:70:MET:CE    | 2:B:107:ARG:CG   | 2.47                     | 0.89              |
| 2:B:243:TRP:CZ2  | 3:M:98:ARG:HD2   | 2.07                     | 0.89              |
| 2:B:267:ASP:O    | 2:B:276:SER:CB   | 2.21                     | 0.89              |
| 2:B:352:ASN:ND2  | 3:M:70:ASN:CB    | 2.35                     | 0.89              |
| 2:B:500:GLN:HB3  | 2:B:503:LEU:HG   | 1.54                     | 0.89              |
| 2:B:501:THR:C    | 2:B:508:ARG:NH2  | 2.31                     | 0.89              |
| 3:M:327:PHE:HE1  | 3:M:336:ASP:HB2  | 1.38                     | 0.89              |
| 3:M:443:SER:CB   | 3:M:447:ILE:HG13 | 2.02                     | 0.89              |
| 1:A:179:LYS:CB   | 4:S:142:ILE:HD12 | 1.84                     | 0.89              |
| 1:A:366:SER:O    | 1:A:370:LYS:HG2  | 1.71                     | 0.89              |
| 2:B:139:LEU:CD1  | 2:B:176:ALA:CB   | 2.50                     | 0.89              |
| 2:B:230:PHE:O    | 2:B:231:ARG:O    | 1.88                     | 0.89              |
| 2:B:309:LEU:HB3  | 2:B:317:VAL:HG12 | 1.54                     | 0.89              |
| 2:B:549:LEU:HD23 | 2:B:607:ILE:O    | 1.71                     | 0.89              |
| 3:M:65:TYR:CZ    | 3:M:86:PRO:HB3   | 2.08                     | 0.89              |
| 3:M:302:TYR:CD2  | 3:M:445:SER:HB3  | 2.07                     | 0.89              |
| 1:A:204:VAL:O    | 1:A:205:SER:C    | 2.09                     | 0.89              |
| 1:A:257:LEU:HD22 | 1:A:278:ILE:HG23 | 1.55                     | 0.89              |
| 1:A:369:SER:HB2  | 1:A:424:TYR:HE2  | 1.38                     | 0.89              |
| 2:B:83:PHE:HZ    | 2:B:119:SER:HB3  | 1.25                     | 0.89              |
| 2:B:178:ILE:HD13 | 2:B:218:CYS:HB2  | 1.53                     | 0.89              |
| 2:B:252:LEU:HB3  | 2:B:302:PHE:CD2  | 2.08                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:472:VAL:CG1  | 2:B:510:GLY:CA   | 2.44                     | 0.89              |
| 1:A:516:ILE:CG2  | 1:A:554:ALA:HB3  | 2.03                     | 0.89              |
| 2:B:472:VAL:HG11 | 2:B:510:GLY:HA3  | 0.89                     | 0.89              |
| 1:A:88:ASN:ND2   | 1:A:120:ILE:CG2  | 2.35                     | 0.88              |
| 2:B:127:LEU:HB3  | 2:B:157:THR:HG23 | 1.54                     | 0.88              |
| 2:B:193:LEU:CG   | 2:B:225:LEU:CG   | 2.26                     | 0.88              |
| 1:A:102:GLN:NE2  | 4:S:166:LYS:NZ   | 2.20                     | 0.88              |
| 2:B:20:ARG:CZ    | 2:B:21:GLU:HG3   | 2.03                     | 0.88              |
| 2:B:193:LEU:HB3  | 2:B:225:LEU:CD1  | 2.03                     | 0.88              |
| 2:B:223:LEU:HB2  | 2:B:259:TYR:CD1  | 2.08                     | 0.88              |
| 3:M:235:LEU:HD13 | 3:M:310:VAL:HG21 | 1.55                     | 0.88              |
| 1:A:111:SER:HB2  | 1:A:152:THR:HG1  | 1.36                     | 0.88              |
| 2:B:103:LEU:CD2  | 3:M:131:ALA:HA   | 2.02                     | 0.88              |
| 3:M:306:LEU:HD11 | 3:M:317:MET:HE1  | 1.53                     | 0.88              |
| 2:B:127:LEU:HD13 | 2:B:157:THR:CB   | 2.03                     | 0.88              |
| 2:B:549:LEU:CD2  | 2:B:611:ALA:CB   | 2.51                     | 0.88              |
| 2:B:552:SER:O    | 2:B:556:LEU:HG   | 1.72                     | 0.88              |
| 3:M:223:HIS:HA   | 3:M:479:PHE:CE2  | 2.09                     | 0.88              |
| 2:B:193:LEU:C    | 2:B:195:ILE:H    | 1.82                     | 0.88              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:CG   | 2.57                     | 0.88              |
| 3:M:272:LEU:HD21 | 3:M:278:ILE:HB   | 1.54                     | 0.88              |
| 2:B:193:LEU:HB3  | 2:B:225:LEU:HD12 | 1.54                     | 0.88              |
| 2:B:549:LEU:HD11 | 2:B:611:ALA:CA   | 2.03                     | 0.88              |
| 3:M:131:ALA:CB   | 3:M:131:ALA:C    | 2.46                     | 0.88              |
| 1:A:609:LEU:HD21 | 1:A:628:VAL:HG21 | 1.54                     | 0.88              |
| 1:A:629:LEU:O    | 1:A:630:PRO:C    | 2.00                     | 0.88              |
| 1:A:638:LEU:CD1  | 2:B:520:SER:CB   | 2.50                     | 0.88              |
| 2:B:534:ILE:HD13 | 2:B:594:ALA:HB3  | 1.55                     | 0.88              |
| 3:M:343:ASN:CA   | 3:M:408:VAL:HG13 | 2.02                     | 0.88              |
| 3:M:347:PHE:CE1  | 3:M:350:VAL:HG11 | 2.09                     | 0.88              |
| 2:B:219:TYR:HE1  | 2:B:226:LEU:HD13 | 1.11                     | 0.88              |
| 3:M:378:ILE:O    | 3:M:413:GLY:CA   | 2.22                     | 0.88              |
| 2:B:139:LEU:HD23 | 2:B:173:VAL:HA   | 0.89                     | 0.88              |
| 2:B:501:THR:C    | 2:B:508:ARG:HH21 | 1.82                     | 0.88              |
| 4:S:54:PRO:HD2   | 4:S:57:LEU:HB2   | 1.56                     | 0.88              |
| 1:A:516:ILE:CG2  | 1:A:554:ALA:CB   | 2.52                     | 0.87              |
| 3:M:327:PHE:CE1  | 3:M:336:ASP:HB2  | 2.09                     | 0.87              |
| 3:M:405:THR:C    | 3:M:407:THR:N    | 2.26                     | 0.87              |
| 1:A:101:GLN:CD   | 4:S:167:ILE:CD1  | 2.48                     | 0.87              |
| 2:B:42:ILE:HA    | 2:B:46:GLN:OE1   | 1.75                     | 0.87              |
| 2:B:215:TYR:CD2  | 2:B:219:TYR:HE1  | 1.92                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:220:GLU:HG3  | 3:M:439:TYR:CD1  | 2.09                     | 0.87              |
| 3:M:290:PHE:CE2  | 3:M:297:PHE:CZ   | 2.62                     | 0.87              |
| 1:A:464:ILE:O    | 1:A:465:SER:C    | 1.98                     | 0.87              |
| 2:B:208:ILE:HG21 | 2:B:236:ILE:HG21 | 1.56                     | 0.87              |
| 3:M:435:LEU:O    | 3:M:479:PHE:CG   | 2.27                     | 0.87              |
| 4:S:75:ILE:HG22  | 4:S:77:TYR:CE1   | 2.09                     | 0.87              |
| 2:B:569:THR:HG22 | 2:B:569:THR:O    | 1.73                     | 0.87              |
| 1:A:174:ARG:NH2  | 4:S:148:ARG:HH22 | 1.73                     | 0.87              |
| 1:A:450:TYR:OH   | 1:A:476:GLN:HG3  | 1.75                     | 0.87              |
| 2:B:25:VAL:N     | 2:B:35:TYR:CD2   | 2.43                     | 0.87              |
| 2:B:86:VAL:CG1   | 2:B:101:ILE:HG23 | 2.05                     | 0.87              |
| 2:B:120:ILE:CD1  | 2:B:150:LEU:HD13 | 2.05                     | 0.87              |
| 2:B:243:TRP:NE1  | 3:M:98:ARG:NE    | 2.22                     | 0.87              |
| 2:B:243:TRP:HD1  | 3:M:274:ASP:OD2  | 1.56                     | 0.87              |
| 2:B:340:ILE:CG1  | 2:B:373:LEU:HD23 | 2.04                     | 0.87              |
| 1:A:370:LYS:O    | 1:A:374:LEU:CD1  | 2.23                     | 0.87              |
| 1:A:633:PHE:CE2  | 2:B:554:LYS:HB2  | 2.10                     | 0.87              |
| 2:B:486:HIS:CG   | 2:B:518:ILE:HD13 | 2.08                     | 0.87              |
| 2:B:553:ALA:CB   | 2:B:614:ILE:HG12 | 2.05                     | 0.87              |
| 1:A:254:ILE:HG13 | 1:A:290:VAL:HG22 | 1.55                     | 0.87              |
| 2:B:208:ILE:HD13 | 2:B:236:ILE:HG21 | 0.89                     | 0.87              |
| 1:A:88:ASN:HB3   | 1:A:120:ILE:HG23 | 1.56                     | 0.86              |
| 2:B:139:LEU:CD1  | 2:B:176:ALA:HB2  | 2.04                     | 0.86              |
| 2:B:243:TRP:HZ3  | 3:M:94:GLU:HB3   | 1.05                     | 0.86              |
| 2:B:328:LEU:CB   | 2:B:333:GLN:HE22 | 1.88                     | 0.86              |
| 2:B:366:LEU:O    | 2:B:367:SER:C    | 1.98                     | 0.86              |
| 2:B:523:PHE:HE1  | 2:B:580:TYR:HB2  | 1.37                     | 0.86              |
| 3:M:479:PHE:H    | 3:M:479:PHE:HD2  | 1.17                     | 0.86              |
| 4:S:35:VAL:HB    | 4:S:77:TYR:OH    | 1.73                     | 0.86              |
| 1:A:339:TYR:HB2  | 1:A:374:LEU:HD11 | 1.57                     | 0.86              |
| 2:B:227:HIS:C    | 2:B:229:HIS:H    | 1.83                     | 0.86              |
| 2:B:352:ASN:HD21 | 3:M:70:ASN:HB3   | 1.36                     | 0.86              |
| 3:M:323:MET:SD   | 3:M:342:LEU:HA   | 2.14                     | 0.86              |
| 2:B:120:ILE:HG13 | 2:B:150:LEU:CD2  | 2.04                     | 0.86              |
| 2:B:537:PHE:CE1  | 2:B:545:ARG:HG2  | 2.08                     | 0.86              |
| 2:B:549:LEU:CD2  | 2:B:611:ALA:CA   | 2.46                     | 0.86              |
| 3:M:235:LEU:HD11 | 3:M:306:LEU:CB   | 2.05                     | 0.86              |
| 1:A:384:LEU:HD22 | 1:A:441:TYR:CD2  | 2.10                     | 0.86              |
| 1:A:420:ILE:HG23 | 1:A:424:TYR:HB2  | 1.57                     | 0.86              |
| 2:B:197:LYS:CA   | 2:B:229:HIS:NE2  | 2.38                     | 0.86              |
| 2:B:293:VAL:O    | 2:B:299:LEU:CD1  | 2.23                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:375:LEU:O    | 2:B:377:TYR:N    | 2.09                     | 0.86              |
| 2:B:549:LEU:HD22 | 2:B:607:ILE:O    | 1.74                     | 0.86              |
| 1:A:368:ARG:NH1  | 1:A:419:ILE:O    | 2.09                     | 0.86              |
| 1:A:595:GLU:N    | 2:B:476:ARG:NH2  | 2.23                     | 0.86              |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:CG   | 2.04                     | 0.86              |
| 2:B:208:ILE:HD13 | 2:B:236:ILE:HG23 | 1.53                     | 0.86              |
| 2:B:563:PHE:CE1  | 2:B:588:ILE:HD12 | 2.09                     | 0.86              |
| 2:B:77:ILE:O     | 2:B:79:VAL:N     | 2.08                     | 0.86              |
| 2:B:127:LEU:CD2  | 2:B:161:LEU:HD21 | 2.06                     | 0.86              |
| 2:B:214:ALA:O    | 2:B:217:GLU:N    | 2.08                     | 0.86              |
| 1:A:100:LEU:O    | 1:A:101:GLN:C    | 2.04                     | 0.86              |
| 1:A:436:CYS:SG   | 1:A:450:TYR:CE2  | 2.68                     | 0.86              |
| 1:A:621:LEU:O    | 1:A:622:PRO:C    | 1.97                     | 0.86              |
| 2:B:135:ARG:NH2  | 2:B:164:ASP:OD1  | 2.08                     | 0.86              |
| 2:B:243:TRP:CZ2  | 3:M:98:ARG:CD    | 2.59                     | 0.86              |
| 2:B:527:PRO:CB   | 2:B:587:ARG:CG   | 2.53                     | 0.86              |
| 1:A:129:LYS:HG2  | 1:A:165:ASP:OD2  | 1.73                     | 0.86              |
| 1:A:183:THR:O    | 1:A:186:PHE:HB3  | 1.76                     | 0.86              |
| 1:A:609:LEU:HG   | 1:A:628:VAL:CB   | 2.05                     | 0.86              |
| 2:B:140:SER:HB2  | 2:B:172:GLU:CD   | 2.01                     | 0.86              |
| 2:B:546:CYS:HB2  | 2:B:607:ILE:CD1  | 2.05                     | 0.86              |
| 2:B:559:ASP:CB   | 2:B:563:PHE:CE1  | 2.56                     | 0.86              |
| 2:B:351:GLU:O    | 3:M:49:ASP:OD2   | 1.94                     | 0.86              |
| 3:M:15:ILE:O     | 3:M:118:TYR:HD1  | 1.59                     | 0.86              |
| 3:M:268:GLY:H    | 3:M:302:TYR:HH   | 1.23                     | 0.86              |
| 1:A:114:PHE:CD2  | 1:A:153:ILE:HG12 | 2.11                     | 0.86              |
| 2:B:38:TYR:HA    | 2:B:42:ILE:CA    | 1.91                     | 0.86              |
| 1:A:316:LEU:CD1  | 1:A:348:PHE:CD2  | 2.58                     | 0.85              |
| 3:M:101:LEU:HD11 | 3:M:106:LYS:O    | 1.75                     | 0.85              |
| 4:S:109:LEU:HD12 | 4:S:113:PHE:CD1  | 2.11                     | 0.85              |
| 1:A:609:LEU:HG   | 1:A:628:VAL:HB   | 1.57                     | 0.85              |
| 2:B:25:VAL:HA    | 2:B:35:TYR:HB3   | 1.56                     | 0.85              |
| 2:B:107:ARG:O    | 2:B:110:GLU:N    | 2.10                     | 0.85              |
| 2:B:178:ILE:CG1  | 2:B:214:ALA:CA   | 2.51                     | 0.85              |
| 2:B:268:LYS:HA   | 2:B:276:SER:HB2  | 1.58                     | 0.85              |
| 3:M:48:ASP:C     | 3:M:75:TRP:CH2   | 2.54                     | 0.85              |
| 2:B:178:ILE:CG2  | 2:B:217:GLU:CB   | 2.52                     | 0.85              |
| 2:B:556:LEU:CB   | 2:B:588:ILE:HD11 | 2.06                     | 0.85              |
| 3:M:306:LEU:O    | 3:M:307:SER:C    | 2.08                     | 0.85              |
| 2:B:243:TRP:CE2  | 3:M:98:ARG:CD    | 2.55                     | 0.85              |
| 3:M:350:VAL:HG13 | 3:M:442:GLN:CG   | 2.07                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189:PHE:HD2  | 1:A:225:LEU:HD11 | 1.40                     | 0.85              |
| 1:A:412:LYS:O    | 1:A:413:SER:C    | 2.19                     | 0.85              |
| 1:A:609:LEU:CG   | 1:A:628:VAL:HG11 | 2.05                     | 0.85              |
| 2:B:83:PHE:HZ    | 2:B:119:SER:CB   | 1.87                     | 0.85              |
| 2:B:161:LEU:HB3  | 2:B:173:VAL:CG2  | 2.05                     | 0.85              |
| 2:B:352:ASN:HD21 | 3:M:70:ASN:CB    | 1.90                     | 0.85              |
| 2:B:493:LEU:HG   | 2:B:511:ILE:HG23 | 1.58                     | 0.85              |
| 1:A:528:ASN:O    | 1:A:529:GLY:C    | 2.10                     | 0.85              |
| 1:A:346:THR:O    | 1:A:347:ASP:C    | 2.10                     | 0.85              |
| 2:B:24:ALA:HB3   | 2:B:35:TYR:CD1   | 1.98                     | 0.85              |
| 2:B:161:LEU:HB3  | 2:B:173:VAL:HG22 | 1.56                     | 0.85              |
| 2:B:256:CYS:SG   | 2:B:328:LEU:HD21 | 2.16                     | 0.85              |
| 3:M:235:LEU:CD1  | 3:M:306:LEU:HB3  | 2.06                     | 0.85              |
| 3:M:282:VAL:N    | 3:M:282:VAL:C    | 2.34                     | 0.85              |
| 4:S:4:ALA:HA     | 4:S:18:LYS:O     | 1.77                     | 0.85              |
| 2:B:151:ALA:CB   | 2:B:180:LEU:HD11 | 2.07                     | 0.85              |
| 2:B:418:TYR:C    | 2:B:418:TYR:HD1  | 1.77                     | 0.85              |
| 2:B:567:GLN:C    | 2:B:569:THR:OG1  | 2.20                     | 0.85              |
| 4:S:8:PHE:HB3    | 4:S:36:TYR:OH    | 1.77                     | 0.85              |
| 4:S:89:VAL:HG11  | 4:S:98:ILE:CG1   | 2.06                     | 0.85              |
| 1:A:121:LEU:HD13 | 1:A:155:THR:CG2  | 2.06                     | 0.84              |
| 1:A:128:LEU:HD13 | 1:A:150:LEU:HG   | 1.59                     | 0.84              |
| 1:A:189:PHE:HB3  | 1:A:225:LEU:CD2  | 2.07                     | 0.84              |
| 2:B:103:LEU:HD21 | 3:M:131:ALA:O    | 1.77                     | 0.84              |
| 2:B:336:ASN:HB3  | 2:B:339:PHE:CE1  | 2.12                     | 0.84              |
| 2:B:497:LEU:CD2  | 2:B:533:LEU:HD21 | 2.07                     | 0.84              |
| 3:M:96:ILE:CG2   | 3:M:125:PHE:CZ   | 2.60                     | 0.84              |
| 3:M:432:THR:HG1  | 3:M:480:GLN:HG3  | 1.35                     | 0.84              |
| 1:A:504:ILE:O    | 1:A:505:ASN:C    | 2.06                     | 0.84              |
| 2:B:123:LEU:HD12 | 2:B:142:LEU:HD23 | 1.58                     | 0.84              |
| 3:M:218:LEU:O    | 3:M:441:GLY:N    | 2.10                     | 0.84              |
| 2:B:13:ASP:OD2   | 3:M:17:GLN:OE1   | 1.96                     | 0.84              |
| 2:B:193:LEU:HD21 | 2:B:225:LEU:HB2  | 1.58                     | 0.84              |
| 1:A:266:VAL:O    | 1:A:267:GLU:CB   | 2.26                     | 0.84              |
| 2:B:243:TRP:CZ2  | 3:M:94:GLU:HG2   | 2.13                     | 0.84              |
| 1:A:84:MET:O     | 1:A:85:ALA:C     | 2.08                     | 0.84              |
| 2:B:136:CYS:HB3  | 2:B:172:GLU:CG   | 2.07                     | 0.84              |
| 2:B:278:PRO:HD2  | 2:B:292:GLU:HG3  | 1.59                     | 0.84              |
| 2:B:537:PHE:CB   | 2:B:598:LEU:HD13 | 2.02                     | 0.84              |
| 2:B:546:CYS:HA   | 2:B:607:ILE:HG23 | 1.58                     | 0.84              |
| 3:M:246:VAL:HB   | 3:M:297:PHE:CZ   | 2.11                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:46:PHE:O     | 4:S:48:SER:N     | 2.10                     | 0.84              |
| 1:A:289:SER:CA   | 4:S:96:LEU:CD1   | 2.55                     | 0.84              |
| 2:B:78:ASP:O     | 2:B:80:GLN:N     | 2.10                     | 0.84              |
| 2:B:127:LEU:CB   | 2:B:157:THR:HG23 | 2.07                     | 0.84              |
| 2:B:245:GLN:CB   | 2:B:309:LEU:HD11 | 2.07                     | 0.84              |
| 2:B:563:PHE:O    | 2:B:566:ALA:HB3  | 1.78                     | 0.84              |
| 3:M:245:ASP:N    | 3:M:472:TYR:CD1  | 2.45                     | 0.84              |
| 1:A:436:CYS:SG   | 1:A:450:TYR:CE1  | 2.70                     | 0.84              |
| 2:B:102:HIS:HE2  | 2:B:138:ALA:HA   | 1.40                     | 0.84              |
| 2:B:285:GLU:O    | 2:B:286:ILE:C    | 2.20                     | 0.84              |
| 1:A:174:ARG:CZ   | 4:S:148:ARG:HH22 | 1.91                     | 0.84              |
| 2:B:143:SER:CB   | 2:B:179:LYS:HB2  | 2.08                     | 0.84              |
| 2:B:167:ALA:O    | 2:B:207:VAL:CG2  | 2.24                     | 0.84              |
| 2:B:566:ALA:C    | 2:B:574:ASN:HD22 | 1.85                     | 0.84              |
| 2:B:276:SER:O    | 2:B:295:ASN:ND2  | 2.10                     | 0.84              |
| 3:M:41:LEU:HD12  | 3:M:52:ASP:N     | 1.93                     | 0.84              |
| 3:M:362:PHE:O    | 3:M:364:VAL:HG13 | 1.77                     | 0.84              |
| 1:A:391:LEU:O    | 1:A:392:MET:C    | 2.00                     | 0.84              |
| 2:B:252:LEU:CB   | 2:B:302:PHE:CE2  | 2.61                     | 0.84              |
| 2:B:418:TYR:OH   | 2:B:432:ALA:HB2  | 1.75                     | 0.84              |
| 2:B:556:LEU:CD2  | 2:B:588:ILE:CG1  | 2.56                     | 0.84              |
| 1:A:88:ASN:CB    | 1:A:120:ILE:HG23 | 2.08                     | 0.83              |
| 1:A:429:VAL:HB   | 1:A:469:LEU:CD1  | 2.08                     | 0.83              |
| 2:B:243:TRP:CH2  | 3:M:94:GLU:HB3   | 1.97                     | 0.83              |
| 2:B:375:LEU:CD2  | 2:B:402:LEU:O    | 2.25                     | 0.83              |
| 1:A:240:LEU:O    | 1:A:241:TYR:C    | 2.07                     | 0.83              |
| 2:B:193:LEU:HD11 | 2:B:225:LEU:CD2  | 2.04                     | 0.83              |
| 2:B:337:THR:CB   | 2:B:373:LEU:HD11 | 2.07                     | 0.83              |
| 2:B:549:LEU:HD22 | 2:B:611:ALA:CB   | 2.08                     | 0.83              |
| 3:M:223:HIS:ND1  | 3:M:476:THR:OG1  | 2.01                     | 0.83              |
| 3:M:344:ILE:HG23 | 3:M:347:PHE:CB   | 2.08                     | 0.83              |
| 1:A:295:VAL:HG11 | 1:A:319:LEU:HD11 | 1.58                     | 0.83              |
| 2:B:108:PHE:CZ   | 2:B:115:LEU:HG   | 2.13                     | 0.83              |
| 2:B:151:ALA:CB   | 2:B:188:TYR:CE1  | 2.61                     | 0.83              |
| 3:M:246:VAL:O    | 3:M:297:PHE:CE2  | 2.31                     | 0.83              |
| 1:A:244:LEU:HD11 | 1:A:281:LEU:HD13 | 1.60                     | 0.83              |
| 1:A:589:SER:O    | 1:A:597:GLN:NE2  | 2.11                     | 0.83              |
| 2:B:20:ARG:CD    | 2:B:35:TYR:OH    | 2.21                     | 0.83              |
| 2:B:243:TRP:HH2  | 3:M:94:GLU:CA    | 1.91                     | 0.83              |
| 2:B:278:PRO:HA   | 2:B:288:TYR:HB2  | 1.57                     | 0.83              |
| 1:A:203:PHE:CZ   | 1:A:221:VAL:HG11 | 2.13                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:215:VAL:HG11 | 1:A:243:ILE:CG2  | 2.06                     | 0.83              |
| 2:B:106:LEU:HD22 | 2:B:144:ASP:HB2  | 1.57                     | 0.83              |
| 2:B:143:SER:HB2  | 2:B:179:LYS:HD2  | 1.60                     | 0.83              |
| 2:B:212:VAL:HG21 | 2:B:248:LEU:CD2  | 2.08                     | 0.83              |
| 2:B:337:THR:HA   | 2:B:373:LEU:CG   | 2.09                     | 0.83              |
| 2:B:44:PRO:CB    | 2:B:82:TYR:OH    | 2.26                     | 0.83              |
| 2:B:170:ARG:HA   | 2:B:199:LEU:CD2  | 2.09                     | 0.83              |
| 1:A:533:ILE:CG1  | 1:A:562:TRP:CH2  | 2.60                     | 0.83              |
| 1:A:638:LEU:HD11 | 2:B:520:SER:N    | 1.91                     | 0.83              |
| 2:B:106:LEU:HD13 | 2:B:144:ASP:CB   | 2.07                     | 0.83              |
| 2:B:337:THR:CA   | 2:B:373:LEU:HD11 | 2.09                     | 0.83              |
| 2:B:568:VAL:O    | 2:B:571:SER:CB   | 2.26                     | 0.83              |
| 2:B:158:VAL:HG13 | 2:B:173:VAL:CG1  | 2.08                     | 0.83              |
| 2:B:245:GLN:HB3  | 2:B:309:LEU:CD1  | 2.08                     | 0.83              |
| 2:B:279:LEU:HG   | 2:B:288:TYR:HD1  | 1.42                     | 0.83              |
| 2:B:458:MET:O    | 2:B:459:GLU:C    | 2.22                     | 0.83              |
| 2:B:478:LEU:O    | 2:B:479:VAL:C    | 2.12                     | 0.83              |
| 3:M:326:HIS:O    | 3:M:338:PHE:HA   | 1.79                     | 0.83              |
| 1:A:298:ILE:HD11 | 1:A:311:THR:HG21 | 1.59                     | 0.82              |
| 1:A:320:HIS:O    | 1:A:321:THR:C    | 2.18                     | 0.82              |
| 2:B:193:LEU:O    | 2:B:195:ILE:N    | 2.11                     | 0.82              |
| 3:M:245:ASP:HB3  | 3:M:472:TYR:HD1  | 1.41                     | 0.82              |
| 1:A:298:ILE:O    | 1:A:299:VAL:C    | 2.19                     | 0.82              |
| 2:B:216:LYS:HB2  | 2:B:251:LEU:CD1  | 2.05                     | 0.82              |
| 3:M:16:PHE:HE1   | 3:M:122:SER:HB2  | 1.44                     | 0.82              |
| 1:A:250:ASN:OD1  | 1:A:285:THR:HB   | 1.79                     | 0.82              |
| 2:B:20:ARG:NE    | 2:B:21:GLU:HB2   | 1.94                     | 0.82              |
| 2:B:560:ILE:HG23 | 2:B:564:LYS:HB2  | 1.62                     | 0.82              |
| 1:A:282:MET:O    | 1:A:283:GLU:C    | 2.18                     | 0.82              |
| 2:B:139:LEU:HG   | 2:B:176:ALA:CB   | 2.09                     | 0.82              |
| 3:M:338:PHE:CD2  | 3:M:415:ILE:HG13 | 2.14                     | 0.82              |
| 4:S:64:ASN:C     | 4:S:66:ASP:H     | 1.86                     | 0.82              |
| 2:B:132:SER:HA   | 2:B:169:VAL:CG2  | 2.09                     | 0.82              |
| 2:B:519:ALA:O    | 2:B:523:PHE:CD2  | 2.32                     | 0.82              |
| 2:B:556:LEU:CD2  | 2:B:588:ILE:HG12 | 2.09                     | 0.82              |
| 3:M:244:VAL:HA   | 3:M:472:TYR:CE2  | 2.14                     | 0.82              |
| 4:S:16:LEU:HD13  | 4:S:125:TRP:CD1  | 2.11                     | 0.82              |
| 1:A:638:LEU:CG   | 2:B:520:SER:CA   | 2.55                     | 0.82              |
| 2:B:24:ALA:HB2   | 2:B:35:TYR:CE1   | 2.15                     | 0.82              |
| 2:B:136:CYS:SG   | 2:B:168:MET:HG2  | 2.19                     | 0.82              |
| 1:A:225:LEU:HB2  | 1:A:233:PHE:CZ   | 2.14                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:545:ARG:HD2  | 2:B:602:ASP:OD2  | 1.80                     | 0.82              |
| 2:B:567:GLN:O    | 2:B:569:THR:CA   | 2.27                     | 0.82              |
| 3:M:323:MET:SD   | 3:M:342:LEU:HG   | 2.19                     | 0.82              |
| 4:S:48:SER:OG    | 4:S:50:PHE:N     | 2.12                     | 0.82              |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:CD2  | 2.09                     | 0.82              |
| 2:B:185:LYS:NZ   | 2:B:221:ASP:OD2  | 2.13                     | 0.82              |
| 2:B:486:HIS:CE1  | 2:B:518:ILE:CB   | 2.63                     | 0.82              |
| 2:B:568:VAL:HG12 | 2:B:571:SER:OG   | 1.79                     | 0.82              |
| 4:S:75:ILE:CG2   | 4:S:77:TYR:CE1   | 2.63                     | 0.82              |
| 2:B:79:VAL:HG23  | 2:B:108:PHE:CZ   | 2.15                     | 0.82              |
| 2:B:219:TYR:CE2  | 2:B:226:LEU:CB   | 2.59                     | 0.82              |
| 2:B:227:HIS:CE1  | 2:B:292:GLU:CG   | 2.62                     | 0.82              |
| 2:B:297:PRO:O    | 2:B:301:LEU:CD1  | 2.28                     | 0.82              |
| 3:M:99:ILE:HG21  | 3:M:124:ILE:CG2  | 2.10                     | 0.82              |
| 1:A:219:VAL:CG2  | 1:A:256:LEU:HD21 | 2.09                     | 0.82              |
| 2:B:127:LEU:HD22 | 2:B:161:LEU:CD2  | 2.09                     | 0.82              |
| 2:B:227:HIS:C    | 2:B:229:HIS:N    | 2.36                     | 0.82              |
| 3:M:258:VAL:HG13 | 3:M:449:VAL:HG13 | 1.62                     | 0.82              |
| 3:M:293:PRO:O    | 3:M:293:PRO:CD   | 2.28                     | 0.82              |
| 1:A:589:SER:O    | 1:A:597:GLN:CG   | 2.28                     | 0.81              |
| 2:B:79:VAL:HG23  | 2:B:108:PHE:CE1  | 2.15                     | 0.81              |
| 2:B:127:LEU:CD1  | 2:B:157:THR:CG2  | 2.20                     | 0.81              |
| 2:B:193:LEU:CD1  | 2:B:225:LEU:HD21 | 1.97                     | 0.81              |
| 2:B:123:LEU:CD1  | 2:B:142:LEU:CD2  | 2.57                     | 0.81              |
| 2:B:172:GLU:O    | 2:B:173:VAL:C    | 2.09                     | 0.81              |
| 2:B:219:TYR:HB3  | 2:B:223:LEU:CD2  | 2.10                     | 0.81              |
| 2:B:247:TYR:OH   | 3:M:137:SER:OG   | 1.95                     | 0.81              |
| 2:B:278:PRO:CA   | 2:B:288:TYR:HB2  | 2.09                     | 0.81              |
| 2:B:545:ARG:HD3  | 2:B:602:ASP:CB   | 2.07                     | 0.81              |
| 3:M:68:VAL:HA    | 3:M:76:CYS:O     | 1.79                     | 0.81              |
| 1:A:163:ALA:CB   | 1:A:199:ASN:HD21 | 1.86                     | 0.81              |
| 1:A:219:VAL:HG11 | 1:A:256:LEU:CD2  | 2.10                     | 0.81              |
| 1:A:258:LYS:HZ3  | 4:S:94:SER:HB3   | 1.42                     | 0.81              |
| 1:A:264:SER:HB2  | 1:A:271:ARG:CD   | 2.10                     | 0.81              |
| 1:A:273:LYS:O    | 1:A:276:PRO:HD2  | 1.79                     | 0.81              |
| 1:A:316:LEU:HD11 | 1:A:341:ILE:HG21 | 1.61                     | 0.81              |
| 1:A:403:LEU:O    | 2:B:3:ASP:CG     | 2.16                     | 0.81              |
| 1:A:605:GLU:OE1  | 1:A:636:TYR:OH   | 1.97                     | 0.81              |
| 2:B:36:THR:CG2   | 2:B:40:GLN:HG3   | 2.10                     | 0.81              |
| 2:B:63:MET:HE2   | 2:B:104:TYR:HB2  | 1.62                     | 0.81              |
| 2:B:98:LYS:HZ1   | 2:B:134:LEU:CB   | 1.90                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:124:GLN:OE1  | 2:B:153:ILE:HG23 | 1.80                     | 0.81              |
| 2:B:181:TYR:HE1  | 2:B:185:LYS:HG3  | 1.41                     | 0.81              |
| 2:B:293:VAL:C    | 2:B:299:LEU:HG   | 2.05                     | 0.81              |
| 2:B:345:ARG:HH12 | 3:M:305:ASP:CG   | 1.88                     | 0.81              |
| 3:M:16:PHE:HA    | 3:M:118:TYR:HE1  | 1.36                     | 0.81              |
| 4:S:10:LYS:HA    | 4:S:84:TYR:CE1   | 2.15                     | 0.81              |
| 2:B:279:LEU:HD12 | 2:B:285:GLU:HG2  | 1.60                     | 0.81              |
| 2:B:367:SER:OG   | 2:B:401:THR:CB   | 2.29                     | 0.81              |
| 2:B:542:PRO:O    | 2:B:607:ILE:CD1  | 2.29                     | 0.81              |
| 2:B:563:PHE:O    | 2:B:567:GLN:N    | 2.12                     | 0.81              |
| 2:B:158:VAL:CG1  | 2:B:177:ILE:HG12 | 1.93                     | 0.81              |
| 1:A:633:PHE:HZ   | 2:B:550:VAL:HG12 | 1.43                     | 0.81              |
| 2:B:236:ILE:HG22 | 2:B:240:LEU:CD1  | 2.09                     | 0.81              |
| 2:B:549:LEU:HD21 | 2:B:610:ARG:C    | 2.06                     | 0.81              |
| 1:A:204:VAL:HG13 | 1:A:239:LEU:HD13 | 1.63                     | 0.81              |
| 2:B:47:LEU:HD22  | 2:B:66:ILE:CG1   | 2.10                     | 0.81              |
| 2:B:120:ILE:HD11 | 2:B:150:LEU:HD13 | 1.60                     | 0.81              |
| 2:B:245:GLN:OE1  | 2:B:309:LEU:HD12 | 1.81                     | 0.81              |
| 2:B:479:VAL:CG1  | 2:B:486:HIS:CD2  | 2.64                     | 0.81              |
| 2:B:494:ALA:HB2  | 2:B:515:PHE:CE2  | 2.16                     | 0.81              |
| 1:A:519:LEU:O    | 1:A:520:GLY:C    | 2.12                     | 0.81              |
| 2:B:232:ARG:HG3  | 2:B:236:ILE:HD11 | 1.62                     | 0.81              |
| 2:B:278:PRO:CD   | 2:B:289:PRO:O    | 2.28                     | 0.81              |
| 2:B:155:LEU:HB2  | 2:B:188:TYR:CD2  | 2.15                     | 0.81              |
| 2:B:162:VAL:HG23 | 2:B:173:VAL:HG11 | 1.61                     | 0.81              |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:CB   | 2.10                     | 0.81              |
| 2:B:566:ALA:O    | 2:B:574:ASN:HB2  | 1.81                     | 0.81              |
| 3:M:100:LEU:O    | 3:M:103:TYR:O    | 1.98                     | 0.81              |
| 1:A:216:SER:HB2  | 1:A:252:ILE:HG12 | 1.61                     | 0.80              |
| 1:A:244:LEU:CG   | 1:A:281:LEU:HD11 | 2.09                     | 0.80              |
| 1:A:332:TYR:CD1  | 1:A:366:SER:OG   | 2.33                     | 0.80              |
| 3:M:131:ALA:CB   | 3:M:131:ALA:N    | 2.42                     | 0.80              |
| 3:M:215:TYR:CG   | 3:M:468:LYS:HA   | 2.16                     | 0.80              |
| 3:M:245:ASP:C    | 3:M:472:TYR:CE1  | 2.59                     | 0.80              |
| 1:A:125:THR:CB   | 1:A:158:LEU:HD13 | 2.11                     | 0.80              |
| 2:B:268:LYS:O    | 2:B:273:SER:OG   | 2.00                     | 0.80              |
| 3:M:131:ALA:C    | 3:M:133:GLU:H    | 1.89                     | 0.80              |
| 1:A:630:PRO:HG2  | 2:B:617:LEU:HD13 | 0.80                     | 0.80              |
| 1:A:633:PHE:CZ   | 2:B:550:VAL:CG1  | 2.64                     | 0.80              |
| 2:B:42:ILE:O     | 2:B:43:ASN:HB2   | 1.82                     | 0.80              |
| 3:M:405:THR:O    | 3:M:407:THR:HG23 | 1.82                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:64:LEU:O     | 1:A:65:ASN:C     | 2.14                     | 0.80              |
| 1:A:189:PHE:HB2  | 1:A:225:LEU:CD2  | 2.08                     | 0.80              |
| 1:A:264:SER:CB   | 1:A:271:ARG:CG   | 2.60                     | 0.80              |
| 1:A:276:PRO:O    | 1:A:278:ILE:O    | 1.99                     | 0.80              |
| 2:B:62:ALA:O     | 2:B:66:ILE:HG13  | 1.80                     | 0.80              |
| 2:B:120:ILE:HA   | 2:B:142:LEU:HD21 | 1.61                     | 0.80              |
| 3:M:48:ASP:HA    | 3:M:75:TRP:HZ2   | 1.45                     | 0.80              |
| 3:M:284:SER:O    | 3:M:285:PRO:C    | 2.09                     | 0.80              |
| 1:A:84:MET:SD    | 1:A:113:SER:CA   | 2.66                     | 0.80              |
| 1:A:275:LEU:CD2  | 1:A:311:THR:OG1  | 2.27                     | 0.80              |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:HD11 | 1.63                     | 0.80              |
| 2:B:109:ALA:O    | 2:B:110:GLU:C    | 2.17                     | 0.80              |
| 4:S:131:VAL:CG2  | 4:S:153:VAL:HG22 | 2.11                     | 0.80              |
| 1:A:258:LYS:NZ   | 4:S:94:SER:N     | 2.29                     | 0.80              |
| 1:A:609:LEU:HG   | 1:A:628:VAL:HG11 | 1.64                     | 0.80              |
| 2:B:280:PRO:HG3  | 2:B:283:TYR:CE1  | 2.15                     | 0.80              |
| 2:B:352:ASN:CG   | 3:M:49:ASP:HA    | 2.07                     | 0.80              |
| 2:B:377:TYR:O    | 2:B:380:LYS:HB2  | 1.81                     | 0.80              |
| 2:B:549:LEU:CD1  | 2:B:611:ALA:CB   | 2.59                     | 0.80              |
| 3:M:99:ILE:HG21  | 3:M:124:ILE:HG23 | 1.62                     | 0.80              |
| 3:M:242:GLY:CA   | 3:M:444:ALA:HB2  | 2.11                     | 0.80              |
| 3:M:244:VAL:HB   | 3:M:300:LEU:HG   | 1.63                     | 0.80              |
| 1:A:323:CYS:CB   | 1:A:355:LEU:HD21 | 2.12                     | 0.80              |
| 2:B:36:THR:O     | 2:B:40:GLN:N     | 2.14                     | 0.80              |
| 2:B:387:ASP:HB3  | 2:B:391:ALA:HB3  | 1.62                     | 0.80              |
| 2:B:193:LEU:CB   | 2:B:225:LEU:HG   | 2.12                     | 0.80              |
| 2:B:140:SER:CB   | 2:B:172:GLU:OE1  | 2.27                     | 0.79              |
| 2:B:188:TYR:O    | 2:B:192:LEU:HD13 | 1.79                     | 0.79              |
| 2:B:522:GLU:O    | 2:B:522:GLU:HG2  | 1.79                     | 0.79              |
| 2:B:227:HIS:CE1  | 2:B:292:GLU:HG2  | 2.16                     | 0.79              |
| 2:B:451:MET:SD   | 2:B:489:ILE:HG12 | 2.22                     | 0.79              |
| 3:M:383:HIS:CG   | 3:M:403:THR:OG1  | 2.34                     | 0.79              |
| 1:A:163:ALA:O    | 1:A:164:ASP:C    | 2.17                     | 0.79              |
| 1:A:179:LYS:HB2  | 4:S:142:ILE:HB   | 1.64                     | 0.79              |
| 2:B:143:SER:C    | 2:B:179:LYS:HD2  | 2.05                     | 0.79              |
| 1:A:200:PHE:CZ   | 1:A:236:LEU:CG   | 2.64                     | 0.79              |
| 1:A:215:VAL:CG1  | 1:A:243:ILE:HG23 | 2.07                     | 0.79              |
| 1:A:552:ILE:O    | 1:A:556:VAL:HG23 | 1.83                     | 0.79              |
| 2:B:20:ARG:NH1   | 2:B:21:GLU:HG2   | 1.97                     | 0.79              |
| 2:B:588:ILE:HG23 | 2:B:618:PHE:HZ   | 1.47                     | 0.79              |
| 3:M:306:LEU:CD1  | 3:M:317:MET:HE1  | 2.12                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:317:MET:HB3  | 3:M:320:ILE:O    | 1.83                     | 0.79              |
| 3:M:350:VAL:CG2  | 3:M:442:GLN:HG2  | 2.11                     | 0.79              |
| 1:A:95:MET:SD    | 1:A:107:TYR:CD2  | 2.76                     | 0.79              |
| 1:A:353:ASP:OD1  | 1:A:378:ILE:HD12 | 1.82                     | 0.79              |
| 1:A:516:ILE:HG22 | 1:A:554:ALA:HB2  | 1.64                     | 0.79              |
| 2:B:116:THR:O    | 2:B:120:ILE:HG12 | 1.83                     | 0.79              |
| 2:B:120:ILE:CG1  | 2:B:150:LEU:HD22 | 2.10                     | 0.79              |
| 2:B:328:LEU:HB2  | 2:B:333:GLN:HE22 | 1.46                     | 0.79              |
| 2:B:567:GLN:CA   | 2:B:569:THR:OG1  | 2.30                     | 0.79              |
| 3:M:245:ASP:N    | 3:M:472:TYR:CG   | 2.49                     | 0.79              |
| 1:A:401:VAL:HG23 | 1:A:418:ILE:O    | 1.81                     | 0.79              |
| 2:B:170:ARG:NH1  | 2:B:198:GLU:HG2  | 1.96                     | 0.79              |
| 2:B:219:TYR:O    | 2:B:220:ALA:C    | 2.23                     | 0.79              |
| 1:A:180:LYS:HZ3  | 4:S:137:GLN:CB   | 1.90                     | 0.79              |
| 1:A:244:LEU:CD1  | 1:A:281:LEU:HD11 | 2.12                     | 0.79              |
| 1:A:404:GLN:HB3  | 2:B:7:ARG:HH21   | 1.41                     | 0.79              |
| 1:A:520:GLY:HA2  | 1:A:558:VAL:HG22 | 1.64                     | 0.79              |
| 2:B:197:LYS:CA   | 2:B:229:HIS:CD2  | 2.65                     | 0.79              |
| 2:B:396:ILE:HG21 | 2:B:432:ALA:HA   | 1.62                     | 0.79              |
| 2:B:513:TRP:O    | 2:B:551:LEU:HD22 | 1.83                     | 0.79              |
| 2:B:534:ILE:O    | 2:B:598:LEU:HD11 | 1.83                     | 0.79              |
| 3:M:220:GLU:OE2  | 3:M:439:TYR:CD1  | 2.36                     | 0.79              |
| 2:B:267:ASP:H    | 2:B:289:PRO:CG   | 1.95                     | 0.79              |
| 2:B:37:TYR:HD2   | 2:B:38:TYR:CD1   | 2.00                     | 0.79              |
| 2:B:178:ILE:CD1  | 2:B:218:CYS:H    | 1.95                     | 0.79              |
| 2:B:490:ILE:HG13 | 2:B:518:ILE:CG2  | 2.12                     | 0.79              |
| 3:M:214:LEU:HD23 | 3:M:214:LEU:C    | 2.08                     | 0.79              |
| 3:M:281:GLY:C    | 3:M:281:GLY:N    | 2.41                     | 0.79              |
| 1:A:332:TYR:CE1  | 1:A:366:SER:HB2  | 2.18                     | 0.78              |
| 1:A:539:ASN:O    | 1:A:540:ILE:C    | 2.18                     | 0.78              |
| 2:B:566:ALA:HB2  | 2:B:581:TYR:CD2  | 2.17                     | 0.78              |
| 3:M:380:ARG:O    | 3:M:411:LEU:HA   | 1.81                     | 0.78              |
| 1:A:581:LEU:CD2  | 1:A:607:LEU:HD11 | 2.13                     | 0.78              |
| 2:B:280:PRO:HG3  | 2:B:283:TYR:CD1  | 2.17                     | 0.78              |
| 1:A:114:PHE:HE1  | 1:A:154:ILE:HG12 | 1.46                     | 0.78              |
| 1:A:136:GLY:O    | 1:A:137:ASN:C    | 2.15                     | 0.78              |
| 1:A:264:SER:HB2  | 1:A:271:ARG:HD3  | 1.63                     | 0.78              |
| 2:B:103:LEU:HD22 | 3:M:131:ALA:HA   | 1.65                     | 0.78              |
| 2:B:534:ILE:HD11 | 2:B:595:VAL:HG23 | 1.63                     | 0.78              |
| 3:M:338:PHE:CE2  | 3:M:415:ILE:HG13 | 2.18                     | 0.78              |
| 1:A:186:PHE:CZ   | 1:A:224:GLU:CG   | 2.63                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:123:LEU:CD1  | 2:B:142:LEU:CG   | 2.58                     | 0.78              |
| 2:B:186:ASN:C    | 2:B:188:TYR:N    | 2.36                     | 0.78              |
| 2:B:199:LEU:C    | 2:B:201:ALA:N    | 2.35                     | 0.78              |
| 2:B:337:THR:CA   | 2:B:373:LEU:CD2  | 2.50                     | 0.78              |
| 4:S:164:ASP:HA   | 4:S:167:ILE:HB   | 1.66                     | 0.78              |
| 1:A:274:LEU:O    | 1:A:275:LEU:C    | 2.21                     | 0.78              |
| 1:A:450:TYR:OH   | 1:A:476:GLN:NE2  | 2.16                     | 0.78              |
| 2:B:25:VAL:HB    | 2:B:36:THR:OG1   | 1.83                     | 0.78              |
| 2:B:135:ARG:HH22 | 2:B:164:ASP:CG   | 1.90                     | 0.78              |
| 2:B:139:LEU:CG   | 2:B:176:ALA:CB   | 2.61                     | 0.78              |
| 3:M:360:LEU:HD23 | 3:M:362:PHE:CZ   | 2.18                     | 0.78              |
| 3:M:383:HIS:CB   | 3:M:403:THR:OG1  | 2.31                     | 0.78              |
| 4:S:43:ASN:O     | 4:S:44:SER:C     | 2.15                     | 0.78              |
| 2:B:63:MET:HG3   | 2:B:100:LEU:HB3  | 1.64                     | 0.78              |
| 2:B:196:LEU:HB3  | 2:B:215:TYR:CZ   | 2.18                     | 0.78              |
| 1:A:121:LEU:HD11 | 1:A:155:THR:H    | 1.49                     | 0.78              |
| 1:A:189:PHE:HB3  | 1:A:225:LEU:HD22 | 1.65                     | 0.78              |
| 1:A:222:ILE:CG2  | 1:A:240:LEU:HD11 | 2.13                     | 0.78              |
| 2:B:136:CYS:HB3  | 2:B:172:GLU:HG3  | 1.66                     | 0.78              |
| 2:B:143:SER:CB   | 2:B:179:LYS:CD   | 2.60                     | 0.78              |
| 2:B:278:PRO:C    | 2:B:288:TYR:CB   | 2.55                     | 0.78              |
| 2:B:374:PHE:HD2  | 2:B:402:LEU:CD1  | 1.91                     | 0.78              |
| 2:B:537:PHE:CZ   | 2:B:545:ARG:HG2  | 2.18                     | 0.78              |
| 1:A:114:PHE:HZ   | 1:A:152:THR:O    | 1.67                     | 0.78              |
| 2:B:21:GLU:CD    | 2:B:39:SER:HB3   | 2.08                     | 0.78              |
| 2:B:106:LEU:CD1  | 2:B:144:ASP:HB3  | 2.14                     | 0.78              |
| 2:B:230:PHE:O    | 2:B:231:ARG:C    | 2.07                     | 0.78              |
| 1:A:114:PHE:CE2  | 1:A:153:ILE:HA   | 2.18                     | 0.78              |
| 1:A:373:GLU:CG   | 1:A:427:LYS:HE2  | 2.13                     | 0.78              |
| 2:B:393:ILE:CG2  | 2:B:431:MET:HG2  | 2.13                     | 0.78              |
| 2:B:162:VAL:CG2  | 2:B:199:LEU:HD11 | 2.13                     | 0.78              |
| 3:M:247:ARG:H    | 3:M:470:ALA:HB2  | 1.49                     | 0.78              |
| 3:M:271:SER:HB3  | 3:M:301:GLU:HG3  | 1.64                     | 0.78              |
| 1:A:176:TYR:HE1  | 4:S:148:ARG:NH2  | 1.81                     | 0.77              |
| 2:B:21:GLU:HA    | 2:B:24:ALA:CB    | 2.14                     | 0.77              |
| 2:B:79:VAL:HB    | 2:B:108:PHE:CE1  | 2.19                     | 0.77              |
| 2:B:293:VAL:O    | 2:B:299:LEU:CB   | 2.32                     | 0.77              |
| 2:B:546:CYS:CA   | 2:B:607:ILE:CG1  | 2.55                     | 0.77              |
| 2:B:553:ALA:HB1  | 2:B:614:ILE:HG12 | 1.65                     | 0.77              |
| 4:S:5:VAL:O      | 4:S:17:VAL:HA    | 1.83                     | 0.77              |
| 1:A:185:LEU:HD13 | 1:A:203:PHE:CE1  | 2.19                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:196:LEU:O    | 1:A:197:ARG:C    | 2.18                     | 0.77              |
| 1:A:566:PHE:C    | 1:A:568:GLU:H    | 1.90                     | 0.77              |
| 2:B:215:TYR:HD1  | 2:B:233:TYR:HE1  | 0.90                     | 0.77              |
| 2:B:566:ALA:C    | 2:B:574:ASN:CB   | 2.57                     | 0.77              |
| 4:S:3:HIS:NE2    | 4:S:90:ASP:OD2   | 2.18                     | 0.77              |
| 1:A:225:LEU:HD12 | 1:A:233:PHE:CE2  | 2.19                     | 0.77              |
| 2:B:70:MET:HE3   | 2:B:107:ARG:HG3  | 1.66                     | 0.77              |
| 2:B:497:LEU:O    | 2:B:499:VAL:N    | 2.17                     | 0.77              |
| 2:B:523:PHE:CG   | 2:B:559:ASP:OD1  | 2.37                     | 0.77              |
| 3:M:323:MET:HB3  | 3:M:340:LEU:HD11 | 1.65                     | 0.77              |
| 4:S:28:GLN:O     | 4:S:32:LEU:HG    | 1.85                     | 0.77              |
| 2:B:20:ARG:NH1   | 2:B:21:GLU:CG    | 2.47                     | 0.77              |
| 2:B:127:LEU:HB3  | 2:B:161:LEU:HD11 | 1.64                     | 0.77              |
| 2:B:316:THR:OG1  | 3:M:90:PHE:HE2   | 1.58                     | 0.77              |
| 3:M:375:LYS:N    | 3:M:416:GLU:O    | 2.16                     | 0.77              |
| 4:S:8:PHE:CD2    | 4:S:8:PHE:N      | 2.50                     | 0.77              |
| 1:A:532:LEU:O    | 1:A:533:ILE:C    | 2.13                     | 0.77              |
| 1:A:567:GLN:O    | 1:A:568:GLU:C    | 2.26                     | 0.77              |
| 1:A:605:GLU:OE2  | 1:A:608:ARG:NH2  | 2.17                     | 0.77              |
| 2:B:66:ILE:HG22  | 2:B:104:TYR:CE1  | 2.19                     | 0.77              |
| 2:B:451:MET:HG3  | 2:B:489:ILE:CD1  | 2.15                     | 0.77              |
| 2:B:486:HIS:NE2  | 2:B:518:ILE:CB   | 2.46                     | 0.77              |
| 4:S:39:ILE:HG23  | 4:S:47:GLN:OE1   | 1.85                     | 0.77              |
| 1:A:638:LEU:HB2  | 2:B:558:TYR:CE1  | 2.10                     | 0.77              |
| 2:B:20:ARG:CZ    | 2:B:21:GLU:CG    | 2.62                     | 0.77              |
| 2:B:256:CYS:CB   | 2:B:328:LEU:CD2  | 2.62                     | 0.77              |
| 2:B:261:PRO:HD2  | 2:B:293:VAL:HG23 | 1.65                     | 0.77              |
| 1:A:436:CYS:CB   | 1:A:450:TYR:CE1  | 2.67                     | 0.77              |
| 2:B:35:TYR:O     | 2:B:39:SER:HB3   | 1.84                     | 0.77              |
| 2:B:310:ILE:HG12 | 2:B:318:ILE:HA   | 1.65                     | 0.77              |
| 2:B:490:ILE:CD1  | 2:B:518:ILE:HG21 | 2.14                     | 0.77              |
| 2:B:523:PHE:HE1  | 2:B:580:TYR:CB   | 1.85                     | 0.77              |
| 2:B:556:LEU:HD22 | 2:B:588:ILE:CG1  | 2.13                     | 0.77              |
| 3:M:323:MET:CE   | 3:M:342:LEU:HB3  | 2.15                     | 0.77              |
| 1:A:289:SER:C    | 4:S:96:LEU:CD1   | 2.58                     | 0.77              |
| 2:B:36:THR:HG23  | 2:B:40:GLN:HG3   | 1.66                     | 0.77              |
| 2:B:174:ALA:HB3  | 2:B:211:ALA:HA   | 1.67                     | 0.77              |
| 2:B:534:ILE:CD1  | 2:B:595:VAL:HG23 | 2.15                     | 0.77              |
| 1:A:84:MET:HB3   | 1:A:113:SER:HB2  | 1.66                     | 0.77              |
| 1:A:320:HIS:HB2  | 1:A:352:PHE:CE2  | 2.20                     | 0.77              |
| 1:A:384:LEU:HD22 | 1:A:441:TYR:CE2  | 2.20                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:21:GLU:OE2   | 2:B:35:TYR:CD2   | 2.37                     | 0.77              |
| 2:B:79:VAL:CG2   | 2:B:108:PHE:CE1  | 2.67                     | 0.77              |
| 2:B:316:THR:HG21 | 3:M:90:PHE:CE2   | 2.18                     | 0.77              |
| 3:M:374:TYR:O    | 3:M:390:ILE:HD12 | 1.85                     | 0.77              |
| 1:A:566:PHE:HZ   | 1:A:618:THR:O    | 1.67                     | 0.77              |
| 2:B:37:TYR:CD2   | 2:B:42:ILE:HA    | 2.20                     | 0.77              |
| 4:S:53:THR:CB    | 4:S:68:VAL:C     | 2.58                     | 0.77              |
| 1:A:215:VAL:HG13 | 1:A:243:ILE:CG2  | 2.08                     | 0.76              |
| 2:B:123:LEU:HD12 | 2:B:142:LEU:HD21 | 1.66                     | 0.76              |
| 2:B:127:LEU:HD23 | 2:B:161:LEU:HD21 | 1.66                     | 0.76              |
| 2:B:345:ARG:NH1  | 3:M:305:ASP:CG   | 2.41                     | 0.76              |
| 1:A:306:GLU:O    | 1:A:307:ASP:C    | 2.22                     | 0.76              |
| 2:B:28:SER:H     | 2:B:32:GLU:HB3   | 1.49                     | 0.76              |
| 2:B:28:SER:N     | 2:B:32:GLU:HB3   | 1.82                     | 0.76              |
| 4:S:130:SER:OG   | 4:S:156:LEU:CD1  | 2.33                     | 0.76              |
| 1:A:404:GLN:CB   | 2:B:7:ARG:NH2    | 2.44                     | 0.76              |
| 1:A:595:GLU:CG   | 2:B:473:ASN:OD1  | 2.33                     | 0.76              |
| 2:B:307:ASN:OD1  | 2:B:339:PHE:HD2  | 1.67                     | 0.76              |
| 2:B:374:PHE:CE1  | 2:B:381:PHE:CE1  | 2.73                     | 0.76              |
| 3:M:48:ASP:O     | 3:M:75:TRP:CH2   | 2.39                     | 0.76              |
| 1:A:110:ALA:O    | 1:A:111:SER:C    | 2.18                     | 0.76              |
| 1:A:332:TYR:HE1  | 1:A:366:SER:HB2  | 1.50                     | 0.76              |
| 1:A:429:VAL:CG1  | 1:A:469:LEU:HD11 | 2.14                     | 0.76              |
| 2:B:106:LEU:CD1  | 2:B:144:ASP:CB   | 2.63                     | 0.76              |
| 2:B:505:ASP:HA   | 2:B:544:THR:OG1  | 1.86                     | 0.76              |
| 2:B:513:TRP:HA   | 2:B:551:LEU:HD21 | 1.61                     | 0.76              |
| 3:M:241:HIS:HB2  | 3:M:476:THR:CG2  | 2.16                     | 0.76              |
| 3:M:243:ILE:H    | 3:M:474:THR:HG22 | 1.51                     | 0.76              |
| 1:A:328:PRO:O    | 1:A:329:ASN:C    | 2.16                     | 0.76              |
| 2:B:143:SER:HB2  | 2:B:179:LYS:CG   | 2.15                     | 0.76              |
| 2:B:245:GLN:CB   | 2:B:309:LEU:CD1  | 2.64                     | 0.76              |
| 2:B:278:PRO:HD3  | 2:B:292:GLU:HB2  | 1.67                     | 0.76              |
| 1:A:174:ARG:NH2  | 4:S:148:ARG:NH2  | 2.34                     | 0.76              |
| 1:A:585:PHE:CE2  | 1:A:603:VAL:CG1  | 2.68                     | 0.76              |
| 2:B:178:ILE:HD12 | 2:B:218:CYS:N    | 1.96                     | 0.76              |
| 2:B:208:ILE:CD1  | 2:B:236:ILE:HD13 | 2.15                     | 0.76              |
| 3:M:225:VAL:HB   | 3:M:237:THR:OG1  | 1.85                     | 0.76              |
| 3:M:306:LEU:CD1  | 3:M:317:MET:CE   | 2.63                     | 0.76              |
| 4:S:8:PHE:CE1    | 4:S:84:TYR:CB    | 2.69                     | 0.76              |
| 1:A:638:LEU:HD21 | 2:B:558:TYR:HB3  | 1.62                     | 0.76              |
| 2:B:16:LYS:CD    | 3:M:119:ASP:OD1  | 2.27                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:20:ARG:NH1   | 2:B:35:TYR:HE1   | 1.84                     | 0.76              |
| 2:B:523:PHE:CE1  | 2:B:580:TYR:HB3  | 2.19                     | 0.76              |
| 2:B:580:TYR:HB3  | 2:B:582:ASP:CG   | 2.11                     | 0.76              |
| 3:M:350:VAL:HG13 | 3:M:442:GLN:HG2  | 1.67                     | 0.76              |
| 1:A:189:PHE:CD2  | 1:A:225:LEU:HD11 | 2.20                     | 0.76              |
| 1:A:408:ILE:HG22 | 4:S:65:ASN:N     | 2.01                     | 0.76              |
| 2:B:29:LYS:HE2   | 2:B:30:LEU:CA    | 2.14                     | 0.76              |
| 2:B:444:THR:O    | 2:B:445:SER:C    | 2.23                     | 0.76              |
| 4:S:53:THR:HB    | 4:S:69:ASN:CB    | 2.16                     | 0.76              |
| 1:A:281:LEU:O    | 1:A:282:MET:C    | 2.17                     | 0.76              |
| 2:B:178:ILE:HD11 | 2:B:215:TYR:HA   | 1.68                     | 0.76              |
| 2:B:500:GLN:CB   | 2:B:503:LEU:HG   | 2.16                     | 0.76              |
| 2:B:560:ILE:HA   | 2:B:563:PHE:HB2  | 1.67                     | 0.76              |
| 3:M:70:ASN:HA    | 3:M:74:TYR:O     | 1.86                     | 0.76              |
| 3:M:245:ASP:OD1  | 3:M:297:PHE:C    | 2.29                     | 0.76              |
| 4:S:25:LEU:O     | 4:S:26:PRO:C     | 2.15                     | 0.76              |
| 2:B:120:ILE:HG23 | 2:B:142:LEU:HD22 | 1.68                     | 0.76              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:CA   | 2.66                     | 0.76              |
| 2:B:475:ILE:HG23 | 2:B:489:ILE:HG21 | 1.68                     | 0.76              |
| 1:A:264:SER:HB2  | 1:A:271:ARG:CG   | 2.16                     | 0.75              |
| 1:A:322:PHE:CD2  | 1:A:330:LEU:HD21 | 2.22                     | 0.75              |
| 2:B:170:ARG:HG2  | 2:B:199:LEU:HD23 | 1.66                     | 0.75              |
| 2:B:243:TRP:CE2  | 3:M:98:ARG:NE    | 2.54                     | 0.75              |
| 2:B:261:PRO:CB   | 2:B:290:SER:HB3  | 2.15                     | 0.75              |
| 2:B:515:PHE:CD2  | 2:B:529:VAL:HG11 | 2.21                     | 0.75              |
| 2:B:566:ALA:C    | 2:B:574:ASN:CG   | 2.54                     | 0.75              |
| 4:S:38:LEU:HD23  | 4:S:68:VAL:HG21  | 1.68                     | 0.75              |
| 2:B:212:VAL:HG23 | 2:B:233:TYR:CE2  | 2.21                     | 0.75              |
| 2:B:487:LEU:CD2  | 2:B:522:GLU:HB3  | 2.17                     | 0.75              |
| 4:S:10:LYS:HA    | 4:S:84:TYR:HE1   | 1.49                     | 0.75              |
| 1:A:180:LYS:HZ3  | 4:S:137:GLN:HB3  | 1.48                     | 0.75              |
| 1:A:182:ILE:HG22 | 1:A:221:VAL:HG21 | 1.68                     | 0.75              |
| 1:A:263:LEU:O    | 1:A:266:VAL:O    | 2.04                     | 0.75              |
| 2:B:63:MET:CG    | 2:B:100:LEU:HB3  | 2.16                     | 0.75              |
| 2:B:267:ASP:HB3  | 2:B:289:PRO:HD3  | 1.67                     | 0.75              |
| 2:B:278:PRO:CG   | 2:B:292:GLU:OE1  | 2.33                     | 0.75              |
| 2:B:353:GLN:CD   | 3:M:50:TYR:CD1   | 2.64                     | 0.75              |
| 2:B:476:ARG:HA   | 2:B:514:LEU:CD1  | 2.15                     | 0.75              |
| 3:M:16:PHE:CA    | 3:M:118:TYR:CE1  | 2.64                     | 0.75              |
| 3:M:437:TYR:N    | 3:M:437:TYR:CD1  | 2.53                     | 0.75              |
| 1:A:114:PHE:O    | 1:A:115:TYR:C    | 2.25                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:373:GLU:HG3  | 1:A:427:LYS:HE2  | 1.66                     | 0.75              |
| 3:M:6:TYR:HA     | 3:M:16:PHE:O     | 1.86                     | 0.75              |
| 2:B:70:MET:CE    | 2:B:107:ARG:HG3  | 2.14                     | 0.75              |
| 3:M:317:MET:O    | 3:M:322:LEU:HB3  | 1.86                     | 0.75              |
| 4:S:32:LEU:O     | 4:S:35:VAL:HG22  | 1.87                     | 0.75              |
| 4:S:71:GLU:O     | 4:S:73:ILE:N     | 2.20                     | 0.75              |
| 1:A:200:PHE:CE1  | 1:A:236:LEU:HG   | 2.21                     | 0.75              |
| 2:B:280:PRO:HG2  | 2:B:283:TYR:CG   | 2.21                     | 0.75              |
| 2:B:297:PRO:O    | 2:B:301:LEU:HD12 | 1.86                     | 0.75              |
| 2:B:549:LEU:HD13 | 2:B:611:ALA:HB2  | 1.69                     | 0.75              |
| 2:B:563:PHE:CD2  | 2:B:584:SER:CB   | 2.67                     | 0.75              |
| 4:S:1:MET:H2     | 4:S:93:GLU:HB2   | 1.51                     | 0.75              |
| 1:A:225:LEU:HD12 | 1:A:233:PHE:CZ   | 2.22                     | 0.75              |
| 2:B:296:ASP:OD1  | 2:B:297:PRO:HD2  | 1.86                     | 0.75              |
| 2:B:418:TYR:CD1  | 2:B:424:PHE:CD1  | 2.74                     | 0.75              |
| 3:M:290:PHE:CZ   | 3:M:293:PRO:HD3  | 2.21                     | 0.75              |
| 1:A:462:GLN:O    | 1:A:463:ASP:C    | 2.25                     | 0.75              |
| 2:B:278:PRO:CB   | 2:B:288:TYR:C    | 2.56                     | 0.75              |
| 2:B:315:PRO:HA   | 2:B:318:ILE:HD12 | 1.69                     | 0.75              |
| 2:B:487:LEU:HD22 | 2:B:522:GLU:HB3  | 1.68                     | 0.75              |
| 2:B:556:LEU:HD23 | 2:B:588:ILE:CG1  | 2.17                     | 0.75              |
| 1:A:88:ASN:O     | 1:A:89:PHE:C     | 2.14                     | 0.75              |
| 2:B:132:SER:HB2  | 2:B:169:VAL:CG2  | 2.17                     | 0.75              |
| 2:B:167:ALA:CB   | 2:B:202:ASP:OD1  | 2.35                     | 0.75              |
| 2:B:212:VAL:C    | 2:B:214:ALA:N    | 2.41                     | 0.75              |
| 2:B:236:ILE:CG2  | 2:B:240:LEU:HD11 | 2.13                     | 0.75              |
| 2:B:344:VAL:HG13 | 2:B:381:PHE:CE1  | 2.20                     | 0.74              |
| 2:B:513:TRP:CG   | 2:B:551:LEU:HD21 | 2.21                     | 0.74              |
| 2:B:531:ARG:HA   | 2:B:591:MET:SD   | 2.27                     | 0.74              |
| 1:A:186:PHE:CD1  | 1:A:224:GLU:HB3  | 2.22                     | 0.74              |
| 2:B:530:LEU:HG   | 2:B:591:MET:HB3  | 1.67                     | 0.74              |
| 2:B:310:ILE:CG2  | 2:B:342:ALA:HB1  | 2.18                     | 0.74              |
| 2:B:351:GLU:OE2  | 3:M:476:THR:O    | 2.05                     | 0.74              |
| 1:A:107:TYR:CD2  | 1:A:128:LEU:HD21 | 2.23                     | 0.74              |
| 3:M:223:HIS:CG   | 3:M:478:ASN:HA   | 2.21                     | 0.74              |
| 1:A:304:LEU:HA   | 1:A:308:ASP:HB2  | 1.70                     | 0.74              |
| 2:B:29:LYS:HE2   | 2:B:30:LEU:H     | 0.72                     | 0.74              |
| 2:B:193:LEU:C    | 2:B:195:ILE:N    | 2.42                     | 0.74              |
| 2:B:317:VAL:O    | 2:B:321:CYS:SG   | 2.46                     | 0.74              |
| 2:B:549:LEU:CD1  | 2:B:611:ALA:HB2  | 2.16                     | 0.74              |
| 2:B:556:LEU:HD23 | 2:B:588:ILE:HG13 | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:566:ALA:CA   | 2:B:574:ASN:ND2  | 2.51                     | 0.74              |
| 3:M:265:ASN:CG   | 3:M:313:SER:HG   | 1.94                     | 0.74              |
| 4:S:98:ILE:O     | 4:S:102:ILE:HG13 | 1.87                     | 0.74              |
| 1:A:158:LEU:HG   | 1:A:162:ILE:CD1  | 2.17                     | 0.74              |
| 1:A:487:MET:O    | 1:A:488:ARG:C    | 2.22                     | 0.74              |
| 1:A:594:PHE:CE1  | 2:B:477:MET:HE2  | 2.23                     | 0.74              |
| 1:A:101:GLN:HE22 | 4:S:167:ILE:HD12 | 1.52                     | 0.74              |
| 1:A:121:LEU:HD21 | 1:A:158:LEU:CB   | 2.06                     | 0.74              |
| 1:A:294:SER:O    | 1:A:298:ILE:HG12 | 1.88                     | 0.74              |
| 1:A:585:PHE:CE2  | 1:A:603:VAL:HG11 | 2.23                     | 0.74              |
| 1:A:264:SER:HB3  | 1:A:271:ARG:CG   | 2.17                     | 0.74              |
| 2:B:108:PHE:CE2  | 2:B:112:ASP:HB3  | 2.23                     | 0.74              |
| 2:B:212:VAL:CG2  | 2:B:248:LEU:CD2  | 2.65                     | 0.74              |
| 2:B:400:SER:HB3  | 2:B:435:SER:HB3  | 1.68                     | 0.74              |
| 3:M:260:LEU:CD2  | 3:M:449:VAL:HG22 | 2.18                     | 0.74              |
| 3:M:267:ILE:HD12 | 3:M:445:SER:OG   | 1.88                     | 0.74              |
| 1:A:196:LEU:O    | 1:A:196:LEU:HD22 | 1.87                     | 0.74              |
| 1:A:316:LEU:HD13 | 1:A:348:PHE:CG   | 2.23                     | 0.74              |
| 1:A:601:VAL:O    | 1:A:602:GLU:C    | 2.12                     | 0.74              |
| 2:B:135:ARG:NH2  | 2:B:164:ASP:CG   | 2.46                     | 0.74              |
| 2:B:279:LEU:H    | 2:B:288:TYR:CB   | 1.91                     | 0.74              |
| 2:B:393:ILE:HG23 | 2:B:431:MET:CG   | 2.17                     | 0.74              |
| 1:A:154:ILE:CG2  | 1:A:191:GLN:CG   | 2.65                     | 0.74              |
| 1:A:365:VAL:O    | 1:A:366:SER:C    | 2.22                     | 0.74              |
| 1:A:436:CYS:HB2  | 1:A:450:TYR:CE1  | 2.23                     | 0.74              |
| 2:B:29:LYS:C     | 2:B:32:GLU:HG3   | 1.86                     | 0.74              |
| 2:B:223:LEU:O    | 2:B:224:GLU:C    | 2.20                     | 0.74              |
| 2:B:237:ILE:HB   | 2:B:248:LEU:HD13 | 1.70                     | 0.74              |
| 2:B:526:CYS:N    | 2:B:527:PRO:CD   | 2.49                     | 0.74              |
| 2:B:563:PHE:HD2  | 2:B:584:SER:HB2  | 1.52                     | 0.74              |
| 3:M:347:PHE:CD1  | 3:M:350:VAL:CB   | 2.70                     | 0.74              |
| 3:M:443:SER:OG   | 3:M:447:ILE:C    | 2.30                     | 0.74              |
| 4:S:8:PHE:HE2    | 4:S:86:THR:N     | 1.85                     | 0.74              |
| 1:A:140:VAL:O    | 1:A:141:VAL:C    | 2.25                     | 0.73              |
| 1:A:215:VAL:O    | 1:A:216:SER:C    | 2.22                     | 0.73              |
| 1:A:638:LEU:CD1  | 2:B:520:SER:HA   | 2.09                     | 0.73              |
| 2:B:316:THR:HG21 | 3:M:90:PHE:CD2   | 2.21                     | 0.73              |
| 3:M:121:ILE:O    | 3:M:125:PHE:CD1  | 2.41                     | 0.73              |
| 3:M:379:LEU:HD23 | 3:M:411:LEU:CG   | 2.16                     | 0.73              |
| 4:S:53:THR:OG1   | 4:S:68:VAL:CA    | 2.35                     | 0.73              |
| 1:A:393:LYS:NZ   | 1:A:397:ASP:OD2  | 2.21                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:399:ASP:O    | 1:A:420:ILE:HB   | 1.88                     | 0.73              |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:HG   | 1.69                     | 0.73              |
| 2:B:267:ASP:O    | 2:B:268:LYS:C    | 2.27                     | 0.73              |
| 2:B:268:LYS:O    | 2:B:273:SER:CB   | 2.36                     | 0.73              |
| 2:B:274:PRO:HG2  | 2:B:295:ASN:HB3  | 1.67                     | 0.73              |
| 2:B:278:PRO:HB3  | 2:B:288:TYR:C    | 2.13                     | 0.73              |
| 2:B:433:VAL:HG11 | 2:B:471:TYR:HA   | 1.69                     | 0.73              |
| 3:M:121:ILE:HG22 | 3:M:125:PHE:CE1  | 2.22                     | 0.73              |
| 3:M:428:VAL:O    | 3:M:429:ASP:C    | 2.29                     | 0.73              |
| 3:M:437:TYR:CD1  | 3:M:479:PHE:CZ   | 2.76                     | 0.73              |
| 2:B:279:LEU:N    | 2:B:288:TYR:CB   | 2.41                     | 0.73              |
| 2:B:545:ARG:CD   | 2:B:602:ASP:HB2  | 2.12                     | 0.73              |
| 4:S:55:PRO:HA    | 4:S:69:ASN:HB3   | 1.69                     | 0.73              |
| 1:A:348:PHE:O    | 1:A:352:PHE:CD1  | 2.42                     | 0.73              |
| 2:B:98:LYS:HZ2   | 2:B:134:LEU:HB3  | 1.50                     | 0.73              |
| 2:B:102:HIS:O    | 2:B:103:LEU:C    | 2.21                     | 0.73              |
| 2:B:106:LEU:HD21 | 2:B:144:ASP:HB3  | 1.68                     | 0.73              |
| 2:B:127:LEU:CG   | 2:B:157:THR:HG21 | 2.18                     | 0.73              |
| 2:B:136:CYS:C    | 2:B:172:GLU:CG   | 2.57                     | 0.73              |
| 2:B:274:PRO:HG2  | 2:B:295:ASN:CB   | 1.90                     | 0.73              |
| 2:B:418:TYR:CD1  | 2:B:424:PHE:CE1  | 2.77                     | 0.73              |
| 1:A:637:GLU:HA   | 2:B:517:GLU:CD   | 2.14                     | 0.73              |
| 2:B:215:TYR:CE1  | 2:B:233:TYR:CE1  | 2.76                     | 0.73              |
| 2:B:501:THR:O    | 2:B:508:ARG:NH2  | 2.21                     | 0.73              |
| 2:B:549:LEU:HD13 | 2:B:611:ALA:CB   | 2.18                     | 0.73              |
| 2:B:559:ASP:HA   | 2:B:562:ASN:HB2  | 1.68                     | 0.73              |
| 1:A:101:GLN:NE2  | 4:S:167:ILE:CD1  | 2.51                     | 0.73              |
| 1:A:185:LEU:CD1  | 1:A:203:PHE:CE1  | 2.72                     | 0.73              |
| 1:A:186:PHE:CE1  | 1:A:224:GLU:HB3  | 2.20                     | 0.73              |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:HA   | 1.69                     | 0.73              |
| 2:B:181:TYR:CZ   | 2:B:185:LYS:HE2  | 2.24                     | 0.73              |
| 2:B:234:CYS:HB3  | 2:B:301:LEU:HB3  | 1.71                     | 0.73              |
| 2:B:239:GLN:CD   | 3:M:279:ASN:C    | 2.56                     | 0.73              |
| 2:B:293:VAL:O    | 2:B:299:LEU:HD12 | 1.88                     | 0.73              |
| 3:M:133:GLU:O    | 3:M:135:ASN:N    | 2.22                     | 0.73              |
| 3:M:331:LEU:HD12 | 3:M:331:LEU:O    | 1.89                     | 0.73              |
| 3:M:351:SER:OG   | 3:M:441:GLY:O    | 2.01                     | 0.73              |
| 4:S:53:THR:HB    | 4:S:69:ASN:HB2   | 1.69                     | 0.73              |
| 1:A:186:PHE:HB2  | 1:A:221:VAL:HG13 | 1.71                     | 0.73              |
| 1:A:498:LEU:O    | 1:A:501:ASN:O    | 2.05                     | 0.73              |
| 2:B:3:ASP:O      | 2:B:7:ARG:HG3    | 1.88                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:25:VAL:CA    | 2:B:35:TYR:HB3   | 2.18                     | 0.73              |
| 2:B:158:VAL:CG1  | 2:B:177:ILE:CD1  | 2.67                     | 0.73              |
| 2:B:186:ASN:C    | 2:B:188:TYR:H    | 1.96                     | 0.73              |
| 3:M:243:ILE:H    | 3:M:474:THR:CG2  | 2.01                     | 0.73              |
| 3:M:245:ASP:N    | 3:M:472:TYR:CE1  | 2.56                     | 0.73              |
| 3:M:320:ILE:HG23 | 3:M:439:TYR:OH   | 1.89                     | 0.73              |
| 2:B:170:ARG:CA   | 2:B:199:LEU:HD22 | 2.18                     | 0.73              |
| 2:B:512:VAL:C    | 2:B:551:LEU:CD1  | 2.45                     | 0.73              |
| 1:A:185:LEU:HB3  | 1:A:203:PHE:HE1  | 1.54                     | 0.73              |
| 1:A:260:PHE:CE1  | 1:A:274:LEU:CD1  | 2.72                     | 0.73              |
| 1:A:404:GLN:O    | 2:B:3:ASP:CA     | 2.37                     | 0.73              |
| 2:B:318:ILE:HD13 | 2:B:346:THR:OG1  | 1.88                     | 0.73              |
| 3:M:290:PHE:HB2  | 3:M:299:LEU:HD11 | 1.70                     | 0.73              |
| 1:A:176:TYR:CE1  | 4:S:143:GLU:OE2  | 2.42                     | 0.73              |
| 1:A:545:HIS:O    | 1:A:546:SER:C    | 2.15                     | 0.73              |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:HD11 | 1.71                     | 0.73              |
| 4:S:6:LEU:HD22   | 4:S:32:LEU:HD22  | 1.70                     | 0.73              |
| 4:S:55:PRO:O     | 4:S:58:LEU:HB3   | 1.88                     | 0.73              |
| 1:A:232:PRO:O    | 1:A:235:GLN:HB2  | 1.88                     | 0.72              |
| 1:A:403:LEU:C    | 2:B:3:ASP:OD2    | 2.31                     | 0.72              |
| 2:B:525:ILE:C    | 2:B:527:PRO:HD2  | 2.14                     | 0.72              |
| 3:M:243:ILE:O    | 3:M:472:TYR:HD2  | 1.71                     | 0.72              |
| 4:S:75:ILE:HG21  | 4:S:77:TYR:CZ    | 2.22                     | 0.72              |
| 1:A:121:LEU:CD1  | 1:A:155:THR:HG23 | 2.18                     | 0.72              |
| 2:B:21:GLU:CD    | 2:B:35:TYR:CG    | 2.65                     | 0.72              |
| 2:B:231:ARG:HH22 | 2:B:279:LEU:HD21 | 1.53                     | 0.72              |
| 3:M:220:GLU:CD   | 3:M:439:TYR:HD1  | 1.97                     | 0.72              |
| 3:M:338:PHE:CE2  | 3:M:415:ILE:CG1  | 2.72                     | 0.72              |
| 3:M:343:ASN:HD22 | 3:M:343:ASN:N    | 1.87                     | 0.72              |
| 4:S:53:THR:OG1   | 4:S:68:VAL:N     | 2.23                     | 0.72              |
| 1:A:638:LEU:HD12 | 2:B:520:SER:HB3  | 1.71                     | 0.72              |
| 2:B:41:ASN:ND2   | 2:B:43:ASN:OD1   | 2.22                     | 0.72              |
| 2:B:79:VAL:C     | 2:B:108:PHE:HE1  | 1.98                     | 0.72              |
| 2:B:181:TYR:C    | 2:B:183:ALA:N    | 2.46                     | 0.72              |
| 1:A:143:VAL:O    | 1:A:147:LEU:HG   | 1.89                     | 0.72              |
| 1:A:350:SER:O    | 1:A:351:ARG:C    | 2.29                     | 0.72              |
| 1:A:394:GLN:O    | 1:A:398:GLU:N    | 2.22                     | 0.72              |
| 1:A:638:LEU:HD22 | 2:B:558:TYR:HA   | 1.64                     | 0.72              |
| 2:B:63:MET:CE    | 2:B:104:TYR:HB2  | 2.19                     | 0.72              |
| 3:M:243:ILE:O    | 3:M:472:TYR:CD2  | 2.41                     | 0.72              |
| 3:M:336:ASP:OD2  | 3:M:415:ILE:HB   | 1.90                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:347:PHE:CG   | 3:M:350:VAL:HB   | 2.23                     | 0.72              |
| 3:M:374:TYR:HE2  | 3:M:393:GLY:HA2  | 1.53                     | 0.72              |
| 2:B:479:VAL:HG21 | 2:B:486:HIS:CD2  | 2.23                     | 0.72              |
| 3:M:223:HIS:CE1  | 3:M:476:THR:H    | 2.08                     | 0.72              |
| 4:S:39:ILE:HD11  | 4:S:77:TYR:CD2   | 2.24                     | 0.72              |
| 1:A:332:TYR:CZ   | 1:A:336:ILE:CD1  | 2.69                     | 0.72              |
| 1:A:332:TYR:CE2  | 1:A:336:ILE:HD11 | 2.24                     | 0.72              |
| 2:B:513:TRP:O    | 2:B:516:GLY:N    | 2.23                     | 0.72              |
| 3:M:5:PHE:O      | 3:M:17:GLN:HA    | 1.90                     | 0.72              |
| 3:M:48:ASP:HA    | 3:M:75:TRP:CZ2   | 2.25                     | 0.72              |
| 3:M:219:LEU:O    | 3:M:474:THR:HG21 | 1.89                     | 0.72              |
| 1:A:375:VAL:O    | 1:A:376:GLU:C    | 2.26                     | 0.72              |
| 2:B:20:ARG:NH1   | 2:B:35:TYR:CE1   | 2.57                     | 0.72              |
| 2:B:151:ALA:HB3  | 2:B:188:TYR:CE1  | 2.25                     | 0.72              |
| 4:S:35:VAL:CB    | 4:S:77:TYR:OH    | 2.37                     | 0.72              |
| 2:B:24:ALA:C     | 2:B:35:TYR:CD2   | 2.67                     | 0.72              |
| 2:B:239:GLN:CD   | 3:M:279:ASN:HA   | 2.13                     | 0.72              |
| 3:M:65:TYR:O     | 3:M:79:SER:HA    | 1.90                     | 0.72              |
| 3:M:224:VAL:HG22 | 3:M:306:LEU:HD12 | 1.71                     | 0.72              |
| 3:M:240:ILE:HG22 | 3:M:444:ALA:HB1  | 1.72                     | 0.72              |
| 3:M:323:MET:HE3  | 3:M:342:LEU:HD23 | 1.71                     | 0.72              |
| 4:S:136:VAL:O    | 4:S:140:MET:N    | 2.22                     | 0.72              |
| 1:A:251:TRP:CH2  | 4:S:100:ASP:N    | 2.45                     | 0.72              |
| 2:B:247:TYR:HH   | 3:M:137:SER:HB3  | 1.54                     | 0.72              |
| 2:B:341:GLU:HB2  | 2:B:377:TYR:OH   | 1.90                     | 0.72              |
| 2:B:399:LEU:HB3  | 2:B:411:ILE:CG2  | 2.20                     | 0.72              |
| 2:B:399:LEU:HB3  | 2:B:411:ILE:HG23 | 1.70                     | 0.72              |
| 3:M:306:LEU:HD22 | 3:M:317:MET:HE3  | 1.71                     | 0.72              |
| 4:S:71:GLU:C     | 4:S:73:ILE:H     | 1.98                     | 0.72              |
| 1:A:298:ILE:CD1  | 1:A:311:THR:HG21 | 2.20                     | 0.71              |
| 2:B:178:ILE:CD1  | 2:B:214:ALA:C    | 2.63                     | 0.71              |
| 2:B:374:PHE:CG   | 2:B:402:LEU:HD21 | 2.25                     | 0.71              |
| 4:S:65:ASN:O     | 4:S:67:GLU:HG3   | 1.90                     | 0.71              |
| 1:A:182:ILE:CG2  | 1:A:221:VAL:HG21 | 2.20                     | 0.71              |
| 1:A:633:PHE:CZ   | 2:B:554:LYS:HE3  | 2.24                     | 0.71              |
| 2:B:219:TYR:CG   | 2:B:226:LEU:CB   | 2.72                     | 0.71              |
| 2:B:267:ASP:C    | 2:B:276:SER:CB   | 2.63                     | 0.71              |
| 2:B:519:ALA:O    | 2:B:523:PHE:CG   | 2.43                     | 0.71              |
| 3:M:244:VAL:HG13 | 3:M:472:TYR:CE2  | 2.25                     | 0.71              |
| 1:A:263:LEU:O    | 1:A:266:VAL:N    | 2.24                     | 0.71              |
| 1:A:420:ILE:HG22 | 1:A:421:PRO:O    | 1.91                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:594:PHE:C    | 2:B:476:ARG:NH2  | 2.47                     | 0.71              |
| 1:A:633:PHE:HZ   | 2:B:550:VAL:CG1  | 2.00                     | 0.71              |
| 2:B:102:HIS:HE1  | 2:B:138:ALA:H    | 1.33                     | 0.71              |
| 2:B:519:ALA:HB1  | 2:B:555:LEU:CD1  | 2.20                     | 0.71              |
| 3:M:131:ALA:C    | 3:M:133:GLU:N    | 2.40                     | 0.71              |
| 3:M:306:LEU:CD2  | 3:M:317:MET:CE   | 2.69                     | 0.71              |
| 1:A:332:TYR:CE2  | 1:A:336:ILE:CD1  | 2.73                     | 0.71              |
| 2:B:199:LEU:C    | 2:B:201:ALA:H    | 1.95                     | 0.71              |
| 2:B:537:PHE:CZ   | 2:B:545:ARG:CG   | 2.73                     | 0.71              |
| 3:M:16:PHE:CZ    | 3:M:18:TYR:HB2   | 2.25                     | 0.71              |
| 3:M:95:THR:HG21  | 3:M:137:SER:HA   | 1.69                     | 0.71              |
| 3:M:96:ILE:O     | 3:M:100:LEU:HG   | 1.91                     | 0.71              |
| 4:S:8:PHE:CE1    | 4:S:84:TYR:HB2   | 2.25                     | 0.71              |
| 4:S:94:SER:O     | 4:S:98:ILE:HG12  | 1.90                     | 0.71              |
| 1:A:509:PRO:HB3  | 1:A:547:VAL:CG2  | 2.20                     | 0.71              |
| 2:B:20:ARG:HG3   | 2:B:21:GLU:H     | 1.55                     | 0.71              |
| 2:B:215:TYR:CD2  | 2:B:219:TYR:CE1  | 2.71                     | 0.71              |
| 2:B:436:LEU:HB3  | 2:B:450:VAL:HG13 | 1.72                     | 0.71              |
| 1:A:638:LEU:HB2  | 2:B:558:TYR:CB   | 2.15                     | 0.71              |
| 2:B:274:PRO:CG   | 2:B:295:ASN:CB   | 2.63                     | 0.71              |
| 2:B:530:LEU:CD2  | 2:B:591:MET:HB3  | 2.20                     | 0.71              |
| 3:M:310:VAL:HG13 | 3:M:315:VAL:O    | 1.91                     | 0.71              |
| 3:M:479:PHE:CD2  | 3:M:479:PHE:N    | 2.59                     | 0.71              |
| 1:A:182:ILE:HG22 | 1:A:221:VAL:CG2  | 2.21                     | 0.71              |
| 2:B:127:LEU:HD22 | 2:B:161:LEU:HD22 | 1.71                     | 0.71              |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:CD1  | 2.20                     | 0.71              |
| 2:B:429:VAL:O    | 2:B:433:VAL:HG23 | 1.90                     | 0.71              |
| 3:M:273:HIS:HB2  | 3:M:298:ARG:O    | 1.91                     | 0.71              |
| 3:M:282:VAL:N    | 3:M:283:PHE:N    | 2.38                     | 0.71              |
| 2:B:37:TYR:HD2   | 2:B:38:TYR:HD1   | 1.37                     | 0.71              |
| 3:M:67:SER:O     | 3:M:77:LEU:HA    | 1.91                     | 0.71              |
| 3:M:233:LEU:HD22 | 3:M:324:SER:HA   | 1.73                     | 0.71              |
| 3:M:379:LEU:CA   | 3:M:412:ARG:O    | 2.33                     | 0.71              |
| 4:S:8:PHE:CE1    | 4:S:84:TYR:HB3   | 2.26                     | 0.71              |
| 4:S:75:ILE:HG21  | 4:S:77:TYR:OH    | 1.91                     | 0.71              |
| 1:A:555:LEU:CD1  | 1:A:581:LEU:HD11 | 2.21                     | 0.71              |
| 2:B:25:VAL:CG1   | 2:B:33:SER:HA    | 2.21                     | 0.71              |
| 2:B:30:LEU:HD12  | 2:B:30:LEU:O     | 1.91                     | 0.71              |
| 2:B:549:LEU:CD1  | 2:B:611:ALA:CA   | 2.67                     | 0.71              |
| 1:A:137:ASN:C    | 1:A:139:ASP:N    | 2.43                     | 0.71              |
| 1:A:266:VAL:O    | 1:A:267:GLU:HB3  | 1.89                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:602:GLU:OE2  | 1:A:633:PHE:CE1  | 2.44                     | 0.71              |
| 1:A:625:LEU:O    | 1:A:626:SER:C    | 2.26                     | 0.71              |
| 2:B:259:TYR:HD2  | 2:B:261:PRO:CG   | 2.00                     | 0.71              |
| 2:B:387:ASP:HB3  | 2:B:391:ALA:CB   | 2.21                     | 0.71              |
| 3:M:224:VAL:HG11 | 3:M:226:PHE:CZ   | 2.26                     | 0.71              |
| 3:M:350:VAL:HA   | 3:M:442:GLN:HB2  | 1.71                     | 0.71              |
| 1:A:179:LYS:HB2  | 4:S:142:ILE:HD12 | 1.71                     | 0.70              |
| 1:A:222:ILE:HD12 | 1:A:240:LEU:HD21 | 1.72                     | 0.70              |
| 1:A:277:LYS:HG3  | 1:A:277:LYS:O    | 1.91                     | 0.70              |
| 1:A:461:CYS:O    | 1:A:462:GLN:O    | 2.09                     | 0.70              |
| 2:B:151:ALA:HB1  | 2:B:188:TYR:CE1  | 2.26                     | 0.70              |
| 2:B:302:PHE:CE2  | 2:B:328:LEU:HD11 | 2.26                     | 0.70              |
| 2:B:550:VAL:CG2  | 2:B:610:ARG:HD3  | 2.21                     | 0.70              |
| 3:M:376:ILE:CG2  | 3:M:379:LEU:CD1  | 2.69                     | 0.70              |
| 4:S:38:LEU:HG    | 4:S:68:VAL:HG23  | 1.72                     | 0.70              |
| 4:S:55:PRO:O     | 4:S:58:LEU:CB    | 2.39                     | 0.70              |
| 1:A:275:LEU:HD13 | 1:A:308:ASP:OD1  | 1.90                     | 0.70              |
| 1:A:450:TYR:HH   | 1:A:476:GLN:HG2  | 1.56                     | 0.70              |
| 1:A:555:LEU:HD13 | 1:A:581:LEU:HD11 | 1.72                     | 0.70              |
| 2:B:24:ALA:HB1   | 2:B:35:TYR:CE1   | 1.94                     | 0.70              |
| 2:B:245:GLN:CD   | 2:B:309:LEU:HD13 | 2.11                     | 0.70              |
| 2:B:508:ARG:HB2  | 2:B:544:THR:HG23 | 1.72                     | 0.70              |
| 3:M:405:THR:O    | 3:M:405:THR:HG22 | 1.92                     | 0.70              |
| 4:S:87:PHE:CE1   | 4:S:102:ILE:HG12 | 2.26                     | 0.70              |
| 1:A:64:LEU:HG    | 1:A:102:GLN:HE22 | 1.53                     | 0.70              |
| 1:A:206:LYS:HE2  | 1:A:206:LYS:HA   | 1.73                     | 0.70              |
| 1:A:279:LEU:O    | 1:A:280:GLU:C    | 2.23                     | 0.70              |
| 2:B:267:ASP:H    | 2:B:289:PRO:HG3  | 1.56                     | 0.70              |
| 2:B:347:VAL:HA   | 2:B:359:LEU:HG   | 1.73                     | 0.70              |
| 2:B:497:LEU:CD2  | 2:B:533:LEU:CD2  | 2.69                     | 0.70              |
| 2:B:515:PHE:O    | 2:B:516:GLY:C    | 2.26                     | 0.70              |
| 3:M:78:ALA:CB    | 3:M:89:CYS:SG    | 2.80                     | 0.70              |
| 1:A:179:LYS:CB   | 4:S:142:ILE:HB   | 2.16                     | 0.70              |
| 1:A:264:SER:HB3  | 1:A:271:ARG:HG2  | 1.73                     | 0.70              |
| 2:B:83:PHE:CE2   | 2:B:119:SER:CB   | 2.68                     | 0.70              |
| 2:B:219:TYR:HE1  | 2:B:226:LEU:CD1  | 1.73                     | 0.70              |
| 2:B:477:MET:O    | 2:B:480:GLN:HB2  | 1.92                     | 0.70              |
| 3:M:272:LEU:HD22 | 3:M:278:ILE:HB   | 1.72                     | 0.70              |
| 3:M:436:GLU:HA   | 3:M:479:PHE:CE2  | 2.26                     | 0.70              |
| 1:A:537:THR:HB   | 1:A:584:PHE:CE1  | 2.26                     | 0.70              |
| 1:A:628:VAL:O    | 1:A:631:SER:OG   | 2.05                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:63:MET:HG2   | 2:B:100:LEU:HB2  | 1.73                     | 0.70              |
| 2:B:143:SER:HB2  | 2:B:179:LYS:CD   | 2.18                     | 0.70              |
| 2:B:325:LEU:HD13 | 2:B:339:PHE:CD2  | 2.25                     | 0.70              |
| 2:B:390:VAL:O    | 2:B:393:ILE:HB   | 1.91                     | 0.70              |
| 2:B:592:TYR:CD2  | 2:B:618:PHE:CD2  | 2.80                     | 0.70              |
| 2:B:613:MET:HE2  | 2:B:617:LEU:HD11 | 1.74                     | 0.70              |
| 3:M:136:VAL:C    | 3:M:138:ASP:H    | 1.96                     | 0.70              |
| 3:M:242:GLY:HA3  | 3:M:444:ALA:CB   | 2.22                     | 0.70              |
| 3:M:344:ILE:HG23 | 3:M:347:PHE:HB2  | 1.73                     | 0.70              |
| 1:A:176:TYR:HE1  | 4:S:148:ARG:HH21 | 1.36                     | 0.70              |
| 2:B:63:MET:HG2   | 2:B:100:LEU:CB   | 2.22                     | 0.70              |
| 2:B:86:VAL:HG13  | 2:B:101:ILE:HG12 | 1.72                     | 0.70              |
| 2:B:316:THR:CG2  | 3:M:90:PHE:HD2   | 1.98                     | 0.70              |
| 2:B:494:ALA:HB2  | 2:B:515:PHE:CZ   | 2.27                     | 0.70              |
| 2:B:545:ARG:CD   | 2:B:602:ASP:CG   | 2.64                     | 0.70              |
| 2:B:6:HIS:CG     | 3:M:25:PRO:C     | 2.46                     | 0.70              |
| 2:B:25:VAL:HG11  | 2:B:36:THR:HB    | 1.74                     | 0.70              |
| 2:B:267:ASP:N    | 2:B:289:PRO:HG3  | 2.07                     | 0.70              |
| 2:B:531:ARG:CA   | 2:B:591:MET:SD   | 2.79                     | 0.70              |
| 2:B:592:TYR:CD2  | 2:B:618:PHE:CE2  | 2.80                     | 0.70              |
| 1:A:186:PHE:CD1  | 1:A:224:GLU:CB   | 2.73                     | 0.70              |
| 1:A:196:LEU:HD22 | 1:A:196:LEU:C    | 2.15                     | 0.70              |
| 1:A:326:GLN:HA   | 1:A:331:ARG:NH2  | 2.05                     | 0.70              |
| 2:B:243:TRP:HZ2  | 3:M:98:ARG:HG3   | 1.56                     | 0.70              |
| 2:B:310:ILE:O    | 2:B:311:TYR:C    | 2.25                     | 0.70              |
| 2:B:513:TRP:CA   | 2:B:551:LEU:HD22 | 2.13                     | 0.70              |
| 2:B:588:ILE:HG23 | 2:B:618:PHE:CE1  | 2.27                     | 0.70              |
| 2:B:212:VAL:C    | 2:B:214:ALA:H    | 1.99                     | 0.70              |
| 2:B:343:LEU:HD21 | 2:B:362:ALA:HB3  | 1.74                     | 0.70              |
| 1:A:103:LYS:O    | 1:A:104:ARG:C    | 2.24                     | 0.70              |
| 1:A:469:LEU:O    | 1:A:470:GLY:C    | 2.28                     | 0.70              |
| 2:B:108:PHE:O    | 2:B:109:ALA:C    | 2.18                     | 0.70              |
| 2:B:162:VAL:HB   | 2:B:195:ILE:HG23 | 1.70                     | 0.70              |
| 2:B:167:ALA:C    | 2:B:207:VAL:HG21 | 2.17                     | 0.70              |
| 3:M:12:ASN:OD1   | 3:M:45:SER:OG    | 2.09                     | 0.70              |
| 3:M:242:GLY:CA   | 3:M:444:ALA:CB   | 2.69                     | 0.70              |
| 3:M:257:ALA:HB3  | 3:M:453:ASP:OD1  | 1.92                     | 0.70              |
| 1:A:421:PRO:HG2  | 1:A:424:TYR:CE1  | 2.26                     | 0.69              |
| 1:A:531:ASP:C    | 1:A:534:LYS:O    | 2.35                     | 0.69              |
| 2:B:267:ASP:C    | 2:B:276:SER:HB2  | 2.16                     | 0.69              |
| 2:B:340:ILE:HG12 | 2:B:373:LEU:CD2  | 2.21                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:508:ARG:CB   | 2:B:544:THR:HG23 | 2.22                     | 0.69              |
| 4:S:1:MET:N      | 4:S:93:GLU:CD    | 2.49                     | 0.69              |
| 1:A:395:PHE:CE1  | 1:A:428:MET:HG3  | 2.27                     | 0.69              |
| 2:B:90:ILE:O     | 2:B:98:LYS:CE    | 2.39                     | 0.69              |
| 2:B:223:LEU:CB   | 2:B:259:TYR:HD1  | 1.54                     | 0.69              |
| 2:B:243:TRP:HE1  | 3:M:98:ARG:HD3   | 1.52                     | 0.69              |
| 2:B:371:GLN:CG   | 2:B:401:THR:O    | 2.40                     | 0.69              |
| 2:B:400:SER:HA   | 2:B:439:CYS:SG   | 2.31                     | 0.69              |
| 2:B:418:TYR:CD1  | 2:B:419:VAL:N    | 2.60                     | 0.69              |
| 2:B:487:LEU:HD21 | 2:B:522:GLU:CB   | 2.22                     | 0.69              |
| 2:B:508:ARG:HB2  | 2:B:544:THR:CG2  | 2.22                     | 0.69              |
| 3:M:214:LEU:O    | 3:M:467:TYR:N    | 2.20                     | 0.69              |
| 3:M:247:ARG:N    | 3:M:470:ALA:HB2  | 2.06                     | 0.69              |
| 3:M:55:MET:O     | 3:M:56:VAL:C     | 2.19                     | 0.69              |
| 3:M:96:ILE:HD12  | 3:M:125:PHE:CD1  | 2.27                     | 0.69              |
| 4:S:53:THR:OG1   | 4:S:68:VAL:C     | 2.35                     | 0.69              |
| 4:S:130:SER:OG   | 4:S:156:LEU:HD12 | 1.92                     | 0.69              |
| 4:S:135:ILE:HG22 | 4:S:141:VAL:HG22 | 1.72                     | 0.69              |
| 1:A:408:ILE:HG21 | 4:S:64:ASN:C     | 2.13                     | 0.69              |
| 2:B:20:ARG:HG3   | 2:B:21:GLU:N     | 2.06                     | 0.69              |
| 2:B:25:VAL:CG2   | 2:B:35:TYR:HD2   | 1.99                     | 0.69              |
| 2:B:132:SER:CA   | 2:B:169:VAL:CG2  | 2.69                     | 0.69              |
| 2:B:534:ILE:HG12 | 2:B:595:VAL:HG22 | 1.75                     | 0.69              |
| 3:M:114:ILE:O    | 3:M:118:TYR:N    | 2.26                     | 0.69              |
| 3:M:128:CYS:O    | 3:M:134:PRO:HA   | 1.92                     | 0.69              |
| 3:M:472:TYR:CD1  | 3:M:472:TYR:N    | 2.58                     | 0.69              |
| 2:B:178:ILE:HD13 | 2:B:218:CYS:CB   | 2.21                     | 0.69              |
| 3:M:276:VAL:HG22 | 3:M:290:PHE:HD1  | 1.56                     | 0.69              |
| 3:M:290:PHE:HB2  | 3:M:299:LEU:CD1  | 2.21                     | 0.69              |
| 3:M:437:TYR:N    | 3:M:437:TYR:HD1  | 1.91                     | 0.69              |
| 1:A:88:ASN:CB    | 1:A:120:ILE:CG2  | 2.67                     | 0.69              |
| 1:A:260:PHE:CE1  | 1:A:274:LEU:HD11 | 2.27                     | 0.69              |
| 2:B:599:ALA:C    | 2:B:601:TYR:N    | 2.44                     | 0.69              |
| 3:M:15:ILE:HG22  | 3:M:114:ILE:HG22 | 1.75                     | 0.69              |
| 1:A:101:GLN:NE2  | 4:S:167:ILE:HD12 | 2.06                     | 0.69              |
| 1:A:244:LEU:HD23 | 1:A:277:LYS:O    | 1.92                     | 0.69              |
| 2:B:374:PHE:HE1  | 2:B:381:PHE:CE1  | 2.10                     | 0.69              |
| 2:B:494:ALA:N    | 2:B:515:PHE:HZ   | 1.90                     | 0.69              |
| 3:M:219:LEU:HG   | 3:M:439:TYR:O    | 1.93                     | 0.69              |
| 3:M:242:GLY:O    | 3:M:301:GLU:HA   | 1.92                     | 0.69              |
| 3:M:265:ASN:OD1  | 3:M:313:SER:HB3  | 1.91                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:94:VAL:O     | 1:A:95:MET:C     | 2.26                     | 0.69              |
| 1:A:103:LYS:HB3  | 1:A:107:TYR:CE1  | 2.28                     | 0.69              |
| 1:A:638:LEU:HD12 | 2:B:520:SER:H    | 1.53                     | 0.69              |
| 2:B:41:ASN:CG    | 2:B:43:ASN:OD1   | 2.36                     | 0.69              |
| 2:B:83:PHE:HE2   | 2:B:119:SER:HB3  | 1.54                     | 0.69              |
| 2:B:178:ILE:C    | 2:B:180:LEU:H    | 2.00                     | 0.69              |
| 2:B:241:ASP:CB   | 3:M:274:ASP:CG   | 2.47                     | 0.69              |
| 2:B:243:TRP:HH2  | 3:M:94:GLU:CB    | 1.85                     | 0.69              |
| 2:B:351:GLU:OE2  | 3:M:476:THR:C    | 2.35                     | 0.69              |
| 2:B:389:ILE:O    | 2:B:390:VAL:C    | 2.23                     | 0.69              |
| 2:B:553:ALA:CB   | 2:B:614:ILE:CG1  | 2.67                     | 0.69              |
| 3:M:74:TYR:HB3   | 3:M:114:ILE:HD11 | 1.74                     | 0.69              |
| 1:A:634:ASN:ND2  | 2:B:554:LYS:HA   | 2.08                     | 0.69              |
| 2:B:25:VAL:CG2   | 2:B:35:TYR:C     | 2.49                     | 0.69              |
| 2:B:136:CYS:CA   | 2:B:172:GLU:HG3  | 2.22                     | 0.69              |
| 2:B:193:LEU:HD11 | 2:B:225:LEU:HD23 | 1.75                     | 0.69              |
| 2:B:458:MET:O    | 2:B:460:SER:N    | 2.25                     | 0.69              |
| 3:M:121:ILE:CG2  | 3:M:125:PHE:CE1  | 2.76                     | 0.69              |
| 4:S:35:VAL:CG1   | 4:S:75:ILE:HD13  | 2.21                     | 0.69              |
| 4:S:112:CYS:HB2  | 4:S:113:PHE:CD1  | 2.26                     | 0.69              |
| 1:A:200:PHE:CE1  | 1:A:236:LEU:CG   | 2.76                     | 0.69              |
| 1:A:236:LEU:C    | 1:A:238:PRO:HD2  | 2.18                     | 0.69              |
| 2:B:139:LEU:HD11 | 2:B:176:ALA:HB1  | 1.73                     | 0.69              |
| 2:B:374:PHE:HD2  | 2:B:402:LEU:HD22 | 1.54                     | 0.69              |
| 2:B:515:PHE:CE2  | 2:B:529:VAL:HG21 | 2.27                     | 0.69              |
| 3:M:454:ILE:HD13 | 3:M:464:THR:HG21 | 1.75                     | 0.69              |
| 1:A:156:PRO:CB   | 1:A:192:TYR:CE1  | 2.71                     | 0.68              |
| 2:B:38:TYR:CA    | 2:B:42:ILE:N     | 2.47                     | 0.68              |
| 2:B:103:LEU:HD21 | 3:M:131:ALA:HA   | 1.74                     | 0.68              |
| 3:M:44:ASP:O     | 3:M:46:SER:N     | 2.26                     | 0.68              |
| 3:M:224:VAL:H    | 3:M:479:PHE:HA   | 1.58                     | 0.68              |
| 1:A:92:LEU:O     | 1:A:127:LEU:CD2  | 2.42                     | 0.68              |
| 1:A:369:SER:HB2  | 1:A:424:TYR:CZ   | 2.28                     | 0.68              |
| 2:B:328:LEU:HB3  | 2:B:333:GLN:HE22 | 1.58                     | 0.68              |
| 3:M:222:PHE:O    | 3:M:479:PHE:HE2  | 1.71                     | 0.68              |
| 1:A:258:LYS:HZ3  | 4:S:94:SER:N     | 1.90                     | 0.68              |
| 1:A:342:GLY:O    | 1:A:343:LYS:C    | 2.34                     | 0.68              |
| 2:B:468:LEU:O    | 2:B:472:VAL:HG23 | 1.94                     | 0.68              |
| 2:B:537:PHE:CD2  | 2:B:537:PHE:C    | 2.71                     | 0.68              |
| 2:B:566:ALA:CA   | 2:B:574:ASN:HB3  | 2.20                     | 0.68              |
| 3:M:356:LEU:C    | 3:M:356:LEU:HD23 | 2.19                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:443:SER:HB3  | 3:M:447:ILE:N    | 2.08                     | 0.68              |
| 4:S:53:THR:CG2   | 4:S:68:VAL:HA    | 2.20                     | 0.68              |
| 1:A:104:ARG:HA   | 1:A:145:ILE:HG21 | 1.74                     | 0.68              |
| 1:A:399:ASP:H    | 1:A:418:ILE:HD11 | 1.57                     | 0.68              |
| 1:A:556:VAL:CG2  | 1:A:603:VAL:CG1  | 2.72                     | 0.68              |
| 2:B:508:ARG:O    | 2:B:509:ALA:C    | 2.30                     | 0.68              |
| 3:M:245:ASP:CA   | 3:M:472:TYR:CE1  | 2.76                     | 0.68              |
| 3:M:306:LEU:HD13 | 3:M:317:MET:HE3  | 1.75                     | 0.68              |
| 3:M:360:LEU:CD2  | 3:M:362:PHE:CE2  | 2.76                     | 0.68              |
| 4:S:47:GLN:O     | 4:S:48:SER:C     | 2.30                     | 0.68              |
| 1:A:176:TYR:CG   | 4:S:143:GLU:OE2  | 2.47                     | 0.68              |
| 1:A:404:GLN:CB   | 2:B:7:ARG:HH21   | 2.05                     | 0.68              |
| 1:A:605:GLU:CG   | 1:A:632:PHE:CD2  | 2.73                     | 0.68              |
| 2:B:196:LEU:C    | 2:B:215:TYR:OH   | 2.35                     | 0.68              |
| 2:B:542:PRO:O    | 2:B:607:ILE:HD13 | 1.93                     | 0.68              |
| 2:B:546:CYS:HA   | 2:B:607:ILE:CG2  | 2.24                     | 0.68              |
| 2:B:566:ALA:C    | 2:B:574:ASN:HB3  | 2.16                     | 0.68              |
| 2:B:589:SER:HA   | 2:B:592:TYR:HD2  | 1.58                     | 0.68              |
| 4:S:70:ASN:O     | 4:S:71:GLU:C     | 2.30                     | 0.68              |
| 4:S:71:GLU:C     | 4:S:73:ILE:N     | 2.50                     | 0.68              |
| 1:A:67:LYS:O     | 1:A:71:VAL:HG23  | 1.94                     | 0.68              |
| 1:A:585:PHE:CE2  | 1:A:607:LEU:HD11 | 2.28                     | 0.68              |
| 2:B:144:ASP:HA   | 2:B:179:LYS:HD3  | 1.74                     | 0.68              |
| 2:B:158:VAL:HG13 | 2:B:177:ILE:HG13 | 1.73                     | 0.68              |
| 2:B:230:PHE:HD2  | 2:B:298:ASP:HB3  | 1.59                     | 0.68              |
| 2:B:418:TYR:O    | 2:B:419:VAL:O    | 2.11                     | 0.68              |
| 2:B:451:MET:HG3  | 2:B:489:ILE:HG12 | 1.74                     | 0.68              |
| 2:B:588:ILE:CG2  | 2:B:618:PHE:CE1  | 2.76                     | 0.68              |
| 1:A:88:ASN:HD22  | 1:A:120:ILE:HG13 | 1.58                     | 0.68              |
| 1:A:253:ILE:HD12 | 1:A:285:THR:HG21 | 1.75                     | 0.68              |
| 2:B:136:CYS:CB   | 2:B:172:GLU:HG3  | 2.24                     | 0.68              |
| 2:B:219:TYR:O    | 2:B:223:LEU:CD2  | 2.41                     | 0.68              |
| 1:A:128:LEU:HD13 | 1:A:150:LEU:CG   | 2.24                     | 0.68              |
| 2:B:563:PHE:C    | 2:B:566:ALA:HB3  | 2.17                     | 0.68              |
| 1:A:480:LEU:C    | 1:A:480:LEU:HD13 | 2.18                     | 0.68              |
| 2:B:16:LYS:CD    | 3:M:118:TYR:CE2  | 2.50                     | 0.68              |
| 2:B:178:ILE:O    | 2:B:180:LEU:N    | 2.27                     | 0.68              |
| 2:B:534:ILE:HG12 | 2:B:595:VAL:CG2  | 2.24                     | 0.68              |
| 1:A:240:LEU:O    | 1:A:242:GLU:O    | 2.11                     | 0.68              |
| 2:B:215:TYR:HE2  | 2:B:229:HIS:HD1  | 1.41                     | 0.68              |
| 2:B:537:PHE:CE1  | 2:B:545:ARG:CG   | 2.77                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:217:ASP:CG   | 3:M:471:LYS:HA   | 2.19                     | 0.68              |
| 1:A:114:PHE:CE1  | 1:A:154:ILE:HG12 | 2.29                     | 0.67              |
| 1:A:237:SER:N    | 1:A:238:PRO:HD2  | 2.09                     | 0.67              |
| 1:A:506:LYS:O    | 1:A:507:GLN:HB2  | 1.94                     | 0.67              |
| 2:B:30:LEU:HD12  | 2:B:30:LEU:C     | 2.18                     | 0.67              |
| 2:B:181:TYR:HE1  | 2:B:222:HIS:CD2  | 2.08                     | 0.67              |
| 2:B:212:VAL:CG1  | 2:B:248:LEU:HD23 | 2.24                     | 0.67              |
| 2:B:501:THR:CA   | 2:B:508:ARG:HH22 | 2.03                     | 0.67              |
| 3:M:212:ASN:O    | 3:M:465:LYS:HB2  | 1.93                     | 0.67              |
| 3:M:302:TYR:HE2  | 3:M:304:VAL:HB   | 1.59                     | 0.67              |
| 4:S:1:MET:H2     | 4:S:93:GLU:CB    | 2.07                     | 0.67              |
| 4:S:75:ILE:CG2   | 4:S:77:TYR:CZ    | 2.77                     | 0.67              |
| 1:A:102:GLN:HE22 | 4:S:166:LYS:CE   | 2.07                     | 0.67              |
| 1:A:333:ILE:O    | 1:A:337:LEU:HG   | 1.95                     | 0.67              |
| 1:A:384:LEU:HG   | 1:A:385:LYS:H    | 1.60                     | 0.67              |
| 1:A:599:ARG:HH11 | 2:B:513:TRP:HZ3  | 1.34                     | 0.67              |
| 2:B:171:GLY:HA2  | 2:B:207:VAL:HG13 | 1.75                     | 0.67              |
| 2:B:226:LEU:HD21 | 2:B:255:TYR:CD1  | 2.25                     | 0.67              |
| 2:B:412:PHE:HE2  | 2:B:446:TRP:HB3  | 1.60                     | 0.67              |
| 2:B:500:GLN:CD   | 2:B:503:LEU:HD21 | 2.19                     | 0.67              |
| 2:B:530:LEU:CG   | 2:B:591:MET:HB3  | 2.24                     | 0.67              |
| 2:B:578:PRO:CD   | 2:B:581:TYR:CE1  | 2.72                     | 0.67              |
| 1:A:103:LYS:O    | 1:A:107:TYR:CD1  | 2.48                     | 0.67              |
| 1:A:323:CYS:SG   | 1:A:334:SER:HB2  | 2.34                     | 0.67              |
| 2:B:77:ILE:CG2   | 2:B:82:TYR:CE1   | 2.78                     | 0.67              |
| 2:B:167:ALA:HA   | 2:B:202:ASP:CG   | 2.17                     | 0.67              |
| 2:B:239:GLN:CD   | 3:M:279:ASN:O    | 2.37                     | 0.67              |
| 3:M:253:ASN:OD1  | 3:M:292:PRO:HG2  | 1.94                     | 0.67              |
| 4:S:17:VAL:HG22  | 4:S:19:PHE:CZ    | 2.28                     | 0.67              |
| 1:A:95:MET:SD    | 1:A:107:TYR:HD2  | 2.15                     | 0.67              |
| 1:A:185:LEU:CB   | 1:A:203:PHE:HE1  | 2.07                     | 0.67              |
| 1:A:585:PHE:CE2  | 1:A:603:VAL:HG12 | 2.30                     | 0.67              |
| 2:B:176:ALA:O    | 2:B:178:ILE:N    | 2.28                     | 0.67              |
| 2:B:252:LEU:HD12 | 2:B:302:PHE:HE1  | 1.58                     | 0.67              |
| 2:B:278:PRO:CA   | 2:B:288:TYR:O    | 2.40                     | 0.67              |
| 3:M:215:TYR:CD1  | 3:M:468:LYS:HA   | 2.28                     | 0.67              |
| 4:S:2:ILE:HG12   | 4:S:98:ILE:HD12  | 1.76                     | 0.67              |
| 1:A:216:SER:CB   | 1:A:252:ILE:HG12 | 2.25                     | 0.67              |
| 2:B:87:VAL:CG1   | 2:B:122:SER:CB   | 2.52                     | 0.67              |
| 2:B:158:VAL:CG1  | 2:B:177:ILE:HD11 | 2.25                     | 0.67              |
| 2:B:337:THR:N    | 2:B:373:LEU:CD2  | 2.56                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:398:ILE:O    | 2:B:401:THR:N    | 2.21                     | 0.67              |
| 3:M:241:HIS:O    | 3:M:474:THR:HB   | 1.94                     | 0.67              |
| 1:A:166:LEU:O    | 1:A:170:LEU:CD2  | 2.42                     | 0.67              |
| 2:B:79:VAL:CB    | 2:B:108:PHE:CE1  | 2.78                     | 0.67              |
| 2:B:243:TRP:CZ3  | 3:M:94:GLU:CG    | 2.73                     | 0.67              |
| 1:A:332:TYR:CE1  | 1:A:366:SER:CB   | 2.77                     | 0.67              |
| 2:B:311:TYR:O    | 2:B:312:SER:C    | 2.37                     | 0.67              |
| 2:B:353:GLN:OE1  | 3:M:50:TYR:HB2   | 1.94                     | 0.67              |
| 2:B:537:PHE:CE1  | 2:B:545:ARG:HB3  | 2.29                     | 0.67              |
| 3:M:219:LEU:HD22 | 3:M:473:LYS:CA   | 2.24                     | 0.67              |
| 1:A:634:ASN:HB3  | 2:B:558:TYR:N    | 2.10                     | 0.67              |
| 2:B:70:MET:SD    | 2:B:107:ARG:HB2  | 2.34                     | 0.67              |
| 2:B:154:ILE:O    | 2:B:158:VAL:HG23 | 1.95                     | 0.67              |
| 1:A:225:LEU:HB3  | 1:A:233:PHE:HE1  | 1.58                     | 0.67              |
| 1:A:581:LEU:CD2  | 1:A:607:LEU:CD1  | 2.69                     | 0.67              |
| 2:B:261:PRO:HD3  | 2:B:293:VAL:CG2  | 2.23                     | 0.67              |
| 2:B:549:LEU:HG   | 2:B:614:ILE:HD12 | 1.77                     | 0.67              |
| 3:M:78:ALA:HB1   | 3:M:89:CYS:SG    | 2.35                     | 0.67              |
| 3:M:428:VAL:O    | 3:M:430:LEU:N    | 2.27                     | 0.67              |
| 4:S:93:GLU:CG    | 4:S:98:ILE:HD11  | 2.25                     | 0.67              |
| 1:A:151:SER:HB2  | 1:A:187:LYS:CB   | 2.19                     | 0.67              |
| 2:B:78:ASP:OD2   | 2:B:81:LEU:HG    | 1.94                     | 0.67              |
| 2:B:303:LEU:HD11 | 2:B:333:GLN:CG   | 2.24                     | 0.67              |
| 2:B:501:THR:HA   | 2:B:508:ARG:NH2  | 2.06                     | 0.67              |
| 2:B:553:ALA:HA   | 2:B:614:ILE:CG2  | 2.25                     | 0.67              |
| 2:B:597:TYR:O    | 2:B:601:TYR:CE1  | 2.48                     | 0.67              |
| 3:M:99:ILE:CG2   | 3:M:124:ILE:HG21 | 2.25                     | 0.67              |
| 1:A:153:ILE:HB   | 1:A:158:LEU:CD2  | 2.25                     | 0.66              |
| 1:A:249:ASN:HB3  | 1:A:252:ILE:HD12 | 1.77                     | 0.66              |
| 1:A:465:SER:N    | 2:B:1:MET:HE1    | 2.10                     | 0.66              |
| 2:B:279:LEU:HG   | 2:B:288:TYR:CD1  | 2.29                     | 0.66              |
| 2:B:592:TYR:OH   | 2:B:619:ASP:OD1  | 2.13                     | 0.66              |
| 3:M:421:GLY:O    | 3:M:422:PRO:C    | 2.22                     | 0.66              |
| 3:M:442:GLN:HG3  | 3:M:443:SER:H    | 1.59                     | 0.66              |
| 1:A:64:LEU:HG    | 1:A:102:GLN:NE2  | 2.06                     | 0.66              |
| 2:B:93:ASN:HA    | 2:B:134:LEU:HD11 | 1.76                     | 0.66              |
| 2:B:116:THR:CG2  | 2:B:150:LEU:HD11 | 2.26                     | 0.66              |
| 2:B:141:ALA:O    | 2:B:142:LEU:C    | 2.35                     | 0.66              |
| 2:B:310:ILE:HG22 | 2:B:342:ALA:HB1  | 1.75                     | 0.66              |
| 2:B:311:TYR:CE2  | 2:B:342:ALA:HB2  | 2.29                     | 0.66              |
| 2:B:580:TYR:HB3  | 2:B:582:ASP:OD1  | 1.96                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:104:PHE:HD1  | 3:M:104:PHE:H    | 1.43                     | 0.66              |
| 4:S:57:LEU:O     | 4:S:67:GLU:O     | 2.12                     | 0.66              |
| 1:A:465:SER:N    | 2:B:1:MET:CE     | 2.58                     | 0.66              |
| 2:B:309:LEU:CB   | 2:B:317:VAL:HG11 | 2.23                     | 0.66              |
| 3:M:278:ILE:HG23 | 3:M:278:ILE:O    | 1.94                     | 0.66              |
| 1:A:107:TYR:CE2  | 1:A:128:LEU:HD23 | 2.31                     | 0.66              |
| 2:B:116:THR:HG22 | 2:B:150:LEU:HD11 | 1.78                     | 0.66              |
| 2:B:123:LEU:HD22 | 2:B:138:ALA:O    | 1.96                     | 0.66              |
| 2:B:274:PRO:CG   | 2:B:295:ASN:HB3  | 2.26                     | 0.66              |
| 2:B:490:ILE:HG22 | 2:B:515:PHE:CE2  | 2.30                     | 0.66              |
| 3:M:323:MET:SD   | 3:M:342:LEU:CB   | 2.84                     | 0.66              |
| 4:S:54:PRO:CD    | 4:S:57:LEU:HB2   | 2.24                     | 0.66              |
| 4:S:64:ASN:C     | 4:S:66:ASP:N     | 2.47                     | 0.66              |
| 1:A:216:SER:O    | 1:A:219:VAL:HB   | 1.96                     | 0.66              |
| 1:A:465:SER:N    | 2:B:1:MET:SD     | 2.68                     | 0.66              |
| 2:B:42:ILE:O     | 2:B:43:ASN:CB    | 2.42                     | 0.66              |
| 2:B:77:ILE:HG22  | 2:B:82:TYR:CE1   | 2.31                     | 0.66              |
| 2:B:216:LYS:CA   | 2:B:251:LEU:HD11 | 2.10                     | 0.66              |
| 2:B:285:GLU:C    | 2:B:286:ILE:O    | 2.21                     | 0.66              |
| 2:B:340:ILE:CG1  | 2:B:373:LEU:CD2  | 2.73                     | 0.66              |
| 2:B:353:GLN:HG2  | 3:M:50:TYR:CE1   | 2.30                     | 0.66              |
| 2:B:451:MET:CG   | 2:B:489:ILE:HG12 | 2.25                     | 0.66              |
| 2:B:483:PRO:HA   | 2:B:486:HIS:HB2  | 1.76                     | 0.66              |
| 2:B:546:CYS:SG   | 2:B:607:ILE:HG12 | 2.35                     | 0.66              |
| 3:M:262:THR:CG2  | 3:M:265:ASN:H    | 2.08                     | 0.66              |
| 1:A:426:ILE:HD13 | 1:A:466:ASP:OD2  | 1.96                     | 0.66              |
| 1:A:461:CYS:C    | 1:A:463:ASP:N    | 2.46                     | 0.66              |
| 2:B:102:HIS:ND1  | 2:B:137:PHE:HB3  | 2.11                     | 0.66              |
| 2:B:108:PHE:CE2  | 2:B:115:LEU:HG   | 2.30                     | 0.66              |
| 2:B:133:GLU:CA   | 2:B:168:MET:SD   | 2.82                     | 0.66              |
| 2:B:374:PHE:HB3  | 2:B:402:LEU:HD21 | 1.73                     | 0.66              |
| 2:B:378:THR:HG23 | 2:B:379:LYS:N    | 2.10                     | 0.66              |
| 2:B:418:TYR:CD1  | 2:B:419:VAL:HA   | 2.31                     | 0.66              |
| 2:B:490:ILE:CG2  | 2:B:515:PHE:CE2  | 2.78                     | 0.66              |
| 3:M:45:SER:CA    | 3:M:47:SER:N     | 2.59                     | 0.66              |
| 3:M:66:PHE:HB3   | 3:M:77:LEU:HD11  | 1.77                     | 0.66              |
| 2:B:232:ARG:HG3  | 2:B:236:ILE:CD1  | 2.25                     | 0.66              |
| 2:B:277:CYS:HA   | 2:B:292:GLU:HA   | 1.76                     | 0.66              |
| 2:B:343:LEU:CD2  | 2:B:366:LEU:HD12 | 2.25                     | 0.66              |
| 2:B:540:GLU:OE1  | 2:B:548:ILE:CD1  | 2.44                     | 0.66              |
| 2:B:559:ASP:O    | 2:B:562:ASN:C    | 2.38                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:271:SER:HB3  | 3:M:301:GLU:CG   | 2.25                     | 0.66              |
| 4:S:109:LEU:O    | 4:S:110:ASP:C    | 2.20                     | 0.66              |
| 1:A:153:ILE:HB   | 1:A:158:LEU:HD21 | 1.78                     | 0.66              |
| 1:A:185:LEU:CB   | 1:A:203:PHE:CE1  | 2.78                     | 0.66              |
| 2:B:169:VAL:O    | 2:B:173:VAL:HG23 | 1.96                     | 0.66              |
| 2:B:189:HIS:NE2  | 2:B:222:HIS:HB3  | 2.10                     | 0.66              |
| 2:B:216:LYS:HG3  | 2:B:251:LEU:CD1  | 2.25                     | 0.66              |
| 2:B:230:PHE:CD2  | 2:B:298:ASP:CB   | 2.77                     | 0.66              |
| 2:B:241:ASP:HB2  | 3:M:274:ASP:CB   | 2.26                     | 0.66              |
| 2:B:268:LYS:O    | 2:B:273:SER:HB3  | 1.95                     | 0.66              |
| 2:B:336:ASN:C    | 2:B:373:LEU:HD21 | 2.20                     | 0.66              |
| 2:B:375:LEU:O    | 2:B:376:PRO:C    | 2.33                     | 0.66              |
| 2:B:487:LEU:CD2  | 2:B:522:GLU:CB   | 2.74                     | 0.66              |
| 2:B:549:LEU:CD2  | 2:B:611:ALA:H    | 1.85                     | 0.66              |
| 2:B:567:GLN:O    | 2:B:569:THR:HB   | 1.93                     | 0.66              |
| 3:M:133:GLU:O    | 3:M:134:PRO:C    | 2.24                     | 0.66              |
| 3:M:372:ILE:CD1  | 3:M:428:VAL:HG22 | 2.26                     | 0.66              |
| 1:A:264:SER:CB   | 1:A:271:ARG:HG3  | 2.24                     | 0.66              |
| 1:A:272:ALA:O    | 1:A:276:PRO:HD3  | 1.95                     | 0.66              |
| 2:B:120:ILE:HA   | 2:B:142:LEU:CD2  | 2.25                     | 0.66              |
| 2:B:243:TRP:CZ3  | 3:M:95:THR:N     | 2.63                     | 0.66              |
| 2:B:343:LEU:HD22 | 2:B:366:LEU:CD1  | 2.25                     | 0.66              |
| 2:B:505:ASP:O    | 2:B:506:ASN:C    | 2.24                     | 0.66              |
| 4:S:53:THR:HB    | 4:S:68:VAL:C     | 2.21                     | 0.66              |
| 1:A:384:LEU:HG   | 1:A:385:LYS:N    | 2.11                     | 0.66              |
| 1:A:555:LEU:CD1  | 1:A:581:LEU:CD1  | 2.73                     | 0.66              |
| 2:B:116:THR:HG21 | 2:B:147:MET:HG3  | 1.77                     | 0.66              |
| 2:B:351:GLU:O    | 3:M:49:ASP:CG    | 2.38                     | 0.66              |
| 2:B:549:LEU:HG   | 2:B:614:ILE:CD1  | 2.25                     | 0.66              |
| 2:B:566:ALA:CA   | 2:B:574:ASN:CB   | 2.70                     | 0.66              |
| 2:B:602:ASP:OD1  | 2:B:603:ASP:N    | 2.28                     | 0.66              |
| 3:M:224:VAL:N    | 3:M:479:PHE:HA   | 2.10                     | 0.66              |
| 3:M:245:ASP:CA   | 3:M:472:TYR:CD1  | 2.78                     | 0.66              |
| 3:M:323:MET:SD   | 3:M:342:LEU:CG   | 2.84                     | 0.66              |
| 1:A:586:GLU:O    | 1:A:587:ASN:O    | 2.13                     | 0.65              |
| 1:A:595:GLU:HA   | 2:B:476:ARG:CZ   | 2.26                     | 0.65              |
| 2:B:21:GLU:OE2   | 2:B:35:TYR:CE1   | 2.38                     | 0.65              |
| 2:B:219:TYR:OH   | 2:B:226:LEU:CA   | 2.32                     | 0.65              |
| 2:B:458:MET:SD   | 2:B:471:TYR:CB   | 2.83                     | 0.65              |
| 3:M:222:PHE:CD1  | 3:M:240:ILE:CG2  | 2.78                     | 0.65              |
| 3:M:245:ASP:HA   | 3:M:297:PHE:O    | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:347:PHE:CZ   | 3:M:350:VAL:HG12 | 2.31                     | 0.65              |
| 4:S:99:LEU:O     | 4:S:102:ILE:HB   | 1.96                     | 0.65              |
| 1:A:92:LEU:CD2   | 1:A:124:ALA:HA   | 2.26                     | 0.65              |
| 2:B:475:ILE:HG23 | 2:B:489:ILE:CG2  | 2.25                     | 0.65              |
| 2:B:580:TYR:O    | 2:B:582:ASP:CG   | 2.39                     | 0.65              |
| 3:M:319:SER:OG   | 3:M:345:GLU:N    | 2.29                     | 0.65              |
| 1:A:370:LYS:HE2  | 1:A:370:LYS:HA   | 1.76                     | 0.65              |
| 1:A:450:TYR:OH   | 1:A:476:GLN:HG2  | 1.96                     | 0.65              |
| 2:B:24:ALA:C     | 2:B:35:TYR:CG    | 2.75                     | 0.65              |
| 2:B:108:PHE:CE2  | 2:B:115:LEU:CG   | 2.79                     | 0.65              |
| 2:B:243:TRP:HZ2  | 3:M:98:ARG:CG    | 2.09                     | 0.65              |
| 2:B:537:PHE:CE1  | 2:B:545:ARG:CB   | 2.79                     | 0.65              |
| 1:A:404:GLN:CB   | 2:B:3:ASP:OD2    | 2.43                     | 0.65              |
| 1:A:438:ALA:O    | 1:A:441:TYR:CD1  | 2.50                     | 0.65              |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:O    | 1.92                     | 0.65              |
| 2:B:219:TYR:CB   | 2:B:226:LEU:HD22 | 2.25                     | 0.65              |
| 2:B:234:CYS:CB   | 2:B:301:LEU:HB3  | 2.26                     | 0.65              |
| 2:B:602:ASP:O    | 2:B:608:ARG:NE   | 2.29                     | 0.65              |
| 4:S:89:VAL:HG11  | 4:S:98:ILE:CD1   | 2.27                     | 0.65              |
| 1:A:121:LEU:CD1  | 1:A:153:ILE:HG22 | 2.26                     | 0.65              |
| 1:A:185:LEU:HB3  | 1:A:203:PHE:CE1  | 2.31                     | 0.65              |
| 1:A:231:GLN:HB2  | 1:A:232:PRO:HD3  | 1.78                     | 0.65              |
| 1:A:292:TYR:CD1  | 1:A:292:TYR:O    | 2.50                     | 0.65              |
| 1:A:460:LEU:O    | 1:A:463:ASP:HB2  | 1.97                     | 0.65              |
| 1:A:637:GLU:CG   | 2:B:517:GLU:HA   | 2.23                     | 0.65              |
| 1:A:638:LEU:CD2  | 2:B:558:TYR:C    | 2.67                     | 0.65              |
| 2:B:132:SER:O    | 2:B:133:GLU:C    | 2.27                     | 0.65              |
| 2:B:276:SER:O    | 2:B:291:TYR:O    | 2.14                     | 0.65              |
| 2:B:278:PRO:HD2  | 2:B:292:GLU:CA   | 2.25                     | 0.65              |
| 2:B:508:ARG:CB   | 2:B:544:THR:CG2  | 2.75                     | 0.65              |
| 3:M:218:LEU:CA   | 3:M:472:TYR:CE2  | 2.78                     | 0.65              |
| 1:A:158:LEU:HG   | 1:A:162:ILE:HD12 | 1.78                     | 0.65              |
| 1:A:170:LEU:HD22 | 1:A:181:ALA:HB1  | 1.78                     | 0.65              |
| 1:A:233:PHE:C    | 1:A:235:GLN:N    | 2.50                     | 0.65              |
| 1:A:254:ILE:CG1  | 1:A:290:VAL:HG22 | 2.26                     | 0.65              |
| 1:A:586:GLU:HB2  | 1:A:604:LEU:CD1  | 2.26                     | 0.65              |
| 2:B:62:ALA:O     | 2:B:66:ILE:CG1   | 2.44                     | 0.65              |
| 2:B:104:TYR:O    | 2:B:107:ARG:HB2  | 1.95                     | 0.65              |
| 2:B:108:PHE:CE2  | 2:B:115:LEU:HB2  | 2.31                     | 0.65              |
| 2:B:243:TRP:CH2  | 3:M:94:GLU:CA    | 2.74                     | 0.65              |
| 2:B:393:ILE:HG23 | 2:B:431:MET:CB   | 2.27                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:217:ASP:N    | 3:M:472:TYR:OH   | 2.30                     | 0.65              |
| 3:M:235:LEU:HD23 | 3:M:235:LEU:C    | 2.22                     | 0.65              |
| 1:A:192:TYR:HD2  | 1:A:195:ALA:H    | 1.43                     | 0.65              |
| 1:A:244:LEU:CG   | 1:A:281:LEU:CD1  | 2.74                     | 0.65              |
| 1:A:258:LYS:HZ3  | 4:S:94:SER:CB    | 2.02                     | 0.65              |
| 1:A:275:LEU:O    | 1:A:277:LYS:N    | 2.29                     | 0.65              |
| 1:A:279:LEU:HD13 | 1:A:314:ALA:HB3  | 1.79                     | 0.65              |
| 2:B:25:VAL:CG2   | 2:B:35:TYR:CD2   | 2.74                     | 0.65              |
| 2:B:29:LYS:O     | 2:B:32:GLU:HG3   | 1.96                     | 0.65              |
| 2:B:129:ASP:O    | 2:B:135:ARG:HD3  | 1.96                     | 0.65              |
| 2:B:252:LEU:HB3  | 2:B:302:PHE:CG   | 2.32                     | 0.65              |
| 3:M:118:TYR:C    | 3:M:118:TYR:CD2  | 2.73                     | 0.65              |
| 3:M:226:PHE:CE1  | 3:M:321:GLY:O    | 2.50                     | 0.65              |
| 2:B:181:TYR:HE1  | 2:B:222:HIS:NE2  | 1.95                     | 0.65              |
| 2:B:513:TRP:HA   | 2:B:551:LEU:HD13 | 1.57                     | 0.65              |
| 4:S:8:PHE:HZ     | 4:S:86:THR:OG1   | 1.72                     | 0.65              |
| 1:A:212:ILE:O    | 1:A:213:SER:C    | 2.26                     | 0.65              |
| 1:A:556:VAL:CG2  | 1:A:603:VAL:HG13 | 2.27                     | 0.65              |
| 1:A:556:VAL:HG22 | 1:A:603:VAL:CG1  | 2.26                     | 0.65              |
| 2:B:245:GLN:HB3  | 2:B:309:LEU:HD11 | 1.71                     | 0.65              |
| 2:B:513:TRP:CB   | 2:B:551:LEU:HD11 | 2.27                     | 0.65              |
| 2:B:546:CYS:HB2  | 2:B:607:ILE:HD11 | 1.79                     | 0.65              |
| 3:M:347:PHE:CE1  | 3:M:350:VAL:CB   | 2.79                     | 0.65              |
| 3:M:347:PHE:CE1  | 3:M:350:VAL:HB   | 2.31                     | 0.65              |
| 4:S:130:SER:CB   | 4:S:156:LEU:HD13 | 2.27                     | 0.65              |
| 1:A:128:LEU:CD1  | 1:A:150:LEU:CD2  | 2.75                     | 0.65              |
| 1:A:258:LYS:HZ3  | 4:S:94:SER:CA    | 2.10                     | 0.65              |
| 1:A:569:ASP:C    | 1:A:571:ARG:N    | 2.54                     | 0.65              |
| 2:B:267:ASP:HB3  | 2:B:289:PRO:CG   | 2.27                     | 0.65              |
| 2:B:352:ASN:HD22 | 3:M:70:ASN:HB3   | 1.54                     | 0.65              |
| 3:M:217:ASP:C    | 3:M:472:TYR:CZ   | 2.75                     | 0.65              |
| 1:A:95:MET:HB2   | 1:A:127:LEU:HD23 | 1.77                     | 0.64              |
| 1:A:383:ASN:O    | 1:A:387:ILE:HG12 | 1.96                     | 0.64              |
| 1:A:460:LEU:O    | 1:A:463:ASP:N    | 2.28                     | 0.64              |
| 1:A:621:LEU:HD13 | 1:A:621:LEU:C    | 2.22                     | 0.64              |
| 2:B:74:ASP:O     | 2:B:77:ILE:HB    | 1.97                     | 0.64              |
| 2:B:343:LEU:HD22 | 2:B:366:LEU:HD12 | 1.78                     | 0.64              |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:CG   | 2.27                     | 0.64              |
| 2:B:472:VAL:O    | 2:B:473:ASN:C    | 2.28                     | 0.64              |
| 2:B:479:VAL:CG1  | 2:B:486:HIS:CG   | 2.66                     | 0.64              |
| 1:A:137:ASN:O    | 1:A:139:ASP:N    | 2.25                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:300:LYS:C    | 1:A:302:ASN:N    | 2.49                     | 0.64              |
| 1:A:536:MET:O    | 1:A:537:THR:O    | 2.15                     | 0.64              |
| 1:A:633:PHE:CZ   | 2:B:550:VAL:HG12 | 2.27                     | 0.64              |
| 2:B:374:PHE:HD2  | 2:B:402:LEU:CG   | 2.11                     | 0.64              |
| 2:B:394:TRP:CZ3  | 2:B:397:GLN:OE1  | 2.49                     | 0.64              |
| 2:B:447:GLU:HG3  | 2:B:482:ASN:ND2  | 2.12                     | 0.64              |
| 3:M:69:ILE:O     | 3:M:75:TRP:HA    | 1.97                     | 0.64              |
| 3:M:214:LEU:HD23 | 3:M:214:LEU:O    | 1.96                     | 0.64              |
| 3:M:221:THR:N    | 3:M:474:THR:HG1  | 1.94                     | 0.64              |
| 3:M:245:ASP:N    | 3:M:472:TYR:CD2  | 2.64                     | 0.64              |
| 1:A:349:ILE:HG21 | 1:A:378:ILE:CG2  | 2.24                     | 0.64              |
| 2:B:176:ALA:C    | 2:B:178:ILE:N    | 2.55                     | 0.64              |
| 2:B:208:ILE:HG21 | 2:B:236:ILE:CG2  | 2.26                     | 0.64              |
| 2:B:267:ASP:HB3  | 2:B:289:PRO:CD   | 2.28                     | 0.64              |
| 2:B:518:ILE:O    | 2:B:518:ILE:CD1  | 2.46                     | 0.64              |
| 2:B:545:ARG:HB2  | 2:B:602:ASP:OD2  | 1.97                     | 0.64              |
| 1:A:566:PHE:C    | 1:A:568:GLU:N    | 2.55                     | 0.64              |
| 3:M:212:ASN:HB3  | 3:M:250:LEU:HD23 | 1.78                     | 0.64              |
| 3:M:306:LEU:HD13 | 3:M:317:MET:CE   | 2.26                     | 0.64              |
| 2:B:226:LEU:CD2  | 2:B:255:TYR:CE1  | 2.70                     | 0.64              |
| 3:M:220:GLU:CG   | 3:M:439:TYR:CD1  | 2.71                     | 0.64              |
| 3:M:223:HIS:CG   | 3:M:476:THR:HG1  | 2.12                     | 0.64              |
| 3:M:323:MET:SD   | 3:M:342:LEU:CA   | 2.85                     | 0.64              |
| 3:M:327:PHE:HE1  | 3:M:336:ASP:CB   | 2.09                     | 0.64              |
| 1:A:185:LEU:HD13 | 1:A:203:PHE:HE1  | 1.63                     | 0.64              |
| 2:B:127:LEU:HB3  | 2:B:161:LEU:CD1  | 2.27                     | 0.64              |
| 2:B:219:TYR:OH   | 2:B:226:LEU:N    | 2.30                     | 0.64              |
| 2:B:525:ILE:C    | 2:B:527:PRO:CD   | 2.71                     | 0.64              |
| 2:B:537:PHE:CE2  | 2:B:598:LEU:O    | 2.51                     | 0.64              |
| 2:B:546:CYS:HA   | 2:B:607:ILE:CG1  | 2.21                     | 0.64              |
| 3:M:105:ASP:O    | 3:M:106:LYS:HB2  | 1.95                     | 0.64              |
| 1:A:136:GLY:O    | 1:A:139:ASP:HB3  | 1.97                     | 0.64              |
| 1:A:608:ARG:NH1  | 1:A:612:GLU:OE2  | 2.30                     | 0.64              |
| 2:B:132:SER:CB   | 2:B:169:VAL:CG2  | 2.76                     | 0.64              |
| 2:B:208:ILE:HG12 | 2:B:236:ILE:CD1  | 2.20                     | 0.64              |
| 2:B:523:PHE:CD1  | 2:B:559:ASP:CG   | 2.75                     | 0.64              |
| 3:M:128:CYS:C    | 3:M:130:GLU:O    | 2.41                     | 0.64              |
| 4:S:73:ILE:CG2   | 4:S:88:ILE:HG23  | 2.26                     | 0.64              |
| 1:A:166:LEU:O    | 1:A:170:LEU:HD22 | 1.98                     | 0.64              |
| 1:A:186:PHE:C    | 1:A:186:PHE:CD2  | 2.75                     | 0.64              |
| 1:A:450:TYR:HH   | 1:A:476:GLN:CG   | 2.08                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:586:GLU:HB2  | 1:A:604:LEU:HD11 | 1.79                     | 0.64              |
| 2:B:25:VAL:CG2   | 2:B:36:THR:CB    | 2.57                     | 0.64              |
| 3:M:245:ASP:O    | 3:M:472:TYR:OH   | 2.14                     | 0.64              |
| 4:S:16:LEU:CD2   | 4:S:128:LEU:HD23 | 2.28                     | 0.64              |
| 4:S:17:VAL:CG2   | 4:S:19:PHE:CE2   | 2.81                     | 0.64              |
| 1:A:207:LEU:O    | 1:A:243:ILE:CD1  | 2.38                     | 0.64              |
| 1:A:581:LEU:HG   | 1:A:585:PHE:CE2  | 2.33                     | 0.64              |
| 2:B:37:TYR:O     | 2:B:38:TYR:C     | 2.40                     | 0.64              |
| 2:B:143:SER:HB3  | 2:B:176:ALA:HA   | 1.79                     | 0.64              |
| 2:B:534:ILE:O    | 2:B:598:LEU:CD1  | 2.45                     | 0.64              |
| 2:B:592:TYR:C    | 2:B:592:TYR:CD1  | 2.76                     | 0.64              |
| 2:B:597:TYR:O    | 2:B:601:TYR:CD1  | 2.51                     | 0.64              |
| 3:M:217:ASP:O    | 3:M:472:TYR:CG   | 2.51                     | 0.64              |
| 4:S:53:THR:HB    | 4:S:69:ASN:CA    | 2.28                     | 0.64              |
| 1:A:279:LEU:CD1  | 1:A:314:ALA:CB   | 2.75                     | 0.64              |
| 2:B:303:LEU:CD1  | 2:B:333:GLN:HB3  | 2.27                     | 0.64              |
| 3:M:262:THR:HG22 | 3:M:264:GLY:N    | 2.13                     | 0.64              |
| 3:M:347:PHE:CE2  | 3:M:350:VAL:O    | 2.51                     | 0.64              |
| 1:A:594:PHE:CZ   | 2:B:477:MET:HE2  | 2.33                     | 0.63              |
| 2:B:501:THR:CA   | 2:B:508:ARG:NH2  | 2.60                     | 0.63              |
| 3:M:58:ARG:C     | 3:M:60:LEU:O     | 2.41                     | 0.63              |
| 1:A:102:GLN:NE2  | 4:S:166:LYS:CE   | 2.61                     | 0.63              |
| 1:A:463:ASP:HA   | 3:M:58:ARG:NH2   | 2.14                     | 0.63              |
| 1:A:637:GLU:O    | 2:B:517:GLU:O    | 2.17                     | 0.63              |
| 2:B:80:GLN:HG2   | 2:B:115:LEU:CD2  | 2.15                     | 0.63              |
| 2:B:253:ILE:HD11 | 2:B:324:ALA:HB2  | 1.80                     | 0.63              |
| 3:M:74:TYR:HB3   | 3:M:114:ILE:CD1  | 2.28                     | 0.63              |
| 3:M:223:HIS:CD2  | 3:M:478:ASN:CA   | 2.77                     | 0.63              |
| 4:S:6:LEU:HA     | 4:S:16:LEU:O     | 1.99                     | 0.63              |
| 1:A:84:MET:HE3   | 1:A:113:SER:O    | 1.97                     | 0.63              |
| 1:A:595:GLU:HG2  | 2:B:473:ASN:OD1  | 1.99                     | 0.63              |
| 2:B:44:PRO:HB3   | 2:B:82:TYR:HH    | 1.61                     | 0.63              |
| 2:B:214:ALA:O    | 2:B:216:LYS:N    | 2.32                     | 0.63              |
| 2:B:226:LEU:O    | 2:B:229:HIS:HB2  | 1.99                     | 0.63              |
| 2:B:276:SER:O    | 2:B:295:ASN:HB2  | 1.98                     | 0.63              |
| 1:A:92:LEU:O     | 1:A:127:LEU:HD21 | 1.98                     | 0.63              |
| 1:A:237:SER:HB2  | 1:A:270:LEU:CD1  | 2.28                     | 0.63              |
| 1:A:438:ALA:O    | 1:A:441:TYR:CE1  | 2.51                     | 0.63              |
| 1:A:581:LEU:HD11 | 1:A:585:PHE:CZ   | 2.33                     | 0.63              |
| 1:A:626:SER:HB2  | 2:B:617:LEU:HD21 | 1.80                     | 0.63              |
| 2:B:230:PHE:HE2  | 2:B:234:CYS:SG   | 2.20                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:243:TRP:HZ2  | 3:M:98:ARG:CD    | 2.09                     | 0.63              |
| 2:B:367:SER:OG   | 2:B:401:THR:HB   | 1.96                     | 0.63              |
| 3:M:373:ALA:O    | 3:M:418:GLU:N    | 2.32                     | 0.63              |
| 1:A:594:PHE:CG   | 2:B:477:MET:SD   | 2.92                     | 0.63              |
| 2:B:87:VAL:O     | 2:B:90:ILE:HG22  | 1.98                     | 0.63              |
| 2:B:132:SER:CB   | 2:B:169:VAL:HG23 | 2.24                     | 0.63              |
| 2:B:353:GLN:C    | 3:M:49:ASP:HB3   | 1.62                     | 0.63              |
| 2:B:486:HIS:CE1  | 2:B:518:ILE:CG1  | 2.82                     | 0.63              |
| 2:B:512:VAL:HG21 | 2:B:548:ILE:HG12 | 1.80                     | 0.63              |
| 3:M:242:GLY:HA3  | 3:M:444:ALA:HB2  | 1.80                     | 0.63              |
| 3:M:244:VAL:N    | 3:M:300:LEU:O    | 2.31                     | 0.63              |
| 3:M:244:VAL:CA   | 3:M:472:TYR:CD2  | 2.68                     | 0.63              |
| 3:M:306:LEU:CD2  | 3:M:317:MET:HE3  | 2.28                     | 0.63              |
| 1:A:128:LEU:HD13 | 1:A:150:LEU:CD2  | 2.29                     | 0.63              |
| 1:A:320:HIS:O    | 1:A:322:PHE:N    | 2.30                     | 0.63              |
| 1:A:402:ILE:HB   | 1:A:421:PRO:HA   | 1.80                     | 0.63              |
| 2:B:25:VAL:CG2   | 2:B:36:THR:HA    | 2.04                     | 0.63              |
| 2:B:132:SER:HA   | 2:B:169:VAL:HG21 | 1.80                     | 0.63              |
| 2:B:162:VAL:CG2  | 2:B:195:ILE:HG22 | 2.01                     | 0.63              |
| 2:B:216:LYS:CG   | 2:B:251:LEU:CD1  | 2.73                     | 0.63              |
| 2:B:249:ILE:HG12 | 2:B:306:LEU:CD2  | 2.28                     | 0.63              |
| 2:B:334:MET:O    | 2:B:335:LYS:C    | 2.38                     | 0.63              |
| 2:B:347:VAL:CG2  | 2:B:359:LEU:HB3  | 2.22                     | 0.63              |
| 2:B:447:GLU:OE1  | 2:B:485:LYS:HG3  | 1.98                     | 0.63              |
| 3:M:215:TYR:HB2  | 3:M:467:TYR:C    | 2.24                     | 0.63              |
| 3:M:217:ASP:O    | 3:M:472:TYR:CD2  | 2.52                     | 0.63              |
| 4:S:39:ILE:HG23  | 4:S:47:GLN:CD    | 2.23                     | 0.63              |
| 1:A:149:GLY:O    | 1:A:152:THR:N    | 2.27                     | 0.63              |
| 1:A:174:ARG:NH1  | 4:S:148:ARG:HH22 | 1.95                     | 0.63              |
| 1:A:186:PHE:HD2  | 1:A:187:LYS:N    | 1.97                     | 0.63              |
| 1:A:319:LEU:O    | 1:A:320:HIS:O    | 2.16                     | 0.63              |
| 1:A:573:GLU:O    | 1:A:577:VAL:HG23 | 1.98                     | 0.63              |
| 2:B:24:ALA:HB1   | 2:B:35:TYR:CG    | 2.19                     | 0.63              |
| 2:B:25:VAL:HG22  | 2:B:35:TYR:CA    | 2.27                     | 0.63              |
| 2:B:261:PRO:C    | 2:B:290:SER:HB3  | 2.24                     | 0.63              |
| 2:B:513:TRP:CA   | 2:B:551:LEU:HD21 | 2.22                     | 0.63              |
| 2:B:520:SER:O    | 2:B:523:PHE:HE2  | 1.81                     | 0.63              |
| 2:B:531:ARG:HB2  | 2:B:591:MET:SD   | 2.39                     | 0.63              |
| 3:M:257:ALA:HB3  | 3:M:453:ASP:CG   | 2.23                     | 0.63              |
| 1:A:225:LEU:HB2  | 1:A:233:PHE:CE1  | 2.28                     | 0.63              |
| 1:A:637:GLU:HG3  | 2:B:517:GLU:HA   | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:638:LEU:CG   | 2:B:520:SER:HA   | 2.27                     | 0.63              |
| 2:B:29:LYS:O     | 2:B:30:LEU:C     | 2.37                     | 0.63              |
| 2:B:104:TYR:O    | 2:B:107:ARG:N    | 2.31                     | 0.63              |
| 2:B:127:LEU:CG   | 2:B:157:THR:CG2  | 2.74                     | 0.63              |
| 2:B:347:VAL:HG11 | 2:B:381:PHE:HE2  | 1.63                     | 0.63              |
| 2:B:431:MET:O    | 2:B:434:LYS:N    | 2.32                     | 0.63              |
| 2:B:486:HIS:CG   | 2:B:518:ILE:CD1  | 2.76                     | 0.63              |
| 1:A:200:PHE:CZ   | 1:A:236:LEU:HG   | 2.33                     | 0.63              |
| 1:A:219:VAL:CG1  | 1:A:256:LEU:CD2  | 2.74                     | 0.63              |
| 1:A:240:LEU:C    | 1:A:242:GLU:O    | 2.42                     | 0.63              |
| 1:A:241:TYR:C    | 1:A:242:GLU:O    | 2.22                     | 0.63              |
| 1:A:323:CYS:SG   | 1:A:338:PHE:HE1  | 2.22                     | 0.63              |
| 1:A:625:LEU:O    | 1:A:627:GLU:N    | 2.31                     | 0.63              |
| 2:B:542:PRO:O    | 2:B:607:ILE:HD11 | 1.98                     | 0.63              |
| 3:M:45:SER:CA    | 3:M:47:SER:H     | 2.12                     | 0.63              |
| 1:A:99:LYS:HG2   | 1:A:101:GLN:H    | 1.63                     | 0.62              |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:HD13 | 1.81                     | 0.62              |
| 2:B:37:TYR:O     | 2:B:40:GLN:C     | 2.41                     | 0.62              |
| 2:B:44:PRO:HG3   | 2:B:77:ILE:HD12  | 1.81                     | 0.62              |
| 2:B:143:SER:CA   | 2:B:179:LYS:HD2  | 2.29                     | 0.62              |
| 2:B:408:VAL:CG1  | 2:B:412:PHE:CE2  | 2.83                     | 0.62              |
| 2:B:430:ILE:O    | 2:B:433:VAL:HB   | 1.98                     | 0.62              |
| 2:B:553:ALA:HA   | 2:B:614:ILE:HG21 | 1.81                     | 0.62              |
| 2:B:584:SER:O    | 2:B:585:GLY:C    | 2.25                     | 0.62              |
| 3:M:44:ASP:O     | 3:M:47:SER:N     | 2.32                     | 0.62              |
| 3:M:94:GLU:O     | 3:M:97:ASP:HB2   | 1.99                     | 0.62              |
| 1:A:258:LYS:NZ   | 4:S:94:SER:H     | 1.96                     | 0.62              |
| 1:A:384:LEU:CG   | 1:A:385:LYS:N    | 2.62                     | 0.62              |
| 1:A:585:PHE:CD2  | 1:A:603:VAL:HG12 | 2.35                     | 0.62              |
| 2:B:36:THR:HG22  | 2:B:40:GLN:HG3   | 1.81                     | 0.62              |
| 2:B:106:LEU:HD13 | 2:B:144:ASP:HB2  | 1.80                     | 0.62              |
| 2:B:133:GLU:O    | 2:B:168:MET:HE2  | 1.99                     | 0.62              |
| 2:B:267:ASP:HB3  | 2:B:289:PRO:HG3  | 1.79                     | 0.62              |
| 2:B:371:GLN:NE2  | 2:B:401:THR:O    | 2.32                     | 0.62              |
| 3:M:219:LEU:HB2  | 3:M:472:TYR:O    | 1.99                     | 0.62              |
| 3:M:220:GLU:OE2  | 3:M:439:TYR:HD1  | 1.77                     | 0.62              |
| 1:A:516:ILE:HG23 | 1:A:554:ALA:HB3  | 1.79                     | 0.62              |
| 3:M:437:TYR:CD1  | 3:M:479:PHE:CE1  | 2.87                     | 0.62              |
| 1:A:114:PHE:C    | 1:A:115:TYR:O    | 2.37                     | 0.62              |
| 2:B:299:LEU:C    | 2:B:299:LEU:HD13 | 2.24                     | 0.62              |
| 2:B:512:VAL:HB   | 2:B:551:LEU:HD12 | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:214:LEU:C    | 3:M:467:TYR:H    | 2.04                     | 0.62              |
| 3:M:316:ARG:HG2  | 3:M:322:LEU:HD13 | 1.80                     | 0.62              |
| 3:M:467:TYR:CG   | 3:M:468:LYS:N    | 2.68                     | 0.62              |
| 4:S:1:MET:H2     | 4:S:93:GLU:CG    | 2.12                     | 0.62              |
| 1:A:533:ILE:HG12 | 1:A:562:TRP:HH2  | 1.62                     | 0.62              |
| 2:B:25:VAL:N     | 2:B:35:TYR:HD2   | 1.97                     | 0.62              |
| 2:B:302:PHE:CD2  | 2:B:328:LEU:HD11 | 2.34                     | 0.62              |
| 2:B:487:LEU:HD21 | 2:B:522:GLU:HB2  | 1.81                     | 0.62              |
| 2:B:580:TYR:HB3  | 2:B:582:ASP:OD2  | 1.98                     | 0.62              |
| 1:A:289:SER:O    | 1:A:290:VAL:O    | 2.17                     | 0.62              |
| 2:B:127:LEU:CD2  | 2:B:161:LEU:CD2  | 2.73                     | 0.62              |
| 2:B:177:ILE:HG21 | 2:B:196:LEU:HG   | 1.81                     | 0.62              |
| 2:B:486:HIS:CD2  | 2:B:518:ILE:HG12 | 2.35                     | 0.62              |
| 2:B:486:HIS:HD1  | 2:B:518:ILE:HD13 | 1.56                     | 0.62              |
| 3:M:224:VAL:H    | 3:M:479:PHE:CB   | 2.12                     | 0.62              |
| 3:M:327:PHE:CE1  | 3:M:336:ASP:OD2  | 2.53                     | 0.62              |
| 1:A:68:THR:HB    | 4:S:166:LYS:O    | 2.00                     | 0.62              |
| 1:A:260:PHE:CZ   | 1:A:274:LEU:CD1  | 2.81                     | 0.62              |
| 1:A:279:LEU:HD11 | 1:A:314:ALA:CB   | 2.29                     | 0.62              |
| 2:B:328:LEU:HB2  | 2:B:333:GLN:NE2  | 2.14                     | 0.62              |
| 2:B:353:GLN:C    | 2:B:355:ASN:N    | 2.48                     | 0.62              |
| 2:B:519:ALA:O    | 2:B:523:PHE:HD2  | 1.77                     | 0.62              |
| 3:M:78:ALA:HB3   | 3:M:89:CYS:SG    | 2.39                     | 0.62              |
| 3:M:350:VAL:CG1  | 3:M:442:GLN:HG2  | 2.30                     | 0.62              |
| 3:M:364:VAL:C    | 3:M:367:ALA:O    | 2.43                     | 0.62              |
| 4:S:38:LEU:HB3   | 4:S:51:LEU:CD1   | 2.30                     | 0.62              |
| 4:S:53:THR:CB    | 4:S:69:ASN:HB2   | 2.28                     | 0.62              |
| 1:A:186:PHE:HA   | 1:A:221:VAL:HG13 | 1.81                     | 0.62              |
| 1:A:349:ILE:O    | 1:A:352:PHE:N    | 2.30                     | 0.62              |
| 2:B:178:ILE:C    | 2:B:180:LEU:N    | 2.58                     | 0.62              |
| 2:B:219:TYR:O    | 2:B:223:LEU:HD21 | 1.99                     | 0.62              |
| 2:B:472:VAL:CG1  | 2:B:510:GLY:C    | 2.73                     | 0.62              |
| 2:B:520:SER:O    | 2:B:523:PHE:CE2  | 2.53                     | 0.62              |
| 3:M:215:TYR:O    | 3:M:246:VAL:HG13 | 2.00                     | 0.62              |
| 1:A:364:ASP:HB3  | 1:A:367:ILE:HD12 | 1.82                     | 0.62              |
| 2:B:141:ALA:C    | 2:B:143:SER:N    | 2.55                     | 0.62              |
| 2:B:311:TYR:HE2  | 2:B:342:ALA:HB2  | 1.65                     | 0.62              |
| 3:M:265:ASN:HA   | 3:M:313:SER:OG   | 2.00                     | 0.62              |
| 3:M:360:LEU:HD23 | 3:M:362:PHE:CE2  | 2.35                     | 0.62              |
| 4:S:5:VAL:HG22   | 4:S:87:PHE:CD2   | 2.34                     | 0.62              |
| 1:A:156:PRO:O    | 1:A:157:SER:C    | 2.31                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:638:LEU:CB   | 2:B:558:TYR:CE1  | 2.69                     | 0.62              |
| 2:B:185:LYS:CE   | 2:B:221:ASP:OD2  | 2.47                     | 0.62              |
| 2:B:592:TYR:CE2  | 2:B:618:PHE:CD2  | 2.87                     | 0.62              |
| 3:M:65:TYR:CG    | 3:M:66:PHE:N     | 2.66                     | 0.62              |
| 3:M:107:ASP:OD1  | 3:M:296:LYS:NZ   | 2.33                     | 0.62              |
| 4:S:132:LEU:O    | 4:S:136:VAL:HG23 | 2.00                     | 0.62              |
| 1:A:121:LEU:HD12 | 1:A:153:ILE:CG2  | 2.29                     | 0.61              |
| 1:A:404:GLN:CG   | 2:B:7:ARG:HH21   | 2.13                     | 0.61              |
| 2:B:25:VAL:CG1   | 2:B:36:THR:CB    | 2.69                     | 0.61              |
| 2:B:63:MET:CG    | 2:B:100:LEU:CB   | 2.78                     | 0.61              |
| 2:B:260:LEU:CA   | 2:B:293:VAL:HG21 | 2.23                     | 0.61              |
| 4:S:49:SER:O     | 4:S:77:TYR:HB2   | 2.00                     | 0.61              |
| 1:A:88:ASN:HB2   | 1:A:120:ILE:HD12 | 1.82                     | 0.61              |
| 1:A:121:LEU:HD23 | 1:A:121:LEU:C    | 2.24                     | 0.61              |
| 1:A:223:CYS:HB2  | 1:A:259:LEU:HD12 | 1.81                     | 0.61              |
| 2:B:178:ILE:HD11 | 2:B:215:TYR:CA   | 2.29                     | 0.61              |
| 2:B:243:TRP:CH2  | 3:M:95:THR:CA    | 2.83                     | 0.61              |
| 2:B:280:PRO:CG   | 2:B:283:TYR:HD1  | 2.10                     | 0.61              |
| 2:B:451:MET:HG3  | 2:B:489:ILE:CG1  | 2.30                     | 0.61              |
| 2:B:530:LEU:HD23 | 2:B:591:MET:CB   | 2.30                     | 0.61              |
| 3:M:320:ILE:O    | 3:M:322:LEU:N    | 2.32                     | 0.61              |
| 4:S:65:ASN:O     | 4:S:67:GLU:N     | 2.33                     | 0.61              |
| 2:B:20:ARG:CG    | 2:B:21:GLU:N     | 2.63                     | 0.61              |
| 2:B:155:LEU:CB   | 2:B:188:TYR:CD2  | 2.83                     | 0.61              |
| 2:B:563:PHE:CD2  | 2:B:584:SER:CA   | 2.83                     | 0.61              |
| 3:M:224:VAL:H    | 3:M:479:PHE:CA   | 2.12                     | 0.61              |
| 4:S:53:THR:HG21  | 4:S:67:GLU:O     | 2.00                     | 0.61              |
| 4:S:87:PHE:CD1   | 4:S:102:ILE:HG12 | 2.36                     | 0.61              |
| 2:B:25:VAL:HG22  | 2:B:35:TYR:CB    | 2.31                     | 0.61              |
| 2:B:95:THR:CG2   | 2:B:137:PHE:HE2  | 2.13                     | 0.61              |
| 2:B:256:CYS:O    | 2:B:257:LYS:C    | 2.35                     | 0.61              |
| 2:B:269:SER:C    | 2:B:270:SER:O    | 2.39                     | 0.61              |
| 2:B:523:PHE:CE1  | 2:B:582:ASP:OD2  | 2.52                     | 0.61              |
| 2:B:563:PHE:HD2  | 2:B:584:SER:HB3  | 1.63                     | 0.61              |
| 3:M:15:ILE:O     | 3:M:118:TYR:CD1  | 2.46                     | 0.61              |
| 3:M:219:LEU:CB   | 3:M:472:TYR:O    | 2.48                     | 0.61              |
| 1:A:438:ALA:O    | 1:A:439:ASP:HB2  | 1.99                     | 0.61              |
| 2:B:293:VAL:HA   | 2:B:299:LEU:HB2  | 1.81                     | 0.61              |
| 2:B:355:ASN:C    | 2:B:359:LEU:HD23 | 2.25                     | 0.61              |
| 2:B:381:PHE:O    | 2:B:395:LYS:HD2  | 2.00                     | 0.61              |
| 2:B:399:LEU:O    | 2:B:400:SER:C    | 2.34                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:424:PHE:CD2  | 2:B:428:VAL:HG11 | 2.35                     | 0.61              |
| 2:B:474:VAL:O    | 2:B:477:MET:N    | 2.33                     | 0.61              |
| 3:M:219:LEU:O    | 3:M:474:THR:CG2  | 2.48                     | 0.61              |
| 1:A:316:LEU:HD13 | 1:A:348:PHE:CD2  | 2.31                     | 0.61              |
| 1:A:495:ILE:HG23 | 1:A:515:CYS:SG   | 2.40                     | 0.61              |
| 2:B:120:ILE:HD11 | 2:B:145:MET:HG3  | 1.83                     | 0.61              |
| 2:B:167:ALA:O    | 2:B:207:VAL:HG11 | 2.00                     | 0.61              |
| 2:B:231:ARG:O    | 2:B:234:CYS:N    | 2.33                     | 0.61              |
| 2:B:261:PRO:HG2  | 2:B:292:GLU:HB3  | 1.82                     | 0.61              |
| 2:B:279:LEU:HD12 | 2:B:285:GLU:CG   | 2.28                     | 0.61              |
| 2:B:336:ASN:HB3  | 2:B:339:PHE:CD1  | 2.35                     | 0.61              |
| 2:B:397:GLN:O    | 2:B:400:SER:OG   | 2.17                     | 0.61              |
| 2:B:562:ASN:O    | 2:B:581:TYR:HD2  | 1.83                     | 0.61              |
| 3:M:134:PRO:O    | 3:M:136:VAL:N    | 2.24                     | 0.61              |
| 3:M:212:ASN:CB   | 3:M:250:LEU:HD23 | 2.30                     | 0.61              |
| 1:A:186:PHE:CD2  | 1:A:187:LYS:N    | 2.69                     | 0.61              |
| 1:A:211:ASP:OD1  | 1:A:213:SER:N    | 2.32                     | 0.61              |
| 2:B:237:ILE:HG21 | 2:B:305:SER:HB3  | 1.82                     | 0.61              |
| 2:B:397:GLN:HE21 | 2:B:431:MET:HE3  | 1.66                     | 0.61              |
| 2:B:604:GLU:HB3  | 2:B:607:ILE:HD12 | 1.81                     | 0.61              |
| 3:M:106:LYS:CB   | 3:M:296:LYS:NZ   | 2.32                     | 0.61              |
| 3:M:253:ASN:HA   | 3:M:292:PRO:HG2  | 1.82                     | 0.61              |
| 3:M:351:SER:CB   | 3:M:440:ILE:O    | 2.43                     | 0.61              |
| 3:M:445:SER:OG   | 3:M:447:ILE:HG23 | 2.01                     | 0.61              |
| 4:S:135:ILE:HG23 | 4:S:141:VAL:HG13 | 1.83                     | 0.61              |
| 1:A:258:LYS:NZ   | 4:S:94:SER:CA    | 2.63                     | 0.61              |
| 1:A:505:ASN:O    | 1:A:506:LYS:C    | 2.38                     | 0.61              |
| 2:B:243:TRP:CD1  | 3:M:274:ASP:OD2  | 2.47                     | 0.61              |
| 2:B:319:LEU:HD13 | 2:B:358:MET:HB3  | 1.83                     | 0.61              |
| 3:M:134:PRO:O    | 3:M:136:VAL:CG2  | 2.49                     | 0.61              |
| 1:A:264:SER:HB2  | 1:A:271:ARG:HG3  | 1.83                     | 0.61              |
| 1:A:405:THR:H    | 2:B:7:ARG:CZ     | 2.10                     | 0.61              |
| 2:B:69:ILE:O     | 2:B:70:MET:C     | 2.39                     | 0.61              |
| 2:B:307:ASN:O    | 2:B:310:ILE:N    | 2.33                     | 0.61              |
| 2:B:475:ILE:HG22 | 2:B:514:LEU:HD21 | 1.82                     | 0.61              |
| 2:B:497:LEU:HD23 | 2:B:533:LEU:CD2  | 2.24                     | 0.61              |
| 2:B:513:TRP:CD2  | 2:B:551:LEU:HD21 | 2.36                     | 0.61              |
| 2:B:589:SER:HG   | 2:B:618:PHE:HE2  | 1.37                     | 0.61              |
| 3:M:218:LEU:O    | 3:M:441:GLY:CA   | 2.49                     | 0.61              |
| 3:M:360:LEU:HD13 | 3:M:433:VAL:HB   | 1.82                     | 0.61              |
| 3:M:433:VAL:HG13 | 3:M:433:VAL:O    | 2.01                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:244:LEU:HD13 | 1:A:256:LEU:HB2  | 1.82                     | 0.61              |
| 1:A:562:TRP:O    | 1:A:565:ASN:N    | 2.24                     | 0.61              |
| 1:A:582:ILE:HG12 | 1:A:607:LEU:HB2  | 1.83                     | 0.61              |
| 2:B:102:HIS:CD2  | 2:B:138:ALA:HA   | 2.26                     | 0.61              |
| 2:B:103:LEU:HD21 | 3:M:131:ALA:C    | 2.25                     | 0.61              |
| 2:B:151:ALA:O    | 2:B:188:TYR:CE2  | 2.54                     | 0.61              |
| 2:B:353:GLN:C    | 2:B:355:ASN:H    | 2.08                     | 0.61              |
| 2:B:568:VAL:O    | 2:B:571:SER:OG   | 2.18                     | 0.61              |
| 4:S:135:ILE:O    | 4:S:141:VAL:CA   | 2.38                     | 0.61              |
| 1:A:292:TYR:CD1  | 1:A:292:TYR:C    | 2.78                     | 0.60              |
| 1:A:633:PHE:CZ   | 2:B:550:VAL:HG13 | 2.34                     | 0.60              |
| 2:B:291:TYR:CE2  | 2:B:294:VAL:HB   | 2.36                     | 0.60              |
| 2:B:292:GLU:O    | 2:B:296:ASP:CB   | 2.49                     | 0.60              |
| 2:B:412:PHE:CZ   | 2:B:450:VAL:CG2  | 2.83                     | 0.60              |
| 3:M:74:TYR:CB    | 3:M:114:ILE:HD11 | 2.30                     | 0.60              |
| 3:M:350:VAL:CG1  | 3:M:442:GLN:HB3  | 2.28                     | 0.60              |
| 3:M:433:VAL:HG12 | 3:M:481:VAL:HB   | 1.82                     | 0.60              |
| 3:M:443:SER:OG   | 3:M:448:TYR:HA   | 2.00                     | 0.60              |
| 4:S:164:ASP:O    | 4:S:165:SER:C    | 2.29                     | 0.60              |
| 1:A:316:LEU:HD11 | 1:A:348:PHE:CD2  | 2.35                     | 0.60              |
| 2:B:139:LEU:HD23 | 2:B:172:GLU:C    | 2.25                     | 0.60              |
| 2:B:230:PHE:CD2  | 2:B:298:ASP:O    | 2.50                     | 0.60              |
| 2:B:345:ARG:NH1  | 3:M:305:ASP:CB   | 2.63                     | 0.60              |
| 2:B:513:TRP:HB2  | 2:B:551:LEU:HD11 | 1.83                     | 0.60              |
| 3:M:223:HIS:HA   | 3:M:479:PHE:CG   | 2.35                     | 0.60              |
| 1:A:484:VAL:O    | 1:A:486:SER:O    | 2.19                     | 0.60              |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:HD21 | 1.81                     | 0.60              |
| 2:B:334:MET:HG3  | 2:B:369:LEU:HD23 | 1.82                     | 0.60              |
| 2:B:335:LYS:HA   | 2:B:370:ASP:OD2  | 2.01                     | 0.60              |
| 2:B:502:SER:O    | 2:B:503:LEU:C    | 2.39                     | 0.60              |
| 2:B:588:ILE:HG21 | 2:B:618:PHE:HE1  | 1.66                     | 0.60              |
| 2:B:189:HIS:NE2  | 2:B:193:LEU:CD1  | 2.60                     | 0.60              |
| 2:B:278:PRO:CG   | 2:B:292:GLU:HB2  | 2.30                     | 0.60              |
| 3:M:6:TYR:N      | 3:M:6:TYR:CD1    | 2.69                     | 0.60              |
| 3:M:258:VAL:HG13 | 3:M:449:VAL:CG1  | 2.30                     | 0.60              |
| 3:M:284:SER:O    | 3:M:286:SER:N    | 2.33                     | 0.60              |
| 3:M:316:ARG:O    | 3:M:317:MET:C    | 2.41                     | 0.60              |
| 3:M:372:ILE:O    | 3:M:372:ILE:HG22 | 2.02                     | 0.60              |
| 3:M:478:ASN:O    | 3:M:479:PHE:C    | 2.42                     | 0.60              |
| 1:A:229:ASN:O    | 1:A:230:PRO:C    | 2.35                     | 0.60              |
| 1:A:244:LEU:HA   | 1:A:256:LEU:HD13 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:323:CYS:HG   | 1:A:338:PHE:HE1  | 1.50                     | 0.60              |
| 1:A:441:TYR:O    | 1:A:442:SER:C    | 2.43                     | 0.60              |
| 1:A:588:LEU:O    | 1:A:589:SER:C    | 2.36                     | 0.60              |
| 2:B:20:ARG:HD2   | 2:B:21:GLU:HB2   | 1.73                     | 0.60              |
| 2:B:396:ILE:HD11 | 2:B:418:TYR:CE2  | 2.37                     | 0.60              |
| 1:A:552:ILE:HG12 | 1:A:585:PHE:CE1  | 2.37                     | 0.60              |
| 3:M:222:PHE:CE1  | 3:M:240:ILE:CG2  | 2.84                     | 0.60              |
| 3:M:383:HIS:HB3  | 3:M:403:THR:OG1  | 2.01                     | 0.60              |
| 1:A:100:LEU:O    | 1:A:101:GLN:O    | 2.20                     | 0.60              |
| 1:A:349:ILE:CG2  | 1:A:378:ILE:CG2  | 2.77                     | 0.60              |
| 1:A:398:GLU:HA   | 1:A:418:ILE:HG13 | 1.84                     | 0.60              |
| 1:A:535:ILE:O    | 1:A:535:ILE:HG22 | 2.01                     | 0.60              |
| 2:B:296:ASP:OD1  | 2:B:297:PRO:CD   | 2.49                     | 0.60              |
| 4:S:70:ASN:HD22  | 4:S:73:ILE:HD12  | 1.66                     | 0.60              |
| 1:A:200:PHE:CE1  | 1:A:236:LEU:HD11 | 2.37                     | 0.60              |
| 1:A:251:TRP:CZ3  | 4:S:96:LEU:O     | 2.54                     | 0.60              |
| 1:A:563:CYS:O    | 1:A:566:PHE:CD2  | 2.55                     | 0.60              |
| 1:A:602:GLU:OE2  | 1:A:633:PHE:HE1  | 1.82                     | 0.60              |
| 2:B:21:GLU:OE2   | 2:B:35:TYR:O     | 2.19                     | 0.60              |
| 2:B:230:PHE:CE2  | 2:B:298:ASP:C    | 2.76                     | 0.60              |
| 2:B:452:LYS:NZ   | 2:B:456:ASP:OD2  | 2.34                     | 0.60              |
| 2:B:497:LEU:HD21 | 2:B:533:LEU:CD2  | 2.32                     | 0.60              |
| 2:B:563:PHE:CD2  | 2:B:584:SER:HB2  | 2.36                     | 0.60              |
| 3:M:44:ASP:CB    | 3:M:50:TYR:CD2   | 2.85                     | 0.60              |
| 3:M:243:ILE:HB   | 3:M:473:LYS:O    | 2.01                     | 0.60              |
| 3:M:288:ILE:CD1  | 3:M:300:LEU:HD22 | 2.32                     | 0.60              |
| 1:A:224:GLU:O    | 1:A:225:LEU:C    | 2.38                     | 0.60              |
| 1:A:605:GLU:OE2  | 1:A:632:PHE:CE2  | 2.54                     | 0.60              |
| 2:B:199:LEU:O    | 2:B:200:MET:C    | 2.44                     | 0.60              |
| 2:B:266:VAL:HG11 | 2:B:275:ARG:HB3  | 1.83                     | 0.60              |
| 2:B:519:ALA:O    | 2:B:523:PHE:CA   | 2.49                     | 0.60              |
| 2:B:602:ASP:O    | 2:B:608:ARG:NH2  | 2.35                     | 0.60              |
| 3:M:243:ILE:HD13 | 3:M:301:GLU:HB3  | 1.84                     | 0.60              |
| 2:B:83:PHE:CZ    | 2:B:105:LEU:HG   | 2.37                     | 0.60              |
| 2:B:108:PHE:CE2  | 2:B:115:LEU:CB   | 2.85                     | 0.60              |
| 2:B:219:TYR:HD1  | 2:B:226:LEU:HD22 | 1.58                     | 0.60              |
| 2:B:340:ILE:HG13 | 2:B:373:LEU:HD23 | 1.82                     | 0.60              |
| 2:B:346:THR:O    | 2:B:349:MET:N    | 2.34                     | 0.60              |
| 2:B:394:TRP:HZ3  | 2:B:397:GLN:OE1  | 1.83                     | 0.60              |
| 2:B:463:LEU:HD13 | 2:B:467:VAL:HG11 | 1.83                     | 0.60              |
| 2:B:577:ASN:O    | 2:B:578:PRO:O    | 2.19                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:53:THR:O     | 4:S:69:ASN:CG    | 2.44                     | 0.60              |
| 1:A:609:LEU:HD13 | 1:A:609:LEU:C    | 2.26                     | 0.59              |
| 2:B:105:LEU:HG   | 2:B:119:SER:CB   | 2.29                     | 0.59              |
| 2:B:136:CYS:HB3  | 2:B:172:GLU:HG2  | 1.82                     | 0.59              |
| 2:B:197:LYS:CB   | 2:B:229:HIS:CD2  | 2.85                     | 0.59              |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:CA   | 2.31                     | 0.59              |
| 2:B:241:ASP:CB   | 3:M:274:ASP:CA   | 2.77                     | 0.59              |
| 2:B:243:TRP:CZ2  | 3:M:95:THR:HA    | 2.37                     | 0.59              |
| 2:B:602:ASP:O    | 2:B:608:ARG:CZ   | 2.50                     | 0.59              |
| 1:A:266:VAL:O    | 1:A:267:GLU:HB2  | 2.02                     | 0.59              |
| 2:B:136:CYS:HA   | 2:B:172:GLU:HB2  | 1.83                     | 0.59              |
| 2:B:165:PRO:HA   | 2:B:170:ARG:HH21 | 1.67                     | 0.59              |
| 3:M:316:ARG:CG   | 3:M:322:LEU:HD13 | 2.31                     | 0.59              |
| 3:M:319:SER:HB3  | 3:M:343:ASN:O    | 2.02                     | 0.59              |
| 4:S:6:LEU:HD21   | 4:S:36:TYR:CE1   | 2.37                     | 0.59              |
| 1:A:244:LEU:CD2  | 1:A:277:LYS:O    | 2.49                     | 0.59              |
| 1:A:513:ARG:CD   | 1:A:550:VAL:HG21 | 2.28                     | 0.59              |
| 2:B:261:PRO:HG2  | 2:B:292:GLU:CB   | 2.31                     | 0.59              |
| 2:B:479:VAL:HG13 | 2:B:486:HIS:CD2  | 2.24                     | 0.59              |
| 3:M:99:ILE:CG2   | 3:M:124:ILE:CG2  | 2.81                     | 0.59              |
| 3:M:262:THR:HG22 | 3:M:265:ASN:H    | 1.67                     | 0.59              |
| 2:B:2:VAL:CG1    | 2:B:6:HIS:NE2    | 2.66                     | 0.59              |
| 2:B:24:ALA:CA    | 2:B:35:TYR:CD2   | 2.86                     | 0.59              |
| 2:B:25:VAL:HG22  | 2:B:35:TYR:HB3   | 1.85                     | 0.59              |
| 2:B:37:TYR:CE2   | 2:B:42:ILE:HA    | 2.37                     | 0.59              |
| 2:B:305:SER:O    | 2:B:309:LEU:HD23 | 2.02                     | 0.59              |
| 2:B:374:PHE:CB   | 2:B:402:LEU:HD21 | 2.32                     | 0.59              |
| 2:B:418:TYR:HD1  | 2:B:424:PHE:CD1  | 2.19                     | 0.59              |
| 2:B:560:ILE:CA   | 2:B:563:PHE:HB2  | 2.32                     | 0.59              |
| 3:M:71:LYS:O     | 3:M:74:TYR:CD2   | 2.55                     | 0.59              |
| 3:M:336:ASP:O    | 3:M:414:CYS:SG   | 2.54                     | 0.59              |
| 2:B:172:GLU:O    | 2:B:174:ALA:N    | 2.36                     | 0.59              |
| 2:B:261:PRO:CD   | 2:B:293:VAL:CG2  | 2.75                     | 0.59              |
| 2:B:490:ILE:HG13 | 2:B:518:ILE:HG12 | 1.84                     | 0.59              |
| 2:B:523:PHE:O    | 2:B:524:LYS:C    | 2.36                     | 0.59              |
| 3:M:100:LEU:HB3  | 3:M:109:LEU:CD2  | 2.32                     | 0.59              |
| 4:S:5:VAL:HG13   | 4:S:87:PHE:CE2   | 2.37                     | 0.59              |
| 4:S:87:PHE:CZ    | 4:S:102:ILE:HG12 | 2.37                     | 0.59              |
| 4:S:126:GLN:NE2  | 4:S:127:THR:OG1  | 2.36                     | 0.59              |
| 1:A:440:ASN:C    | 1:A:442:SER:H    | 2.09                     | 0.59              |
| 1:A:582:ILE:HG23 | 1:A:604:LEU:HG   | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:167:ALA:O    | 2:B:207:VAL:CG1  | 2.51                     | 0.59              |
| 2:B:185:LYS:O    | 2:B:186:ASN:C    | 2.23                     | 0.59              |
| 2:B:303:LEU:HD11 | 2:B:333:GLN:HB3  | 1.84                     | 0.59              |
| 2:B:519:ALA:HB1  | 2:B:555:LEU:HD12 | 1.83                     | 0.59              |
| 1:A:289:SER:HB3  | 4:S:96:LEU:HB3   | 1.85                     | 0.59              |
| 1:A:599:ARG:CZ   | 2:B:513:TRP:CE3  | 2.86                     | 0.59              |
| 2:B:231:ARG:O    | 2:B:233:TYR:N    | 2.36                     | 0.59              |
| 2:B:473:ASN:O    | 2:B:476:ARG:HB3  | 2.02                     | 0.59              |
| 2:B:599:ALA:O    | 2:B:601:TYR:N    | 2.36                     | 0.59              |
| 3:M:306:LEU:CD1  | 3:M:317:MET:HE3  | 2.32                     | 0.59              |
| 3:M:461:GLY:C    | 3:M:462:LYS:O    | 2.27                     | 0.59              |
| 4:S:17:VAL:HG21  | 4:S:19:PHE:CE2   | 2.38                     | 0.59              |
| 1:A:150:LEU:HB3  | 1:A:162:ILE:CD1  | 2.33                     | 0.59              |
| 1:A:553:LEU:HD22 | 2:B:610:ARG:HH21 | 1.67                     | 0.59              |
| 2:B:162:VAL:O    | 2:B:163:THR:C    | 2.40                     | 0.59              |
| 2:B:291:TYR:HE2  | 2:B:294:VAL:HB   | 1.68                     | 0.59              |
| 3:M:16:PHE:CE1   | 3:M:122:SER:HB2  | 2.32                     | 0.59              |
| 3:M:245:ASP:N    | 3:M:472:TYR:CZ   | 2.71                     | 0.59              |
| 3:M:338:PHE:CD2  | 3:M:415:ILE:CG1  | 2.85                     | 0.59              |
| 2:B:37:TYR:CD2   | 2:B:38:TYR:HD1   | 2.20                     | 0.59              |
| 2:B:256:CYS:SG   | 2:B:299:LEU:HD23 | 2.43                     | 0.59              |
| 3:M:66:PHE:HA    | 3:M:78:ALA:O     | 2.03                     | 0.59              |
| 3:M:95:THR:OG1   | 3:M:137:SER:CB   | 2.43                     | 0.59              |
| 3:M:115:VAL:O    | 3:M:116:ASN:C    | 2.44                     | 0.59              |
| 4:S:31:LEU:O     | 4:S:35:VAL:HG13  | 2.03                     | 0.59              |
| 4:S:49:SER:C     | 4:S:77:TYR:HB2   | 2.27                     | 0.59              |
| 1:A:461:CYS:SG   | 1:A:469:LEU:HB3  | 2.42                     | 0.59              |
| 2:B:2:VAL:HA     | 2:B:5:ILE:HD12   | 1.84                     | 0.59              |
| 2:B:56:SER:O     | 2:B:57:ARG:C     | 2.43                     | 0.59              |
| 2:B:549:LEU:HD23 | 2:B:610:ARG:HB2  | 1.85                     | 0.59              |
| 3:M:217:ASP:HB2  | 3:M:470:ALA:O    | 2.03                     | 0.59              |
| 3:M:220:GLU:CD   | 3:M:222:PHE:CE1  | 2.81                     | 0.59              |
| 1:A:203:PHE:CE2  | 1:A:221:VAL:HG11 | 2.38                     | 0.58              |
| 1:A:464:ILE:HG23 | 1:A:465:SER:HA   | 1.85                     | 0.58              |
| 2:B:230:PHE:HD2  | 2:B:298:ASP:CB   | 2.12                     | 0.58              |
| 2:B:577:ASN:O    | 2:B:578:PRO:C    | 2.39                     | 0.58              |
| 3:M:44:ASP:C     | 3:M:46:SER:N     | 2.60                     | 0.58              |
| 3:M:214:LEU:HD11 | 3:M:452:ILE:HG21 | 1.85                     | 0.58              |
| 3:M:376:ILE:HG21 | 3:M:379:LEU:CD1  | 2.32                     | 0.58              |
| 3:M:379:LEU:HB3  | 3:M:411:LEU:HD11 | 1.84                     | 0.58              |
| 4:S:17:VAL:HG21  | 4:S:19:PHE:HZ    | 1.63                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:LEU:HD11 | 1:A:314:ALA:HB1  | 1.85                     | 0.58              |
| 1:A:429:VAL:HG11 | 1:A:473:ILE:HD11 | 1.85                     | 0.58              |
| 1:A:609:LEU:CD2  | 1:A:628:VAL:CG1  | 2.71                     | 0.58              |
| 2:B:25:VAL:HG11  | 2:B:36:THR:HG1   | 1.64                     | 0.58              |
| 2:B:219:TYR:CD2  | 2:B:226:LEU:CB   | 2.77                     | 0.58              |
| 2:B:352:ASN:ND2  | 3:M:48:ASP:O     | 2.36                     | 0.58              |
| 3:M:48:ASP:C     | 3:M:75:TRP:CZ2   | 2.81                     | 0.58              |
| 3:M:48:ASP:C     | 3:M:75:TRP:HH2   | 2.08                     | 0.58              |
| 3:M:245:ASP:O    | 3:M:246:VAL:HG22 | 2.03                     | 0.58              |
| 3:M:302:TYR:CE2  | 3:M:445:SER:CB   | 2.86                     | 0.58              |
| 3:M:317:MET:HB2  | 3:M:322:LEU:H    | 1.67                     | 0.58              |
| 3:M:374:TYR:HB3  | 3:M:417:TYR:HD2  | 1.68                     | 0.58              |
| 3:M:403:THR:CG2  | 3:M:407:THR:OG1  | 2.52                     | 0.58              |
| 1:A:107:TYR:CD2  | 1:A:128:LEU:CD2  | 2.86                     | 0.58              |
| 1:A:134:TYR:O    | 1:A:135:ASP:C    | 2.42                     | 0.58              |
| 1:A:297:CYS:O    | 1:A:298:ILE:C    | 2.40                     | 0.58              |
| 2:B:21:GLU:CD    | 2:B:39:SER:CB    | 2.66                     | 0.58              |
| 2:B:321:CYS:O    | 2:B:325:LEU:HG   | 2.03                     | 0.58              |
| 2:B:374:PHE:CZ   | 2:B:381:PHE:CE1  | 2.92                     | 0.58              |
| 1:A:114:PHE:CE2  | 1:A:152:THR:C    | 2.82                     | 0.58              |
| 1:A:170:LEU:HB3  | 1:A:206:LYS:HD2  | 1.85                     | 0.58              |
| 1:A:291:ILE:HG21 | 1:A:322:PHE:CE1  | 2.39                     | 0.58              |
| 1:A:303:MET:HG2  | 1:A:308:ASP:OD2  | 2.03                     | 0.58              |
| 1:A:556:VAL:HG22 | 1:A:603:VAL:HG13 | 1.85                     | 0.58              |
| 1:A:570:LYS:O    | 1:A:571:ARG:HB2  | 2.03                     | 0.58              |
| 2:B:123:LEU:O    | 2:B:127:LEU:CG   | 2.48                     | 0.58              |
| 2:B:431:MET:C    | 2:B:433:VAL:H    | 2.10                     | 0.58              |
| 2:B:479:VAL:HG22 | 2:B:486:HIS:CG   | 2.37                     | 0.58              |
| 2:B:545:ARG:CD   | 2:B:602:ASP:OD2  | 2.52                     | 0.58              |
| 2:B:563:PHE:CD1  | 2:B:588:ILE:HD12 | 2.38                     | 0.58              |
| 3:M:244:VAL:O    | 3:M:299:LEU:HB3  | 2.04                     | 0.58              |
| 3:M:341:SER:OG   | 3:M:343:ASN:ND2  | 2.35                     | 0.58              |
| 1:A:260:PHE:CE1  | 1:A:274:LEU:HD12 | 2.39                     | 0.58              |
| 1:A:512:LEU:HD13 | 1:A:543:TYR:CE1  | 2.39                     | 0.58              |
| 1:A:516:ILE:HD13 | 1:A:551:LEU:HA   | 1.84                     | 0.58              |
| 2:B:325:LEU:HB3  | 2:B:334:MET:SD   | 2.43                     | 0.58              |
| 2:B:475:ILE:HG22 | 2:B:514:LEU:CD2  | 2.33                     | 0.58              |
| 2:B:486:HIS:NE2  | 2:B:490:ILE:HD11 | 2.17                     | 0.58              |
| 2:B:566:ALA:N    | 2:B:574:ASN:ND2  | 2.42                     | 0.58              |
| 3:M:216:VAL:O    | 3:M:216:VAL:HG23 | 2.03                     | 0.58              |
| 3:M:217:ASP:O    | 3:M:472:TYR:CD1  | 2.57                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:290:PHE:CE2  | 3:M:297:PHE:CE1  | 2.91                     | 0.58              |
| 3:M:437:TYR:CE1  | 3:M:479:PHE:CE1  | 2.91                     | 0.58              |
| 4:S:8:PHE:CE2    | 4:S:86:THR:OG1   | 2.45                     | 0.58              |
| 4:S:16:LEU:HD23  | 4:S:128:LEU:CD2  | 2.33                     | 0.58              |
| 1:A:71:VAL:CG1   | 1:A:105:VAL:HG12 | 2.33                     | 0.58              |
| 1:A:531:ASP:O    | 1:A:534:LYS:O    | 2.20                     | 0.58              |
| 1:A:556:VAL:CG2  | 1:A:603:VAL:HG11 | 2.33                     | 0.58              |
| 2:B:396:ILE:CD1  | 2:B:418:TYR:CE2  | 2.86                     | 0.58              |
| 3:M:48:ASP:O     | 3:M:75:TRP:CZ2   | 2.57                     | 0.58              |
| 3:M:245:ASP:HB3  | 3:M:472:TYR:CE1  | 2.35                     | 0.58              |
| 3:M:269:ILE:C    | 3:M:302:TYR:CE1  | 2.82                     | 0.58              |
| 3:M:276:VAL:CG2  | 3:M:299:LEU:HD12 | 2.33                     | 0.58              |
| 3:M:433:VAL:CG1  | 3:M:481:VAL:HB   | 2.33                     | 0.58              |
| 4:S:47:GLN:HG2   | 4:S:84:TYR:CE2   | 2.39                     | 0.58              |
| 1:A:429:VAL:HG11 | 1:A:469:LEU:HD11 | 1.83                     | 0.58              |
| 2:B:141:ALA:O    | 2:B:143:SER:N    | 2.37                     | 0.58              |
| 2:B:162:VAL:CG2  | 2:B:199:LEU:CD1  | 2.81                     | 0.58              |
| 2:B:178:ILE:HG22 | 2:B:179:LYS:N    | 2.17                     | 0.58              |
| 2:B:374:PHE:HE2  | 2:B:402:LEU:CD1  | 2.05                     | 0.58              |
| 3:M:16:PHE:CA    | 3:M:118:TYR:CD1  | 2.84                     | 0.58              |
| 3:M:99:ILE:CD1   | 3:M:128:CYS:SG   | 2.92                     | 0.58              |
| 3:M:315:VAL:O    | 3:M:315:VAL:HG12 | 2.03                     | 0.58              |
| 1:A:85:ALA:O     | 1:A:88:ASN:HB2   | 2.03                     | 0.58              |
| 1:A:176:TYR:CD1  | 4:S:143:GLU:OE2  | 2.55                     | 0.58              |
| 2:B:136:CYS:SG   | 2:B:168:MET:O    | 2.62                     | 0.58              |
| 2:B:278:PRO:CA   | 2:B:288:TYR:HB3  | 2.20                     | 0.58              |
| 4:S:105:PHE:CZ   | 4:S:128:LEU:HD11 | 2.39                     | 0.58              |
| 1:A:80:TYR:HB2   | 1:A:82:PHE:CD2   | 2.39                     | 0.58              |
| 1:A:186:PHE:CA   | 1:A:221:VAL:HG13 | 2.34                     | 0.58              |
| 1:A:520:GLY:HA2  | 1:A:558:VAL:CG2  | 2.34                     | 0.58              |
| 1:A:630:PRO:CG   | 2:B:617:LEU:HD11 | 1.98                     | 0.58              |
| 2:B:334:MET:C    | 2:B:336:ASN:N    | 2.34                     | 0.58              |
| 2:B:415:LEU:O    | 2:B:418:TYR:N    | 2.33                     | 0.58              |
| 2:B:418:TYR:OH   | 2:B:432:ALA:CB   | 2.51                     | 0.58              |
| 2:B:553:ALA:CB   | 2:B:614:ILE:CD1  | 2.70                     | 0.58              |
| 3:M:100:LEU:HD11 | 3:M:121:ILE:HG23 | 1.86                     | 0.58              |
| 3:M:218:LEU:N    | 3:M:218:LEU:HD12 | 2.18                     | 0.58              |
| 3:M:223:HIS:HE1  | 3:M:476:THR:H    | 1.52                     | 0.58              |
| 4:S:14:PRO:HA    | 4:S:36:TYR:OH    | 2.03                     | 0.58              |
| 4:S:93:GLU:OE1   | 4:S:93:GLU:HA    | 2.04                     | 0.58              |
| 1:A:204:VAL:HG13 | 1:A:239:LEU:HD11 | 1.81                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:244:LEU:O    | 1:A:245:VAL:C    | 2.46                     | 0.58              |
| 1:A:260:PHE:CD2  | 1:A:274:LEU:CG   | 2.81                     | 0.58              |
| 1:A:274:LEU:O    | 1:A:277:LYS:N    | 2.36                     | 0.58              |
| 1:A:609:LEU:CG   | 1:A:628:VAL:HB   | 2.31                     | 0.58              |
| 2:B:197:LYS:N    | 2:B:229:HIS:CE1  | 2.72                     | 0.58              |
| 2:B:469:ASP:OD1  | 2:B:506:ASN:HB2  | 2.04                     | 0.58              |
| 2:B:563:PHE:O    | 2:B:566:ALA:CB   | 2.49                     | 0.58              |
| 3:M:379:LEU:HD22 | 3:M:397:TRP:CE2  | 2.39                     | 0.58              |
| 1:A:78:GLU:O     | 1:A:80:TYR:O     | 2.21                     | 0.57              |
| 1:A:244:LEU:HD11 | 1:A:281:LEU:HD12 | 1.84                     | 0.57              |
| 1:A:323:CYS:SG   | 1:A:355:LEU:HD21 | 2.43                     | 0.57              |
| 2:B:90:ILE:HD11  | 2:B:102:HIS:CD2  | 2.38                     | 0.57              |
| 2:B:137:PHE:O    | 2:B:140:SER:HB3  | 2.04                     | 0.57              |
| 2:B:253:ILE:HG12 | 2:B:324:ALA:CB   | 2.34                     | 0.57              |
| 2:B:267:ASP:O    | 2:B:269:SER:N    | 2.36                     | 0.57              |
| 3:M:134:PRO:O    | 3:M:136:VAL:CA   | 2.52                     | 0.57              |
| 4:S:157:ASN:O    | 4:S:161:GLU:HG3  | 2.04                     | 0.57              |
| 1:A:71:VAL:HG12  | 1:A:105:VAL:HG12 | 1.84                     | 0.57              |
| 1:A:147:LEU:HD22 | 1:A:166:LEU:HD23 | 1.84                     | 0.57              |
| 1:A:247:ILE:HG21 | 1:A:252:ILE:CG2  | 2.33                     | 0.57              |
| 1:A:516:ILE:HD13 | 1:A:551:LEU:CA   | 2.34                     | 0.57              |
| 2:B:161:LEU:HB3  | 2:B:173:VAL:HG21 | 1.83                     | 0.57              |
| 2:B:217:GLU:O    | 2:B:218:CYS:C    | 2.47                     | 0.57              |
| 2:B:513:TRP:CB   | 2:B:551:LEU:HD21 | 2.34                     | 0.57              |
| 3:M:293:PRO:HB2  | 3:M:294:ASP:O    | 2.03                     | 0.57              |
| 3:M:374:TYR:CB   | 3:M:417:TYR:CD2  | 2.87                     | 0.57              |
| 1:A:83:ASP:CG    | 1:A:85:ALA:H     | 2.12                     | 0.57              |
| 2:B:13:ASP:O     | 2:B:14:THR:C     | 2.47                     | 0.57              |
| 2:B:177:ILE:HB   | 2:B:196:LEU:HD21 | 1.87                     | 0.57              |
| 2:B:344:VAL:HG13 | 2:B:381:PHE:CZ   | 2.39                     | 0.57              |
| 2:B:526:CYS:N    | 2:B:527:PRO:HD3  | 2.17                     | 0.57              |
| 2:B:577:ASN:C    | 2:B:578:PRO:O    | 2.48                     | 0.57              |
| 4:S:53:THR:CG2   | 4:S:67:GLU:O     | 2.52                     | 0.57              |
| 4:S:109:LEU:CD1  | 4:S:113:PHE:CD1  | 2.87                     | 0.57              |
| 1:A:190:LEU:HD11 | 1:A:228:LYS:HE3  | 1.86                     | 0.57              |
| 1:A:555:LEU:HD13 | 1:A:581:LEU:HD13 | 1.81                     | 0.57              |
| 2:B:268:LYS:CA   | 2:B:276:SER:HB2  | 2.33                     | 0.57              |
| 2:B:310:ILE:HG23 | 2:B:318:ILE:HG23 | 1.87                     | 0.57              |
| 2:B:546:CYS:N    | 2:B:607:ILE:HD13 | 2.19                     | 0.57              |
| 1:A:480:LEU:O    | 1:A:483:LYS:O    | 2.22                     | 0.57              |
| 2:B:243:TRP:CZ2  | 3:M:98:ARG:NE    | 2.71                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:267:ASP:H    | 2:B:289:PRO:HB3  | 1.68                     | 0.57              |
| 2:B:277:CYS:SG   | 2:B:292:GLU:HG3  | 2.45                     | 0.57              |
| 3:M:338:PHE:CD2  | 3:M:415:ILE:CD1  | 2.87                     | 0.57              |
| 1:A:326:GLN:HA   | 1:A:331:ARG:HH21 | 1.68                     | 0.57              |
| 1:A:371:ALA:O    | 1:A:374:LEU:HB2  | 2.04                     | 0.57              |
| 1:A:464:ILE:O    | 2:B:1:MET:SD     | 2.62                     | 0.57              |
| 2:B:140:SER:O    | 2:B:143:SER:N    | 2.35                     | 0.57              |
| 2:B:151:ALA:C    | 2:B:188:TYR:CE2  | 2.66                     | 0.57              |
| 2:B:185:LYS:HE2  | 2:B:221:ASP:OD2  | 2.04                     | 0.57              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:HA   | 2.33                     | 0.57              |
| 2:B:512:VAL:HG13 | 2:B:533:LEU:HD13 | 1.86                     | 0.57              |
| 2:B:560:ILE:CG2  | 2:B:564:LYS:HB2  | 2.32                     | 0.57              |
| 4:S:60:SER:O     | 4:S:66:ASP:HB2   | 2.03                     | 0.57              |
| 1:A:151:SER:O    | 1:A:152:THR:C    | 2.41                     | 0.57              |
| 1:A:373:GLU:HG2  | 1:A:427:LYS:HE2  | 1.86                     | 0.57              |
| 1:A:638:LEU:CD2  | 2:B:558:TYR:CA   | 2.50                     | 0.57              |
| 2:B:37:TYR:CD2   | 2:B:38:TYR:CD1   | 2.90                     | 0.57              |
| 2:B:166:SER:O    | 2:B:170:ARG:HG3  | 2.04                     | 0.57              |
| 2:B:188:TYR:HB3  | 2:B:192:LEU:HD13 | 1.86                     | 0.57              |
| 2:B:409:LYS:O    | 2:B:413:LYS:HG3  | 2.04                     | 0.57              |
| 2:B:431:MET:O    | 2:B:433:VAL:N    | 2.38                     | 0.57              |
| 2:B:482:ASN:N    | 2:B:483:PRO:HD3  | 2.20                     | 0.57              |
| 3:M:97:ASP:O     | 3:M:100:LEU:HB2  | 2.04                     | 0.57              |
| 3:M:374:TYR:CE1  | 3:M:376:ILE:HD11 | 2.40                     | 0.57              |
| 1:A:170:LEU:O    | 1:A:206:LYS:HD2  | 2.04                     | 0.57              |
| 1:A:185:LEU:HB2  | 1:A:203:PHE:CZ   | 2.40                     | 0.57              |
| 1:A:244:LEU:HD23 | 1:A:277:LYS:HG3  | 1.86                     | 0.57              |
| 1:A:298:ILE:CD1  | 1:A:311:THR:CG2  | 2.83                     | 0.57              |
| 1:A:429:VAL:HG21 | 1:A:469:LEU:HD21 | 1.87                     | 0.57              |
| 2:B:293:VAL:O    | 2:B:299:LEU:HB3  | 2.04                     | 0.57              |
| 2:B:519:ALA:CB   | 2:B:555:LEU:HD13 | 2.35                     | 0.57              |
| 2:B:567:GLN:N    | 2:B:574:ASN:ND2  | 2.52                     | 0.57              |
| 2:B:575:ASN:C    | 2:B:576:GLN:O    | 2.31                     | 0.57              |
| 3:M:319:SER:CB   | 3:M:343:ASN:O    | 2.53                     | 0.57              |
| 3:M:419:ASN:OD1  | 3:M:424:PHE:CD2  | 2.57                     | 0.57              |
| 1:A:154:ILE:HG21 | 1:A:191:GLN:CG   | 2.34                     | 0.57              |
| 1:A:323:CYS:HB2  | 1:A:355:LEU:HD21 | 1.87                     | 0.57              |
| 2:B:285:GLU:O    | 2:B:286:ILE:O    | 2.21                     | 0.57              |
| 2:B:418:TYR:CD1  | 2:B:419:VAL:CA   | 2.88                     | 0.57              |
| 2:B:520:SER:HB3  | 2:B:558:TYR:CD2  | 2.40                     | 0.57              |
| 2:B:588:ILE:CG2  | 2:B:618:PHE:CZ   | 2.81                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:354:ASP:O    | 3:M:438:SER:O    | 2.22                     | 0.57              |
| 4:S:131:VAL:HG22 | 4:S:153:VAL:CG2  | 2.25                     | 0.57              |
| 1:A:114:PHE:O    | 1:A:115:TYR:O    | 2.22                     | 0.57              |
| 1:A:253:ILE:CD1  | 1:A:285:THR:HG21 | 2.34                     | 0.57              |
| 1:A:595:GLU:HG2  | 2:B:473:ASN:CG   | 2.30                     | 0.57              |
| 2:B:103:LEU:CD2  | 3:M:131:ALA:O    | 2.51                     | 0.57              |
| 2:B:147:MET:O    | 2:B:148:SER:C    | 2.41                     | 0.57              |
| 2:B:307:ASN:OD1  | 2:B:339:PHE:CE2  | 2.57                     | 0.57              |
| 2:B:351:GLU:C    | 3:M:49:ASP:OD2   | 2.47                     | 0.57              |
| 2:B:361:GLN:O    | 2:B:364:HIS:HB3  | 2.05                     | 0.57              |
| 3:M:224:VAL:HG22 | 3:M:306:LEU:CD1  | 2.35                     | 0.57              |
| 3:M:405:THR:C    | 3:M:407:THR:H    | 2.12                     | 0.57              |
| 4:S:110:ASP:O    | 4:S:114:THR:HA   | 2.05                     | 0.57              |
| 1:A:322:PHE:HB3  | 1:A:330:LEU:HD21 | 1.86                     | 0.56              |
| 1:A:429:VAL:CG2  | 1:A:469:LEU:HD11 | 2.33                     | 0.56              |
| 2:B:234:CYS:CB   | 2:B:301:LEU:CB   | 2.82                     | 0.56              |
| 2:B:343:LEU:HD21 | 2:B:362:ALA:CB   | 2.35                     | 0.56              |
| 3:M:69:ILE:HG21  | 3:M:97:ASP:OD2   | 2.05                     | 0.56              |
| 3:M:375:LYS:HE3  | 3:M:418:GLU:OE1  | 2.05                     | 0.56              |
| 3:M:378:ILE:O    | 3:M:413:GLY:HA2  | 2.03                     | 0.56              |
| 1:A:260:PHE:O    | 1:A:262:ASN:N    | 2.35                     | 0.56              |
| 1:A:268:PRO:HG3  | 1:A:271:ARG:HH21 | 1.69                     | 0.56              |
| 1:A:402:ILE:HG12 | 1:A:406:GLY:HA2  | 1.86                     | 0.56              |
| 1:A:498:LEU:HB3  | 1:A:504:ILE:HG13 | 1.85                     | 0.56              |
| 1:A:563:CYS:HA   | 1:A:566:PHE:HD2  | 1.68                     | 0.56              |
| 2:B:18:ILE:H     | 2:B:18:ILE:HD13  | 1.70                     | 0.56              |
| 2:B:42:ILE:HG22  | 2:B:43:ASN:O     | 2.05                     | 0.56              |
| 2:B:227:HIS:O    | 2:B:298:ASP:OD2  | 2.22                     | 0.56              |
| 2:B:284:ASN:O    | 2:B:284:ASN:CG   | 2.45                     | 0.56              |
| 3:M:220:GLU:OE1  | 3:M:443:SER:O    | 2.23                     | 0.56              |
| 3:M:302:TYR:CE2  | 3:M:445:SER:HB2  | 2.40                     | 0.56              |
| 1:A:114:PHE:CE1  | 1:A:153:ILE:HA   | 2.38                     | 0.56              |
| 1:A:450:TYR:CE1  | 1:A:454:ILE:HD11 | 2.41                     | 0.56              |
| 1:A:609:LEU:CG   | 1:A:628:VAL:CB   | 2.82                     | 0.56              |
| 2:B:108:PHE:HE2  | 2:B:112:ASP:HB3  | 1.69                     | 0.56              |
| 2:B:127:LEU:HD23 | 2:B:135:ARG:O    | 2.05                     | 0.56              |
| 2:B:247:TYR:HE1  | 3:M:137:SER:OG   | 1.82                     | 0.56              |
| 2:B:454:LEU:O    | 2:B:457:HIS:HB2  | 2.05                     | 0.56              |
| 3:M:217:ASP:N    | 3:M:472:TYR:CZ   | 2.73                     | 0.56              |
| 3:M:217:ASP:O    | 3:M:472:TYR:CE2  | 2.58                     | 0.56              |
| 3:M:235:LEU:HD11 | 3:M:306:LEU:HD13 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:265:ASN:HA   | 3:M:313:SER:HG   | 1.69                     | 0.56              |
| 3:M:300:LEU:C    | 3:M:300:LEU:HD12 | 2.31                     | 0.56              |
| 3:M:386:PHE:HB2  | 3:M:397:TRP:CD1  | 2.40                     | 0.56              |
| 4:S:16:LEU:HD22  | 4:S:128:LEU:HD23 | 1.85                     | 0.56              |
| 4:S:137:GLN:C    | 4:S:140:MET:H    | 2.13                     | 0.56              |
| 1:A:101:GLN:OE1  | 4:S:167:ILE:HD12 | 2.01                     | 0.56              |
| 1:A:318:ARG:O    | 1:A:322:PHE:HD1  | 1.88                     | 0.56              |
| 1:A:515:CYS:O    | 1:A:519:LEU:HG   | 2.05                     | 0.56              |
| 1:A:556:VAL:HG21 | 1:A:603:VAL:CG1  | 2.34                     | 0.56              |
| 2:B:87:VAL:O     | 2:B:88:LYS:C     | 2.44                     | 0.56              |
| 2:B:162:VAL:CG1  | 2:B:195:ILE:HG23 | 2.36                     | 0.56              |
| 2:B:200:MET:CG   | 2:B:232:ARG:HB3  | 2.27                     | 0.56              |
| 2:B:241:ASP:HB2  | 3:M:274:ASP:CA   | 2.35                     | 0.56              |
| 2:B:267:ASP:CA   | 2:B:289:PRO:HG3  | 2.35                     | 0.56              |
| 2:B:453:TRP:HE3  | 2:B:453:TRP:HA   | 1.71                     | 0.56              |
| 3:M:7:ILE:HA     | 3:M:75:TRP:O     | 2.05                     | 0.56              |
| 3:M:222:PHE:HB2  | 3:M:479:PHE:CZ   | 2.39                     | 0.56              |
| 3:M:224:VAL:O    | 3:M:480:GLN:N    | 2.36                     | 0.56              |
| 3:M:372:ILE:HD12 | 3:M:428:VAL:HG22 | 1.85                     | 0.56              |
| 1:A:125:THR:CG2  | 1:A:158:LEU:CD1  | 2.84                     | 0.56              |
| 1:A:154:ILE:HG22 | 1:A:191:GLN:HG3  | 1.84                     | 0.56              |
| 1:A:202:LYS:O    | 1:A:205:SER:N    | 2.39                     | 0.56              |
| 1:A:295:VAL:HG11 | 1:A:337:LEU:HD13 | 1.86                     | 0.56              |
| 1:A:332:TYR:OH   | 1:A:336:ILE:HD11 | 2.03                     | 0.56              |
| 2:B:171:GLY:HA3  | 2:B:207:VAL:HA   | 1.86                     | 0.56              |
| 3:M:350:VAL:CB   | 3:M:442:GLN:HG2  | 2.35                     | 0.56              |
| 4:S:9:ASN:ND2    | 4:S:118:GLU:OE1  | 2.39                     | 0.56              |
| 1:A:404:GLN:C    | 2:B:7:ARG:CZ     | 2.76                     | 0.56              |
| 1:A:637:GLU:HG3  | 2:B:516:GLY:C    | 2.30                     | 0.56              |
| 2:B:151:ALA:CB   | 2:B:180:LEU:CD1  | 2.81                     | 0.56              |
| 2:B:182:ARG:CG   | 2:B:217:GLU:HB3  | 2.35                     | 0.56              |
| 2:B:215:TYR:HB3  | 2:B:226:LEU:CD1  | 2.36                     | 0.56              |
| 2:B:252:LEU:CB   | 2:B:302:PHE:CD1  | 2.89                     | 0.56              |
| 2:B:276:SER:C    | 2:B:295:ASN:ND2  | 2.49                     | 0.56              |
| 2:B:311:TYR:HB2  | 3:M:269:ILE:HD13 | 1.87                     | 0.56              |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:HD12 | 1.87                     | 0.56              |
| 3:M:220:GLU:C    | 3:M:474:THR:OG1  | 2.43                     | 0.56              |
| 1:A:254:ILE:HG12 | 1:A:290:VAL:HA   | 1.86                     | 0.56              |
| 1:A:416:ILE:O    | 1:A:417:PRO:C    | 2.40                     | 0.56              |
| 1:A:633:PHE:HE2  | 2:B:554:LYS:HB2  | 1.65                     | 0.56              |
| 2:B:171:GLY:CA   | 2:B:207:VAL:CG1  | 2.73                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:214:ALA:C    | 2:B:216:LYS:N    | 2.61                     | 0.56              |
| 2:B:292:GLU:HG3  | 2:B:296:ASP:HB2  | 1.88                     | 0.56              |
| 2:B:453:TRP:HA   | 2:B:453:TRP:CE3  | 2.41                     | 0.56              |
| 2:B:550:VAL:CG2  | 2:B:610:ARG:CD   | 2.83                     | 0.56              |
| 4:S:8:PHE:N      | 4:S:8:PHE:HD2    | 2.03                     | 0.56              |
| 1:A:121:LEU:CD1  | 1:A:153:ILE:CG2  | 2.83                     | 0.56              |
| 1:A:128:LEU:CD1  | 1:A:150:LEU:HD23 | 2.36                     | 0.56              |
| 1:A:532:LEU:O    | 1:A:533:ILE:O    | 2.24                     | 0.56              |
| 2:B:90:ILE:HD11  | 2:B:123:LEU:CD2  | 2.36                     | 0.56              |
| 2:B:276:SER:OG   | 2:B:289:PRO:CG   | 2.53                     | 0.56              |
| 2:B:355:ASN:O    | 2:B:358:MET:N    | 2.38                     | 0.56              |
| 2:B:545:ARG:CD   | 2:B:602:ASP:CB   | 2.76                     | 0.56              |
| 3:M:217:ASP:CB   | 3:M:470:ALA:O    | 2.54                     | 0.56              |
| 3:M:443:SER:HB3  | 3:M:447:ILE:HG12 | 1.80                     | 0.56              |
| 4:S:8:PHE:CD2    | 4:S:84:TYR:O     | 2.58                     | 0.56              |
| 1:A:190:LEU:CD1  | 1:A:228:LYS:HG3  | 2.31                     | 0.56              |
| 1:A:384:LEU:HD12 | 1:A:385:LYS:N    | 2.20                     | 0.56              |
| 2:B:57:ARG:O     | 2:B:60:ARG:HB3   | 2.05                     | 0.56              |
| 2:B:127:LEU:CB   | 2:B:157:THR:CG2  | 2.81                     | 0.56              |
| 2:B:523:PHE:CE2  | 2:B:580:TYR:CE1  | 2.94                     | 0.56              |
| 2:B:589:SER:HG   | 2:B:618:PHE:HZ   | 1.45                     | 0.56              |
| 3:M:319:SER:HA   | 3:M:343:ASN:O    | 2.05                     | 0.56              |
| 3:M:376:ILE:HG22 | 3:M:379:LEU:HD12 | 1.88                     | 0.56              |
| 4:S:1:MET:H2     | 4:S:93:GLU:CD    | 2.12                     | 0.56              |
| 4:S:38:LEU:HB3   | 4:S:51:LEU:HD13  | 1.88                     | 0.56              |
| 1:A:420:ILE:HG23 | 1:A:424:TYR:CB   | 2.33                     | 0.56              |
| 1:A:606:PHE:CD2  | 1:A:629:LEU:HD11 | 2.41                     | 0.56              |
| 2:B:42:ILE:HG22  | 2:B:43:ASN:N     | 2.20                     | 0.56              |
| 2:B:175:LEU:O    | 2:B:178:ILE:HB   | 2.06                     | 0.56              |
| 2:B:197:LYS:O    | 2:B:199:LEU:N    | 2.39                     | 0.56              |
| 2:B:247:TYR:CE1  | 3:M:136:VAL:HG13 | 2.41                     | 0.56              |
| 2:B:303:LEU:HD11 | 2:B:333:GLN:CD   | 2.30                     | 0.56              |
| 2:B:404:ASN:O    | 2:B:408:VAL:HG23 | 2.06                     | 0.56              |
| 2:B:523:PHE:CE1  | 2:B:580:TYR:HB2  | 2.17                     | 0.56              |
| 3:M:244:VAL:CA   | 3:M:472:TYR:CE2  | 2.88                     | 0.56              |
| 1:A:186:PHE:CB   | 1:A:221:VAL:HG13 | 2.35                     | 0.55              |
| 1:A:244:LEU:CA   | 1:A:256:LEU:HD13 | 2.35                     | 0.55              |
| 1:A:292:TYR:CE1  | 1:A:296:ASN:HB2  | 2.42                     | 0.55              |
| 2:B:50:LEU:HG    | 2:B:58:GLU:O     | 2.06                     | 0.55              |
| 2:B:167:ALA:HB1  | 2:B:202:ASP:OD2  | 2.05                     | 0.55              |
| 2:B:212:VAL:HG11 | 2:B:248:LEU:HD23 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:340:ILE:HG13 | 2:B:373:LEU:CG   | 2.37                     | 0.55              |
| 2:B:431:MET:C    | 2:B:433:VAL:N    | 2.62                     | 0.55              |
| 3:M:253:ASN:OD1  | 3:M:292:PRO:CG   | 2.54                     | 0.55              |
| 3:M:262:THR:C    | 3:M:264:GLY:H    | 2.14                     | 0.55              |
| 1:A:225:LEU:CG   | 1:A:233:PHE:CZ   | 2.90                     | 0.55              |
| 2:B:219:TYR:CG   | 2:B:226:LEU:CD2  | 2.83                     | 0.55              |
| 2:B:306:LEU:HD12 | 2:B:325:LEU:CD2  | 2.37                     | 0.55              |
| 2:B:604:GLU:O    | 2:B:607:ILE:HB   | 2.06                     | 0.55              |
| 3:M:41:LEU:HB3   | 3:M:50:TYR:O     | 2.06                     | 0.55              |
| 1:A:64:LEU:HA    | 1:A:102:GLN:HE22 | 1.70                     | 0.55              |
| 1:A:128:LEU:HB2  | 1:A:150:LEU:HD21 | 1.87                     | 0.55              |
| 1:A:332:TYR:CE2  | 1:A:336:ILE:HD12 | 2.39                     | 0.55              |
| 1:A:438:ALA:O    | 1:A:439:ASP:CB   | 2.54                     | 0.55              |
| 1:A:638:LEU:HD11 | 2:B:519:ALA:C    | 2.31                     | 0.55              |
| 2:B:30:LEU:C     | 2:B:32:GLU:H     | 2.14                     | 0.55              |
| 2:B:50:LEU:HD23  | 2:B:62:ALA:HB2   | 1.89                     | 0.55              |
| 2:B:112:ASP:C    | 2:B:112:ASP:OD1  | 2.49                     | 0.55              |
| 2:B:139:LEU:HD11 | 2:B:158:VAL:HG22 | 1.88                     | 0.55              |
| 2:B:141:ALA:O    | 2:B:144:ASP:N    | 2.40                     | 0.55              |
| 2:B:155:LEU:HD13 | 2:B:155:LEU:C    | 2.30                     | 0.55              |
| 2:B:155:LEU:HG   | 2:B:188:TYR:HD2  | 1.70                     | 0.55              |
| 2:B:278:PRO:HA   | 2:B:288:TYR:O    | 2.00                     | 0.55              |
| 2:B:559:ASP:HB2  | 2:B:563:PHE:HD1  | 1.58                     | 0.55              |
| 3:M:220:GLU:HG2  | 3:M:439:TYR:HB2  | 1.88                     | 0.55              |
| 3:M:245:ASP:N    | 3:M:472:TYR:CE2  | 2.75                     | 0.55              |
| 3:M:437:TYR:HD1  | 3:M:479:PHE:CZ   | 2.21                     | 0.55              |
| 1:A:260:PHE:CD1  | 1:A:274:LEU:HD12 | 2.42                     | 0.55              |
| 1:A:332:TYR:CE1  | 1:A:366:SER:OG   | 2.55                     | 0.55              |
| 1:A:558:VAL:O    | 1:A:561:ASN:N    | 2.37                     | 0.55              |
| 1:A:566:PHE:C    | 1:A:566:PHE:CD1  | 2.83                     | 0.55              |
| 1:A:603:VAL:O    | 1:A:606:PHE:HB2  | 2.07                     | 0.55              |
| 2:B:127:LEU:HD13 | 2:B:157:THR:HG21 | 0.59                     | 0.55              |
| 2:B:231:ARG:NH2  | 2:B:297:PRO:HD2  | 2.21                     | 0.55              |
| 2:B:537:PHE:CE2  | 2:B:598:LEU:HB3  | 2.37                     | 0.55              |
| 2:B:572:GLU:O    | 2:B:575:ASN:N    | 2.34                     | 0.55              |
| 3:M:9:ASP:HB3    | 3:M:15:ILE:HD11  | 1.88                     | 0.55              |
| 3:M:215:TYR:CD1  | 3:M:467:TYR:O    | 2.59                     | 0.55              |
| 3:M:215:TYR:HD1  | 3:M:467:TYR:O    | 1.89                     | 0.55              |
| 3:M:347:PHE:CD1  | 3:M:350:VAL:CG1  | 2.88                     | 0.55              |
| 4:S:55:PRO:HB3   | 4:S:71:GLU:CG    | 2.37                     | 0.55              |
| 1:A:185:LEU:CD1  | 1:A:203:PHE:HE1  | 2.16                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:634:ASN:HB3  | 2:B:558:TYR:HD1  | 1.70                     | 0.55              |
| 2:B:195:ILE:C    | 2:B:197:LYS:N    | 2.62                     | 0.55              |
| 3:M:219:LEU:HD22 | 3:M:474:THR:N    | 2.22                     | 0.55              |
| 4:S:55:PRO:HG3   | 4:S:71:GLU:HG2   | 1.89                     | 0.55              |
| 1:A:158:LEU:HG   | 1:A:162:ILE:HD11 | 1.89                     | 0.55              |
| 2:B:237:ILE:HG13 | 2:B:248:LEU:HD12 | 1.87                     | 0.55              |
| 2:B:262:LYS:O    | 2:B:264:THR:N    | 2.40                     | 0.55              |
| 2:B:299:LEU:O    | 2:B:302:PHE:CB   | 2.52                     | 0.55              |
| 4:S:38:LEU:CD2   | 4:S:68:VAL:CG2   | 2.85                     | 0.55              |
| 1:A:102:GLN:HE21 | 4:S:166:LYS:HD2  | 1.69                     | 0.55              |
| 1:A:370:LYS:O    | 1:A:374:LEU:HD12 | 2.05                     | 0.55              |
| 2:B:87:VAL:HG13  | 2:B:122:SER:OG   | 2.07                     | 0.55              |
| 2:B:249:ILE:CD1  | 2:B:321:CYS:SG   | 2.95                     | 0.55              |
| 2:B:523:PHE:HB2  | 2:B:559:ASP:CG   | 2.30                     | 0.55              |
| 3:M:377:LYS:NZ   | 3:M:416:GLU:OE1  | 2.34                     | 0.55              |
| 3:M:429:ASP:O    | 3:M:430:LEU:C    | 2.45                     | 0.55              |
| 4:S:43:ASN:HB3   | 4:S:46:PHE:CD1   | 2.42                     | 0.55              |
| 1:A:219:VAL:HG13 | 1:A:256:LEU:HD23 | 1.85                     | 0.55              |
| 2:B:70:MET:HE1   | 2:B:107:ARG:CB   | 2.00                     | 0.55              |
| 2:B:252:LEU:HB3  | 2:B:302:PHE:CZ   | 2.27                     | 0.55              |
| 2:B:531:ARG:CB   | 2:B:591:MET:SD   | 2.95                     | 0.55              |
| 3:M:100:LEU:HD22 | 3:M:121:ILE:HG12 | 1.89                     | 0.55              |
| 3:M:271:SER:N    | 3:M:301:GLU:O    | 2.31                     | 0.55              |
| 3:M:288:ILE:HD12 | 3:M:300:LEU:CD2  | 2.37                     | 0.55              |
| 4:S:4:ALA:HB2    | 4:S:19:PHE:HD2   | 1.72                     | 0.55              |
| 1:A:318:ARG:O    | 1:A:322:PHE:CD1  | 2.60                     | 0.55              |
| 1:A:349:ILE:O    | 1:A:350:SER:C    | 2.49                     | 0.55              |
| 1:A:391:LEU:O    | 1:A:392:MET:O    | 2.22                     | 0.55              |
| 1:A:435:ILE:HG23 | 1:A:441:TYR:CE2  | 2.42                     | 0.55              |
| 1:A:570:LYS:HD2  | 1:A:614:LEU:HB3  | 1.89                     | 0.55              |
| 1:A:626:SER:O    | 1:A:630:PRO:CD   | 2.55                     | 0.55              |
| 2:B:249:ILE:HG12 | 2:B:306:LEU:HD23 | 1.88                     | 0.55              |
| 2:B:341:GLU:HG2  | 2:B:345:ARG:HE   | 1.72                     | 0.55              |
| 2:B:515:PHE:HA   | 2:B:518:ILE:HG22 | 1.89                     | 0.55              |
| 2:B:599:ALA:O    | 2:B:602:ASP:N    | 2.29                     | 0.55              |
| 4:S:46:PHE:O     | 4:S:47:GLN:C     | 2.29                     | 0.55              |
| 1:A:264:SER:CB   | 1:A:271:ARG:HD3  | 2.33                     | 0.55              |
| 2:B:374:PHE:CD2  | 2:B:402:LEU:HD13 | 2.40                     | 0.55              |
| 2:B:550:VAL:HG22 | 2:B:610:ARG:CD   | 2.26                     | 0.55              |
| 1:A:401:VAL:CG2  | 1:A:418:ILE:N    | 2.70                     | 0.54              |
| 1:A:602:GLU:CD   | 1:A:633:PHE:HE1  | 2.15                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:103:LEU:HD21 | 3:M:131:ALA:CA   | 2.38                     | 0.54              |
| 2:B:189:HIS:NE2  | 2:B:222:HIS:CB   | 2.69                     | 0.54              |
| 2:B:223:LEU:HB3  | 2:B:259:TYR:HD1  | 0.75                     | 0.54              |
| 2:B:332:LEU:HG   | 2:B:332:LEU:O    | 2.07                     | 0.54              |
| 3:M:290:PHE:CZ   | 3:M:297:PHE:CE1  | 2.96                     | 0.54              |
| 1:A:125:THR:CG2  | 1:A:158:LEU:HD13 | 2.36                     | 0.54              |
| 1:A:174:ARG:HH22 | 4:S:148:ARG:NH2  | 2.04                     | 0.54              |
| 1:A:586:GLU:O    | 1:A:588:LEU:N    | 2.34                     | 0.54              |
| 2:B:136:CYS:O    | 2:B:172:GLU:HB3  | 2.07                     | 0.54              |
| 2:B:226:LEU:O    | 2:B:226:LEU:HD12 | 2.07                     | 0.54              |
| 2:B:596:LEU:HD13 | 2:B:611:ALA:O    | 2.06                     | 0.54              |
| 3:M:56:VAL:N     | 3:M:64:LYS:HB2   | 2.22                     | 0.54              |
| 3:M:403:THR:HG22 | 3:M:407:THR:OG1  | 2.06                     | 0.54              |
| 1:A:375:VAL:HA   | 1:A:378:ILE:HG12 | 1.88                     | 0.54              |
| 1:A:404:GLN:O    | 2:B:4:S:SER:N    | 2.40                     | 0.54              |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:CD2  | 2.37                     | 0.54              |
| 2:B:461:HIS:O    | 2:B:462:ASN:O    | 2.21                     | 0.54              |
| 2:B:493:LEU:HD21 | 2:B:511:ILE:HA   | 1.88                     | 0.54              |
| 3:M:99:ILE:HG22  | 3:M:124:ILE:HD13 | 1.88                     | 0.54              |
| 3:M:338:PHE:HD2  | 3:M:415:ILE:HG13 | 1.70                     | 0.54              |
| 1:A:418:ILE:O    | 1:A:418:ILE:HG12 | 2.07                     | 0.54              |
| 1:A:450:TYR:OH   | 1:A:476:GLN:CD   | 2.50                     | 0.54              |
| 1:A:485:PRO:O    | 1:A:488:ARG:HG3  | 2.08                     | 0.54              |
| 2:B:292:GLU:O    | 2:B:296:ASP:HB3  | 2.07                     | 0.54              |
| 2:B:337:THR:CB   | 2:B:373:LEU:CD1  | 2.83                     | 0.54              |
| 2:B:490:ILE:CD1  | 2:B:514:LEU:HG   | 2.38                     | 0.54              |
| 2:B:519:ALA:HB1  | 2:B:555:LEU:HD13 | 1.88                     | 0.54              |
| 2:B:519:ALA:C    | 2:B:523:PHE:HB3  | 2.23                     | 0.54              |
| 2:B:530:LEU:HD23 | 2:B:591:MET:HB3  | 1.87                     | 0.54              |
| 3:M:222:PHE:CE1  | 3:M:240:ILE:HG23 | 2.38                     | 0.54              |
| 3:M:272:LEU:N    | 3:M:272:LEU:HD12 | 2.23                     | 0.54              |
| 1:A:166:LEU:O    | 1:A:170:LEU:HD23 | 2.08                     | 0.54              |
| 1:A:223:CYS:O    | 1:A:226:SER:OG   | 2.15                     | 0.54              |
| 1:A:301:GLY:O    | 1:A:302:ASN:CB   | 2.54                     | 0.54              |
| 1:A:446:ASP:CG   | 1:A:448:GLU:O    | 2.50                     | 0.54              |
| 2:B:18:ILE:O     | 2:B:23:ALA:CB    | 2.55                     | 0.54              |
| 2:B:29:LYS:CD    | 2:B:30:LEU:N     | 2.59                     | 0.54              |
| 2:B:436:LEU:HB3  | 2:B:450:VAL:CG1  | 2.38                     | 0.54              |
| 3:M:44:ASP:HB3   | 3:M:50:TYR:CD2   | 2.43                     | 0.54              |
| 3:M:376:ILE:HD12 | 3:M:415:ILE:HG12 | 1.88                     | 0.54              |
| 4:S:53:THR:HB    | 4:S:69:ASN:N     | 2.22                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:220:SER:O    | 1:A:223:CYS:CB   | 2.52                     | 0.54              |
| 1:A:279:LEU:HD13 | 1:A:314:ALA:CB   | 2.38                     | 0.54              |
| 1:A:281:LEU:O    | 1:A:282:MET:O    | 2.26                     | 0.54              |
| 1:A:395:PHE:CG   | 1:A:428:MET:HE2  | 2.42                     | 0.54              |
| 1:A:461:CYS:O    | 1:A:463:ASP:N    | 2.39                     | 0.54              |
| 1:A:529:GLY:C    | 1:A:562:TRP:CZ2  | 2.86                     | 0.54              |
| 1:A:627:GLU:O    | 1:A:630:PRO:HD2  | 2.08                     | 0.54              |
| 2:B:176:ALA:C    | 2:B:178:ILE:H    | 2.15                     | 0.54              |
| 2:B:278:PRO:CD   | 2:B:292:GLU:CA   | 2.86                     | 0.54              |
| 3:M:16:PHE:HB2   | 3:M:118:TYR:CD1  | 2.42                     | 0.54              |
| 3:M:74:TYR:CB    | 3:M:114:ILE:CD1  | 2.85                     | 0.54              |
| 3:M:136:VAL:O    | 3:M:138:ASP:N    | 2.41                     | 0.54              |
| 3:M:248:SER:C    | 3:M:249:TYR:CD1  | 2.86                     | 0.54              |
| 3:M:252:ASP:C    | 3:M:254:PRO:HD2  | 2.33                     | 0.54              |
| 3:M:362:PHE:O    | 3:M:363:ASN:O    | 2.26                     | 0.54              |
| 3:M:374:TYR:HB3  | 3:M:417:TYR:CD2  | 2.42                     | 0.54              |
| 1:A:147:LEU:HD13 | 1:A:181:ALA:HA   | 1.89                     | 0.54              |
| 1:A:309:PHE:CZ   | 1:A:348:PHE:CZ   | 2.95                     | 0.54              |
| 1:A:453:VAL:O    | 1:A:457:LEU:HG   | 2.06                     | 0.54              |
| 1:A:502:ASP:O    | 3:M:59:ASP:OD2   | 2.26                     | 0.54              |
| 2:B:223:LEU:HD13 | 2:B:259:TYR:H    | 1.62                     | 0.54              |
| 2:B:418:TYR:O    | 2:B:418:TYR:HD1  | 1.89                     | 0.54              |
| 2:B:476:ARG:CA   | 2:B:514:LEU:HD13 | 2.31                     | 0.54              |
| 2:B:534:ILE:CG2  | 2:B:594:ALA:HB3  | 2.15                     | 0.54              |
| 2:B:537:PHE:CZ   | 2:B:545:ARG:HD3  | 2.42                     | 0.54              |
| 3:M:476:THR:HG1  | 3:M:477:GLY:N    | 2.05                     | 0.54              |
| 1:A:84:MET:CE    | 1:A:113:SER:O    | 2.55                     | 0.54              |
| 1:A:554:ALA:O    | 1:A:557:LYS:HB2  | 2.08                     | 0.54              |
| 2:B:241:ASP:CB   | 3:M:274:ASP:CB   | 2.85                     | 0.54              |
| 2:B:435:SER:O    | 2:B:438:ARG:N    | 2.39                     | 0.54              |
| 2:B:557:SER:O    | 2:B:560:ILE:N    | 2.40                     | 0.54              |
| 2:B:589:SER:OG   | 2:B:618:PHE:CZ   | 2.52                     | 0.54              |
| 3:M:15:ILE:CG2   | 3:M:114:ILE:HG22 | 2.37                     | 0.54              |
| 3:M:327:PHE:HE1  | 3:M:336:ASP:OD2  | 1.89                     | 0.54              |
| 1:A:158:LEU:CD1  | 1:A:162:ILE:HG13 | 2.37                     | 0.54              |
| 1:A:488:ARG:HD2  | 1:A:522:PHE:CE2  | 2.43                     | 0.54              |
| 1:A:589:SER:HB2  | 1:A:601:VAL:CG2  | 2.38                     | 0.54              |
| 2:B:177:ILE:HD11 | 2:B:195:ILE:HG21 | 1.88                     | 0.54              |
| 2:B:310:ILE:HG21 | 2:B:342:ALA:HB1  | 1.90                     | 0.54              |
| 2:B:374:PHE:CD2  | 2:B:402:LEU:HD22 | 2.34                     | 0.54              |
| 3:M:217:ASP:C    | 3:M:472:TYR:CE2  | 2.86                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:296:LYS:HG3  | 3:M:296:LYS:O    | 2.06                     | 0.54              |
| 2:B:260:LEU:O    | 2:B:261:PRO:C    | 2.39                     | 0.54              |
| 2:B:271:GLU:C    | 2:B:273:SER:N    | 2.54                     | 0.54              |
| 2:B:508:ARG:O    | 2:B:509:ALA:O    | 2.25                     | 0.54              |
| 3:M:7:ILE:CD1    | 3:M:121:ILE:HG21 | 2.38                     | 0.54              |
| 3:M:233:LEU:CD2  | 3:M:323:MET:O    | 2.55                     | 0.54              |
| 3:M:360:LEU:CD2  | 3:M:362:PHE:CZ   | 2.91                     | 0.54              |
| 4:S:50:PHE:HA    | 4:S:77:TYR:HD1   | 1.73                     | 0.54              |
| 4:S:83:LEU:HD11  | 4:S:116:VAL:CG1  | 2.38                     | 0.54              |
| 4:S:136:VAL:O    | 4:S:139:GLY:C    | 2.50                     | 0.54              |
| 1:A:153:ILE:CG2  | 1:A:158:LEU:HD23 | 2.37                     | 0.53              |
| 1:A:233:PHE:O    | 1:A:234:ILE:O    | 2.22                     | 0.53              |
| 1:A:245:VAL:O    | 1:A:245:VAL:HG22 | 2.08                     | 0.53              |
| 1:A:552:ILE:HG22 | 1:A:603:VAL:HG21 | 1.90                     | 0.53              |
| 1:A:638:LEU:HD12 | 2:B:520:SER:CB   | 2.26                     | 0.53              |
| 2:B:79:VAL:HB    | 2:B:108:PHE:HE1  | 1.69                     | 0.53              |
| 2:B:336:ASN:C    | 2:B:373:LEU:CD2  | 2.81                     | 0.53              |
| 2:B:490:ILE:HG13 | 2:B:518:ILE:CG1  | 2.36                     | 0.53              |
| 3:M:131:ALA:HB3  | 3:M:135:ASN:HB2  | 1.90                     | 0.53              |
| 3:M:219:LEU:HD13 | 3:M:473:LYS:HA   | 1.90                     | 0.53              |
| 3:M:302:TYR:CE2  | 3:M:304:VAL:HB   | 2.40                     | 0.53              |
| 4:S:1:MET:SD     | 4:S:20:TYR:CE2   | 3.02                     | 0.53              |
| 1:A:395:PHE:CZ   | 1:A:428:MET:HG3  | 2.44                     | 0.53              |
| 2:B:155:LEU:CB   | 2:B:188:TYR:HD2  | 2.20                     | 0.53              |
| 2:B:367:SER:OG   | 2:B:401:THR:OG1  | 2.25                     | 0.53              |
| 2:B:515:PHE:HE2  | 2:B:529:VAL:HG21 | 1.72                     | 0.53              |
| 2:B:556:LEU:HD12 | 2:B:614:ILE:CG2  | 2.38                     | 0.53              |
| 3:M:317:MET:HB2  | 3:M:322:LEU:N    | 2.24                     | 0.53              |
| 4:S:5:VAL:CG1    | 4:S:87:PHE:CE2   | 2.91                     | 0.53              |
| 1:A:121:LEU:HD12 | 1:A:153:ILE:HG22 | 1.89                     | 0.53              |
| 1:A:223:CYS:HB2  | 1:A:259:LEU:CD1  | 2.38                     | 0.53              |
| 1:A:375:VAL:HG11 | 1:A:387:ILE:HG21 | 1.90                     | 0.53              |
| 2:B:50:LEU:HB3   | 2:B:62:ALA:HB2   | 1.89                     | 0.53              |
| 2:B:80:GLN:CG    | 2:B:115:LEU:HD21 | 2.18                     | 0.53              |
| 2:B:81:LEU:C     | 2:B:83:PHE:N     | 2.55                     | 0.53              |
| 2:B:105:LEU:CG   | 2:B:119:SER:HB2  | 2.34                     | 0.53              |
| 2:B:174:ALA:CB   | 2:B:211:ALA:CA   | 2.75                     | 0.53              |
| 2:B:234:CYS:SG   | 2:B:298:ASP:O    | 2.67                     | 0.53              |
| 2:B:267:ASP:O    | 2:B:276:SER:OG   | 2.25                     | 0.53              |
| 2:B:310:ILE:HG23 | 2:B:318:ILE:HG12 | 1.91                     | 0.53              |
| 2:B:310:ILE:HD11 | 2:B:321:CYS:HB2  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:549:LEU:CG   | 2:B:611:ALA:HB2  | 2.38                     | 0.53              |
| 2:B:572:GLU:C    | 2:B:574:ASN:N    | 2.66                     | 0.53              |
| 2:B:599:ALA:C    | 2:B:601:TYR:H    | 2.16                     | 0.53              |
| 3:M:338:PHE:CE2  | 3:M:415:ILE:HD11 | 2.43                     | 0.53              |
| 3:M:371:GLU:O    | 3:M:419:ASN:OD1  | 2.26                     | 0.53              |
| 4:S:83:LEU:HD12  | 4:S:116:VAL:HG11 | 1.90                     | 0.53              |
| 1:A:304:LEU:C    | 1:A:304:LEU:HD23 | 2.33                     | 0.53              |
| 2:B:36:THR:HA    | 2:B:39:SER:OG    | 2.09                     | 0.53              |
| 2:B:237:ILE:HD12 | 2:B:248:LEU:CB   | 2.39                     | 0.53              |
| 2:B:378:THR:CG2  | 2:B:379:LYS:N    | 2.71                     | 0.53              |
| 2:B:519:ALA:O    | 2:B:523:PHE:N    | 2.41                     | 0.53              |
| 3:M:96:ILE:HD11  | 3:M:125:PHE:HA   | 1.91                     | 0.53              |
| 3:M:121:ILE:O    | 3:M:125:PHE:HD1  | 1.90                     | 0.53              |
| 3:M:350:VAL:HA   | 3:M:442:GLN:CB   | 2.38                     | 0.53              |
| 3:M:437:TYR:HB3  | 3:M:439:TYR:CE2  | 2.43                     | 0.53              |
| 4:S:32:LEU:O     | 4:S:35:VAL:CG2   | 2.55                     | 0.53              |
| 4:S:130:SER:CB   | 4:S:156:LEU:CD1  | 2.86                     | 0.53              |
| 1:A:95:MET:HB2   | 1:A:127:LEU:CD2  | 2.38                     | 0.53              |
| 1:A:179:LYS:CE   | 4:S:140:MET:C    | 2.81                     | 0.53              |
| 2:B:2:VAL:HG13   | 2:B:6:HIS:NE2    | 2.24                     | 0.53              |
| 2:B:8:ILE:HG22   | 2:B:12:LEU:HD11  | 1.90                     | 0.53              |
| 2:B:237:ILE:CG2  | 2:B:238:LYS:N    | 2.71                     | 0.53              |
| 2:B:476:ARG:O    | 2:B:480:GLN:HG3  | 2.08                     | 0.53              |
| 2:B:560:ILE:O    | 2:B:563:PHE:N    | 2.41                     | 0.53              |
| 2:B:566:ALA:HB2  | 2:B:581:TYR:HD2  | 1.71                     | 0.53              |
| 3:M:213:GLU:C    | 3:M:467:TYR:HB2  | 2.34                     | 0.53              |
| 3:M:220:GLU:CD   | 3:M:222:PHE:CZ   | 2.87                     | 0.53              |
| 3:M:221:THR:CB   | 3:M:474:THR:OG1  | 2.57                     | 0.53              |
| 3:M:276:VAL:HG22 | 3:M:290:PHE:CD1  | 2.40                     | 0.53              |
| 3:M:375:LYS:CE   | 3:M:418:GLU:OE1  | 2.57                     | 0.53              |
| 4:S:47:GLN:HG2   | 4:S:84:TYR:HE2   | 1.74                     | 0.53              |
| 1:A:384:LEU:HD12 | 1:A:384:LEU:C    | 2.34                     | 0.53              |
| 1:A:403:LEU:C    | 2:B:3:ASP:CB     | 2.67                     | 0.53              |
| 2:B:29:LYS:HD3   | 2:B:30:LEU:H     | 1.72                     | 0.53              |
| 2:B:117:LEU:HD23 | 2:B:150:LEU:CD2  | 2.39                     | 0.53              |
| 2:B:181:TYR:HD2  | 2:B:218:CYS:HA   | 1.73                     | 0.53              |
| 2:B:189:HIS:CE1  | 2:B:222:HIS:ND1  | 2.76                     | 0.53              |
| 2:B:335:LYS:O    | 2:B:373:LEU:HD22 | 2.09                     | 0.53              |
| 3:M:442:GLN:CG   | 3:M:443:SER:H    | 2.21                     | 0.53              |
| 1:A:446:ASP:O    | 1:A:448:GLU:O    | 2.27                     | 0.53              |
| 2:B:108:PHE:CD2  | 2:B:115:LEU:HB2  | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:151:ALA:CA   | 2:B:180:LEU:CD1  | 2.67                     | 0.53              |
| 2:B:151:ALA:HB1  | 2:B:188:TYR:CD1  | 2.44                     | 0.53              |
| 2:B:455:ILE:O    | 2:B:459:GLU:N    | 2.38                     | 0.53              |
| 3:M:250:LEU:HD13 | 3:M:254:PRO:HG2  | 1.89                     | 0.53              |
| 4:S:65:ASN:O     | 4:S:66:ASP:C     | 2.46                     | 0.53              |
| 4:S:130:SER:HB2  | 4:S:156:LEU:HD13 | 1.89                     | 0.53              |
| 1:A:207:LEU:HD23 | 1:A:239:LEU:HB3  | 1.91                     | 0.53              |
| 2:B:17:VAL:O     | 2:B:18:ILE:O     | 2.26                     | 0.53              |
| 2:B:50:LEU:CG    | 2:B:62:ALA:HB2   | 2.39                     | 0.53              |
| 2:B:126:SER:O    | 2:B:135:ARG:HG2  | 2.09                     | 0.53              |
| 3:M:214:LEU:C    | 3:M:467:TYR:HB3  | 2.33                     | 0.53              |
| 3:M:262:THR:O    | 3:M:264:GLY:N    | 2.36                     | 0.53              |
| 1:A:153:ILE:HG22 | 1:A:158:LEU:HD23 | 1.91                     | 0.53              |
| 1:A:174:ARG:CZ   | 4:S:148:ARG:NH2  | 2.69                     | 0.53              |
| 1:A:322:PHE:HD2  | 1:A:330:LEU:HD21 | 1.69                     | 0.53              |
| 1:A:441:TYR:C    | 1:A:443:SER:N    | 2.56                     | 0.53              |
| 1:A:529:GLY:HA3  | 1:A:562:TRP:CZ2  | 2.44                     | 0.53              |
| 2:B:325:LEU:HD13 | 2:B:339:PHE:CG   | 2.43                     | 0.53              |
| 3:M:223:HIS:HB3  | 3:M:477:GLY:O    | 2.09                     | 0.53              |
| 3:M:306:LEU:O    | 3:M:307:SER:O    | 2.27                     | 0.53              |
| 3:M:306:LEU:HD22 | 3:M:317:MET:CE   | 2.33                     | 0.53              |
| 1:A:187:LYS:O    | 1:A:190:LEU:HB3  | 2.08                     | 0.53              |
| 1:A:289:SER:O    | 1:A:291:ILE:N    | 2.39                     | 0.53              |
| 1:A:402:ILE:CB   | 1:A:421:PRO:HA   | 2.39                     | 0.53              |
| 1:A:509:PRO:HB3  | 1:A:547:VAL:HG21 | 1.90                     | 0.53              |
| 2:B:390:VAL:HA   | 2:B:393:ILE:HD12 | 1.91                     | 0.53              |
| 2:B:592:TYR:CE2  | 2:B:618:PHE:CE2  | 2.97                     | 0.53              |
| 3:M:245:ASP:C    | 3:M:246:VAL:CG2  | 2.81                     | 0.53              |
| 3:M:290:PHE:CE1  | 3:M:297:PHE:CD1  | 2.97                     | 0.53              |
| 2:B:219:TYR:C    | 2:B:221:ASP:N    | 2.58                     | 0.52              |
| 2:B:246:SER:O    | 2:B:249:ILE:HB   | 2.08                     | 0.52              |
| 3:M:306:LEU:HD21 | 3:M:317:MET:CE   | 2.39                     | 0.52              |
| 1:A:97:SER:C     | 1:A:98:ASN:O     | 2.32                     | 0.52              |
| 1:A:196:LEU:O    | 1:A:197:ARG:O    | 2.27                     | 0.52              |
| 1:A:435:ILE:CG2  | 1:A:441:TYR:CE2  | 2.93                     | 0.52              |
| 1:A:533:ILE:HG12 | 1:A:562:TRP:CZ2  | 2.43                     | 0.52              |
| 2:B:25:VAL:CG2   | 2:B:35:TYR:HB3   | 2.39                     | 0.52              |
| 2:B:132:SER:HB2  | 2:B:166:SER:OG   | 2.09                     | 0.52              |
| 2:B:245:GLN:NE2  | 2:B:309:LEU:CD1  | 2.69                     | 0.52              |
| 2:B:483:PRO:O    | 2:B:486:HIS:HB3  | 2.09                     | 0.52              |
| 2:B:490:ILE:O    | 2:B:515:PHE:CZ   | 2.62                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:537:PHE:CZ   | 2:B:545:ARG:CD   | 2.92                     | 0.52              |
| 2:B:556:LEU:HB3  | 2:B:588:ILE:HD11 | 1.89                     | 0.52              |
| 2:B:563:PHE:CZ   | 2:B:588:ILE:HB   | 2.44                     | 0.52              |
| 2:B:564:LYS:CD   | 2:B:621:GLY:O    | 2.50                     | 0.52              |
| 3:M:243:ILE:HD13 | 3:M:301:GLU:CB   | 2.39                     | 0.52              |
| 1:A:207:LEU:CD1  | 1:A:243:ILE:HG13 | 2.39                     | 0.52              |
| 1:A:237:SER:HB2  | 1:A:270:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:506:LYS:O    | 1:A:507:GLN:CB   | 2.56                     | 0.52              |
| 2:B:154:ILE:HB   | 2:B:180:LEU:HD13 | 1.91                     | 0.52              |
| 2:B:334:MET:O    | 2:B:336:ASN:C    | 2.51                     | 0.52              |
| 2:B:458:MET:SD   | 2:B:475:ILE:HD11 | 2.49                     | 0.52              |
| 2:B:549:LEU:CG   | 2:B:614:ILE:HD12 | 2.38                     | 0.52              |
| 2:B:564:LYS:O    | 2:B:567:GLN:N    | 2.42                     | 0.52              |
| 3:M:84:LYS:O     | 3:M:88:ASP:HB3   | 2.08                     | 0.52              |
| 3:M:224:VAL:CG1  | 3:M:226:PHE:CE1  | 2.92                     | 0.52              |
| 3:M:235:LEU:HD11 | 3:M:306:LEU:CD1  | 2.40                     | 0.52              |
| 3:M:253:ASN:N    | 3:M:254:PRO:CD   | 2.72                     | 0.52              |
| 3:M:347:PHE:HE1  | 3:M:350:VAL:HG11 | 1.65                     | 0.52              |
| 3:M:374:TYR:HE1  | 3:M:376:ILE:CG1  | 2.23                     | 0.52              |
| 4:S:57:LEU:O     | 4:S:59:LEU:HA    | 2.09                     | 0.52              |
| 1:A:183:THR:OG1  | 4:S:137:GLN:O    | 2.28                     | 0.52              |
| 1:A:401:VAL:CG2  | 1:A:418:ILE:H    | 2.23                     | 0.52              |
| 2:B:29:LYS:O     | 2:B:32:GLU:CG    | 2.56                     | 0.52              |
| 2:B:83:PHE:O     | 2:B:87:VAL:HG23  | 2.10                     | 0.52              |
| 2:B:592:TYR:HH   | 2:B:619:ASP:CG   | 2.16                     | 0.52              |
| 3:M:276:VAL:HG21 | 3:M:299:LEU:HD12 | 1.90                     | 0.52              |
| 3:M:283:PHE:CE2  | 3:M:289:THR:HB   | 2.44                     | 0.52              |
| 3:M:327:PHE:CE1  | 3:M:336:ASP:CB   | 2.89                     | 0.52              |
| 3:M:343:ASN:HD22 | 3:M:343:ASN:H    | 1.56                     | 0.52              |
| 4:S:3:HIS:O      | 4:S:19:PHE:HA    | 2.10                     | 0.52              |
| 1:A:341:ILE:O    | 1:A:344:ILE:HB   | 2.10                     | 0.52              |
| 1:A:609:LEU:CG   | 1:A:628:VAL:CG1  | 2.66                     | 0.52              |
| 1:A:637:GLU:CG   | 2:B:516:GLY:C    | 2.83                     | 0.52              |
| 2:B:25:VAL:CG2   | 2:B:36:THR:H     | 1.91                     | 0.52              |
| 2:B:90:ILE:CD1   | 2:B:123:LEU:HD23 | 2.40                     | 0.52              |
| 2:B:126:SER:O    | 2:B:127:LEU:C    | 2.47                     | 0.52              |
| 2:B:197:LYS:N    | 2:B:229:HIS:NE2  | 2.57                     | 0.52              |
| 2:B:216:LYS:HG3  | 2:B:251:LEU:HD12 | 1.90                     | 0.52              |
| 2:B:279:LEU:O    | 2:B:280:PRO:C    | 2.52                     | 0.52              |
| 2:B:340:ILE:HD13 | 2:B:366:LEU:HD13 | 1.92                     | 0.52              |
| 2:B:470:ALA:O    | 2:B:473:ASN:N    | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:570:GLY:C    | 2:B:571:SER:O    | 2.35                     | 0.52              |
| 3:M:44:ASP:C     | 3:M:47:SER:H     | 2.18                     | 0.52              |
| 3:M:243:ILE:N    | 3:M:474:THR:HG22 | 2.21                     | 0.52              |
| 3:M:290:PHE:CZ   | 3:M:297:PHE:CZ   | 2.98                     | 0.52              |
| 2:B:132:SER:HA   | 2:B:169:VAL:HG22 | 1.90                     | 0.52              |
| 2:B:146:LYS:O    | 2:B:147:MET:SD   | 2.67                     | 0.52              |
| 2:B:208:ILE:CD1  | 2:B:236:ILE:HG23 | 2.28                     | 0.52              |
| 2:B:237:ILE:HD12 | 2:B:248:LEU:HB2  | 1.92                     | 0.52              |
| 2:B:241:ASP:HB3  | 3:M:274:ASP:CA   | 2.32                     | 0.52              |
| 2:B:452:LYS:NZ   | 2:B:456:ASP:OD1  | 2.42                     | 0.52              |
| 4:S:146:VAL:O    | 4:S:150:VAL:HG23 | 2.10                     | 0.52              |
| 2:B:14:THR:O     | 2:B:15:ALA:C     | 2.53                     | 0.52              |
| 2:B:102:HIS:ND1  | 2:B:137:PHE:O    | 2.41                     | 0.52              |
| 2:B:180:LEU:HD23 | 2:B:192:LEU:HD21 | 1.90                     | 0.52              |
| 2:B:215:TYR:HB3  | 2:B:226:LEU:HD13 | 1.91                     | 0.52              |
| 2:B:270:SER:O    | 2:B:273:SER:HB2  | 2.09                     | 0.52              |
| 2:B:311:TYR:CD1  | 3:M:269:ILE:HD11 | 2.44                     | 0.52              |
| 2:B:545:ARG:NH1  | 2:B:602:ASP:HA   | 2.24                     | 0.52              |
| 2:B:596:LEU:HD22 | 2:B:615:SER:OG   | 2.09                     | 0.52              |
| 3:M:217:ASP:O    | 3:M:472:TYR:CE1  | 2.63                     | 0.52              |
| 3:M:240:ILE:CG2  | 3:M:444:ALA:O    | 2.52                     | 0.52              |
| 3:M:265:ASN:O    | 3:M:266:ASP:C    | 2.47                     | 0.52              |
| 3:M:374:TYR:HA   | 3:M:417:TYR:HA   | 1.92                     | 0.52              |
| 4:S:55:PRO:HB3   | 4:S:71:GLU:HG3   | 1.91                     | 0.52              |
| 1:A:128:LEU:HD12 | 1:A:150:LEU:CD2  | 2.40                     | 0.52              |
| 2:B:41:ASN:HB3   | 2:B:43:ASN:CG    | 2.32                     | 0.52              |
| 2:B:208:ILE:CG2  | 2:B:236:ILE:HG21 | 2.35                     | 0.52              |
| 2:B:267:ASP:CB   | 2:B:289:PRO:HG3  | 2.40                     | 0.52              |
| 2:B:340:ILE:CD1  | 2:B:366:LEU:HB3  | 2.40                     | 0.52              |
| 3:M:228:LYS:NZ   | 3:M:326:HIS:HA   | 2.25                     | 0.52              |
| 4:S:10:LYS:CA    | 4:S:84:TYR:HE1   | 2.22                     | 0.52              |
| 4:S:149:ILE:O    | 4:S:153:VAL:HG23 | 2.10                     | 0.52              |
| 1:A:250:ASN:OD1  | 1:A:285:THR:CB   | 2.54                     | 0.52              |
| 2:B:73:ASP:O     | 2:B:75:ASP:N     | 2.43                     | 0.52              |
| 2:B:120:ILE:CG1  | 2:B:150:LEU:HD13 | 2.39                     | 0.52              |
| 2:B:139:LEU:HD23 | 2:B:173:VAL:N    | 2.23                     | 0.52              |
| 2:B:155:LEU:HB2  | 2:B:188:TYR:HD2  | 1.70                     | 0.52              |
| 2:B:200:MET:HE1  | 2:B:228:GLY:O    | 2.10                     | 0.52              |
| 2:B:433:VAL:HG22 | 2:B:471:TYR:CZ   | 2.45                     | 0.52              |
| 3:M:95:THR:HG1   | 3:M:137:SER:HB2  | 1.73                     | 0.52              |
| 3:M:217:ASP:O    | 3:M:472:TYR:CZ   | 2.63                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:342:LEU:O    | 3:M:409:PRO:HD2  | 2.10                     | 0.52              |
| 3:M:350:VAL:HG22 | 3:M:442:GLN:CG   | 2.28                     | 0.52              |
| 3:M:442:GLN:HG3  | 3:M:443:SER:N    | 2.23                     | 0.52              |
| 4:S:57:LEU:HD23  | 4:S:66:ASP:HA    | 1.92                     | 0.52              |
| 1:A:216:SER:O    | 4:S:140:MET:HE2  | 2.10                     | 0.52              |
| 1:A:244:LEU:HG   | 1:A:281:LEU:CD1  | 2.29                     | 0.52              |
| 1:A:263:LEU:O    | 1:A:266:VAL:C    | 2.52                     | 0.52              |
| 1:A:301:GLY:O    | 1:A:302:ASN:HB3  | 2.10                     | 0.52              |
| 1:A:599:ARG:CZ   | 2:B:547:GLN:HE22 | 2.22                     | 0.52              |
| 2:B:311:TYR:CB   | 3:M:269:ILE:CD1  | 2.87                     | 0.52              |
| 2:B:374:PHE:CB   | 2:B:402:LEU:CD2  | 2.81                     | 0.52              |
| 2:B:490:ILE:HD12 | 2:B:518:ILE:HG21 | 1.89                     | 0.52              |
| 3:M:58:ARG:O     | 3:M:60:LEU:O     | 2.27                     | 0.52              |
| 3:M:218:LEU:HG   | 3:M:244:VAL:HG22 | 1.92                     | 0.52              |
| 4:S:48:SER:HG    | 4:S:50:PHE:H     | 1.52                     | 0.52              |
| 1:A:395:PHE:CZ   | 1:A:428:MET:HB2  | 2.45                     | 0.51              |
| 3:M:302:TYR:CE2  | 3:M:445:SER:HB3  | 2.44                     | 0.51              |
| 3:M:344:ILE:H    | 3:M:408:VAL:HG22 | 1.75                     | 0.51              |
| 3:M:350:VAL:CG1  | 3:M:442:GLN:CB   | 2.80                     | 0.51              |
| 3:M:374:TYR:CB   | 3:M:417:TYR:HD2  | 2.23                     | 0.51              |
| 1:A:121:LEU:HG   | 1:A:153:ILE:HG21 | 1.91                     | 0.51              |
| 1:A:237:SER:HB2  | 1:A:270:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:275:LEU:C    | 1:A:275:LEU:HD23 | 2.35                     | 0.51              |
| 1:A:289:SER:CA   | 4:S:96:LEU:HD11  | 2.39                     | 0.51              |
| 2:B:189:HIS:CD2  | 2:B:222:HIS:CG   | 2.98                     | 0.51              |
| 2:B:253:ILE:CG1  | 2:B:324:ALA:HB2  | 2.40                     | 0.51              |
| 2:B:534:ILE:O    | 2:B:535:GLN:C    | 2.54                     | 0.51              |
| 3:M:64:LYS:HE3   | 3:M:66:PHE:CZ    | 2.44                     | 0.51              |
| 3:M:114:ILE:HG23 | 3:M:121:ILE:CD1  | 2.41                     | 0.51              |
| 3:M:443:SER:OG   | 3:M:448:TYR:N    | 2.43                     | 0.51              |
| 1:A:101:GLN:CD   | 4:S:167:ILE:HD12 | 2.29                     | 0.51              |
| 1:A:569:ASP:C    | 1:A:571:ARG:H    | 2.18                     | 0.51              |
| 2:B:18:ILE:O     | 2:B:23:ALA:HB2   | 2.10                     | 0.51              |
| 2:B:37:TYR:O     | 2:B:40:GLN:N     | 2.43                     | 0.51              |
| 2:B:188:TYR:HB3  | 2:B:192:LEU:CD1  | 2.41                     | 0.51              |
| 2:B:223:LEU:CD1  | 2:B:258:GLN:CA   | 2.87                     | 0.51              |
| 2:B:574:ASN:O    | 2:B:576:GLN:O    | 2.28                     | 0.51              |
| 3:M:4:SER:HB3    | 3:M:79:SER:OG    | 2.11                     | 0.51              |
| 3:M:52:ASP:O     | 3:M:53:HIS:HB3   | 2.11                     | 0.51              |
| 3:M:443:SER:OG   | 3:M:447:ILE:O    | 2.27                     | 0.51              |
| 1:A:288:THR:O    | 1:A:291:ILE:HB   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:373:GLU:HG2  | 1:A:427:LYS:CE   | 2.40                     | 0.51              |
| 1:A:397:ASP:O    | 1:A:418:ILE:HG13 | 2.11                     | 0.51              |
| 1:A:485:PRO:C    | 1:A:486:SER:O    | 2.48                     | 0.51              |
| 2:B:203:THR:HG22 | 2:B:232:ARG:HH22 | 1.74                     | 0.51              |
| 2:B:204:ASP:O    | 2:B:207:VAL:HB   | 2.10                     | 0.51              |
| 2:B:589:SER:HA   | 2:B:592:TYR:CD2  | 2.43                     | 0.51              |
| 3:M:241:HIS:CB   | 3:M:476:THR:CG2  | 2.86                     | 0.51              |
| 3:M:242:GLY:HA3  | 3:M:444:ALA:HB3  | 1.91                     | 0.51              |
| 1:A:200:PHE:CE1  | 1:A:236:LEU:CD1  | 2.93                     | 0.51              |
| 1:A:257:LEU:CD2  | 1:A:278:ILE:CG2  | 2.55                     | 0.51              |
| 1:A:291:ILE:O    | 1:A:295:VAL:HG23 | 2.11                     | 0.51              |
| 2:B:98:LYS:HB2   | 2:B:134:LEU:HD22 | 1.92                     | 0.51              |
| 2:B:162:VAL:HG23 | 2:B:173:VAL:CG1  | 2.37                     | 0.51              |
| 3:M:64:LYS:HZ2   | 3:M:79:SER:HB2   | 1.75                     | 0.51              |
| 3:M:342:LEU:HD12 | 3:M:342:LEU:N    | 2.25                     | 0.51              |
| 4:S:24:ASP:HB3   | 4:S:26:PRO:HD2   | 1.91                     | 0.51              |
| 1:A:176:TYR:CE1  | 4:S:148:ARG:NH2  | 2.69                     | 0.51              |
| 1:A:401:VAL:HG23 | 1:A:418:ILE:C    | 2.35                     | 0.51              |
| 2:B:219:TYR:O    | 2:B:223:LEU:HG   | 2.10                     | 0.51              |
| 2:B:322:CYS:SG   | 2:B:362:ALA:HB1  | 2.51                     | 0.51              |
| 2:B:433:VAL:CG1  | 2:B:474:VAL:CG2  | 2.69                     | 0.51              |
| 2:B:486:HIS:NE2  | 2:B:518:ILE:CG1  | 2.73                     | 0.51              |
| 2:B:519:ALA:HA   | 2:B:526:CYS:SG   | 2.51                     | 0.51              |
| 2:B:563:PHE:O    | 2:B:566:ALA:CA   | 2.58                     | 0.51              |
| 3:M:44:ASP:HB2   | 3:M:50:TYR:CD2   | 2.45                     | 0.51              |
| 3:M:46:SER:O     | 3:M:47:SER:C     | 2.43                     | 0.51              |
| 3:M:54:SER:HB2   | 3:M:66:PHE:CE1   | 2.46                     | 0.51              |
| 3:M:103:TYR:O    | 3:M:104:PHE:HB2  | 2.11                     | 0.51              |
| 3:M:253:ASN:O    | 3:M:254:PRO:C    | 2.53                     | 0.51              |
| 1:A:79:MET:HB3   | 4:S:25:LEU:HD11  | 1.92                     | 0.51              |
| 1:A:167:PHE:CE1  | 1:A:202:LYS:HD3  | 2.46                     | 0.51              |
| 1:A:183:THR:OG1  | 4:S:137:GLN:C    | 2.50                     | 0.51              |
| 2:B:55:ASN:O     | 2:B:59:VAL:HG23  | 2.11                     | 0.51              |
| 2:B:215:TYR:CZ   | 2:B:229:HIS:HB3  | 2.46                     | 0.51              |
| 2:B:223:LEU:HD22 | 2:B:255:TYR:CD1  | 2.46                     | 0.51              |
| 2:B:337:THR:CA   | 2:B:373:LEU:CD1  | 2.78                     | 0.51              |
| 2:B:340:ILE:HB   | 2:B:373:LEU:HG   | 1.93                     | 0.51              |
| 2:B:440:GLY:C    | 2:B:442:LEU:N    | 2.66                     | 0.51              |
| 2:B:481:LYS:C    | 2:B:483:PRO:HD3  | 2.35                     | 0.51              |
| 2:B:567:GLN:N    | 2:B:574:ASN:HD22 | 2.06                     | 0.51              |
| 3:M:235:LEU:CD1  | 3:M:306:LEU:HD13 | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:270:PRO:CA   | 3:M:302:TYR:CD1  | 2.94                     | 0.51              |
| 3:M:270:PRO:CA   | 3:M:302:TYR:HD1  | 2.24                     | 0.51              |
| 3:M:270:PRO:HA   | 3:M:302:TYR:CD1  | 2.46                     | 0.51              |
| 1:A:103:LYS:HB3  | 1:A:107:TYR:HE1  | 1.76                     | 0.51              |
| 2:B:44:PRO:HG3   | 2:B:77:ILE:CD1   | 2.41                     | 0.51              |
| 2:B:77:ILE:HG23  | 2:B:82:TYR:CE1   | 2.45                     | 0.51              |
| 2:B:162:VAL:O    | 2:B:164:ASP:N    | 2.43                     | 0.51              |
| 2:B:177:ILE:HD11 | 2:B:195:ILE:CG2  | 2.41                     | 0.51              |
| 2:B:367:SER:OG   | 2:B:401:THR:HG21 | 2.10                     | 0.51              |
| 2:B:397:GLN:NE2  | 2:B:431:MET:HE3  | 2.25                     | 0.51              |
| 2:B:411:ILE:O    | 2:B:414:GLU:N    | 2.40                     | 0.51              |
| 2:B:450:VAL:O    | 2:B:453:TRP:HB2  | 2.11                     | 0.51              |
| 3:M:51:LEU:N     | 3:M:51:LEU:HD12  | 2.26                     | 0.51              |
| 3:M:213:GLU:CB   | 3:M:467:TYR:HB2  | 2.41                     | 0.51              |
| 3:M:233:LEU:CD2  | 3:M:324:SER:HA   | 2.39                     | 0.51              |
| 3:M:272:LEU:HD22 | 3:M:278:ILE:CB   | 2.40                     | 0.51              |
| 3:M:372:ILE:HD12 | 3:M:428:VAL:CG2  | 2.41                     | 0.51              |
| 1:A:68:THR:OG1   | 4:S:166:LYS:HB3  | 2.11                     | 0.51              |
| 1:A:88:ASN:ND2   | 1:A:120:ILE:HG13 | 2.25                     | 0.51              |
| 1:A:121:LEU:HD13 | 1:A:155:THR:OG1  | 2.11                     | 0.51              |
| 1:A:241:TYR:C    | 1:A:241:TYR:CD2  | 2.88                     | 0.51              |
| 2:B:17:VAL:O     | 2:B:18:ILE:C     | 2.54                     | 0.51              |
| 2:B:181:TYR:CZ   | 2:B:222:HIS:CD2  | 2.96                     | 0.51              |
| 2:B:303:LEU:HD11 | 2:B:333:GLN:CB   | 2.41                     | 0.51              |
| 2:B:311:TYR:HB3  | 3:M:269:ILE:HD12 | 1.92                     | 0.51              |
| 2:B:556:LEU:CA   | 2:B:588:ILE:CD1  | 2.53                     | 0.51              |
| 3:M:56:VAL:H     | 3:M:64:LYS:HB2   | 1.76                     | 0.51              |
| 3:M:99:ILE:O     | 3:M:103:TYR:CD1  | 2.64                     | 0.51              |
| 3:M:443:SER:OG   | 3:M:448:TYR:CA   | 2.58                     | 0.51              |
| 4:S:73:ILE:CG2   | 4:S:88:ILE:CG2   | 2.88                     | 0.51              |
| 1:A:128:LEU:HD12 | 1:A:150:LEU:HD23 | 1.91                     | 0.51              |
| 1:A:260:PHE:CD1  | 1:A:274:LEU:CD1  | 2.94                     | 0.51              |
| 2:B:191:GLU:C    | 2:B:193:LEU:N    | 2.67                     | 0.51              |
| 2:B:193:LEU:CB   | 2:B:225:LEU:CD1  | 2.84                     | 0.51              |
| 2:B:196:LEU:HB3  | 2:B:215:TYR:OH   | 2.10                     | 0.51              |
| 2:B:308:CYS:O    | 2:B:311:TYR:N    | 2.44                     | 0.51              |
| 2:B:508:ARG:HB3  | 2:B:544:THR:CG2  | 2.40                     | 0.51              |
| 3:M:224:VAL:HB   | 3:M:226:PHE:CE1  | 2.46                     | 0.51              |
| 4:S:38:LEU:HD23  | 4:S:68:VAL:CG2   | 2.39                     | 0.51              |
| 4:S:49:SER:O     | 4:S:77:TYR:O     | 2.29                     | 0.51              |
| 4:S:61:ASN:O     | 4:S:62:GLU:C     | 2.53                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189:PHE:O    | 1:A:190:LEU:C    | 2.51                     | 0.50              |
| 1:A:223:CYS:CB   | 1:A:259:LEU:HG   | 2.41                     | 0.50              |
| 1:A:253:ILE:O    | 1:A:257:LEU:HG   | 2.11                     | 0.50              |
| 1:A:436:CYS:CB   | 1:A:450:TYR:CZ   | 2.94                     | 0.50              |
| 2:B:120:ILE:HD12 | 2:B:142:LEU:CD2  | 2.41                     | 0.50              |
| 2:B:227:HIS:C    | 2:B:298:ASP:OD2  | 2.54                     | 0.50              |
| 2:B:513:TRP:HE1  | 2:B:517:GLU:HG3  | 1.76                     | 0.50              |
| 2:B:534:ILE:CG1  | 2:B:595:VAL:CG2  | 2.89                     | 0.50              |
| 2:B:592:TYR:CZ   | 2:B:619:ASP:OD1  | 2.64                     | 0.50              |
| 3:M:260:LEU:HD21 | 3:M:449:VAL:HG22 | 1.91                     | 0.50              |
| 1:A:107:TYR:CE2  | 1:A:128:LEU:CD2  | 2.94                     | 0.50              |
| 1:A:150:LEU:HB3  | 1:A:162:ILE:HD13 | 1.93                     | 0.50              |
| 1:A:402:ILE:CG2  | 1:A:421:PRO:HA   | 2.41                     | 0.50              |
| 2:B:181:TYR:CE1  | 2:B:222:HIS:NE2  | 2.70                     | 0.50              |
| 2:B:249:ILE:HD13 | 2:B:321:CYS:SG   | 2.52                     | 0.50              |
| 2:B:286:ILE:CG2  | 2:B:288:TYR:CE2  | 2.94                     | 0.50              |
| 2:B:353:GLN:HB3  | 3:M:50:TYR:CG    | 2.38                     | 0.50              |
| 2:B:449:HIS:O    | 2:B:453:TRP:CD1  | 2.64                     | 0.50              |
| 2:B:486:HIS:HA   | 2:B:489:ILE:HD12 | 1.92                     | 0.50              |
| 2:B:560:ILE:HG22 | 2:B:561:ASP:N    | 2.25                     | 0.50              |
| 3:M:226:PHE:N    | 3:M:480:GLN:O    | 2.41                     | 0.50              |
| 3:M:374:TYR:HB2  | 3:M:417:TYR:CD2  | 2.46                     | 0.50              |
| 4:S:64:ASN:C     | 4:S:64:ASN:N     | 2.64                     | 0.50              |
| 1:A:512:LEU:HD13 | 1:A:543:TYR:CZ   | 2.46                     | 0.50              |
| 1:A:604:LEU:HD23 | 1:A:604:LEU:C    | 2.35                     | 0.50              |
| 2:B:20:ARG:NH1   | 2:B:21:GLU:HG3   | 2.19                     | 0.50              |
| 2:B:51:LEU:HD11  | 2:B:66:ILE:HD13  | 1.93                     | 0.50              |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:HD21 | 1.93                     | 0.50              |
| 2:B:231:ARG:C    | 2:B:233:TYR:N    | 2.65                     | 0.50              |
| 2:B:396:ILE:CD1  | 2:B:418:TYR:HE2  | 2.23                     | 0.50              |
| 3:M:6:TYR:CD1    | 3:M:77:LEU:HD23  | 2.47                     | 0.50              |
| 3:M:9:ASP:C      | 3:M:9:ASP:OD1    | 2.54                     | 0.50              |
| 3:M:235:LEU:HD22 | 3:M:307:SER:HA   | 1.93                     | 0.50              |
| 3:M:241:HIS:O    | 3:M:474:THR:CB   | 2.59                     | 0.50              |
| 3:M:271:SER:C    | 3:M:272:LEU:HD12 | 2.36                     | 0.50              |
| 4:S:83:LEU:CD1   | 4:S:116:VAL:HG11 | 2.41                     | 0.50              |
| 1:A:109:ALA:O    | 1:A:112:GLN:N    | 2.45                     | 0.50              |
| 1:A:298:ILE:HD11 | 1:A:311:THR:CG2  | 2.34                     | 0.50              |
| 1:A:425:LYS:HD2  | 1:A:428:MET:HE3  | 1.92                     | 0.50              |
| 2:B:77:ILE:HG22  | 2:B:82:TYR:HE1   | 1.74                     | 0.50              |
| 2:B:157:THR:O    | 2:B:160:LYS:N    | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:172:GLU:OE1  | 2:B:175:LEU:HD12 | 2.12                     | 0.50              |
| 2:B:193:LEU:CB   | 2:B:225:LEU:CG   | 2.83                     | 0.50              |
| 2:B:219:TYR:CE1  | 2:B:226:LEU:HD12 | 2.32                     | 0.50              |
| 2:B:343:LEU:CD2  | 2:B:363:ILE:HD13 | 2.33                     | 0.50              |
| 4:S:38:LEU:CD2   | 4:S:68:VAL:HG21  | 2.39                     | 0.50              |
| 1:A:271:ARG:NH1  | 1:A:302:ASN:O    | 2.44                     | 0.50              |
| 1:A:625:LEU:C    | 1:A:627:GLU:N    | 2.69                     | 0.50              |
| 2:B:38:TYR:CD1   | 2:B:38:TYR:N     | 2.76                     | 0.50              |
| 2:B:79:VAL:CB    | 2:B:108:PHE:HE1  | 2.20                     | 0.50              |
| 2:B:120:ILE:CD1  | 2:B:142:LEU:HD23 | 2.42                     | 0.50              |
| 2:B:452:LYS:NZ   | 2:B:456:ASP:CG   | 2.69                     | 0.50              |
| 2:B:553:ALA:CA   | 2:B:614:ILE:HG21 | 2.41                     | 0.50              |
| 2:B:559:ASP:C    | 2:B:563:PHE:HB2  | 2.36                     | 0.50              |
| 3:M:19:LEU:CD2   | 3:M:24:ALA:HB3   | 2.42                     | 0.50              |
| 3:M:260:LEU:HD23 | 3:M:449:VAL:HG22 | 1.92                     | 0.50              |
| 1:A:91:ILE:HG22  | 1:A:95:MET:HE2   | 1.93                     | 0.50              |
| 2:B:103:LEU:CD2  | 3:M:131:ALA:C    | 2.85                     | 0.50              |
| 2:B:114:ASN:O    | 2:B:117:LEU:HB2  | 2.12                     | 0.50              |
| 2:B:139:LEU:HD21 | 2:B:173:VAL:O    | 2.12                     | 0.50              |
| 2:B:161:LEU:CB   | 2:B:173:VAL:HG22 | 2.35                     | 0.50              |
| 2:B:247:TYR:HE1  | 3:M:136:VAL:HG13 | 1.76                     | 0.50              |
| 2:B:276:SER:OG   | 2:B:289:PRO:HG3  | 2.12                     | 0.50              |
| 2:B:311:TYR:CD1  | 3:M:269:ILE:CD1  | 2.94                     | 0.50              |
| 2:B:520:SER:C    | 2:B:523:PHE:CD2  | 2.90                     | 0.50              |
| 2:B:578:PRO:CD   | 2:B:581:TYR:CD1  | 2.84                     | 0.50              |
| 3:M:4:SER:HA     | 3:M:18:TYR:O     | 2.11                     | 0.50              |
| 4:S:89:VAL:HG11  | 4:S:98:ILE:HD12  | 1.93                     | 0.50              |
| 1:A:260:PHE:CE2  | 1:A:274:LEU:HD11 | 2.44                     | 0.50              |
| 1:A:556:VAL:HG22 | 1:A:603:VAL:HG11 | 1.93                     | 0.50              |
| 2:B:62:ALA:O     | 2:B:66:ILE:CD1   | 2.60                     | 0.50              |
| 2:B:325:LEU:O    | 2:B:326:TYR:C    | 2.39                     | 0.50              |
| 2:B:346:THR:O    | 2:B:350:THR:N    | 2.44                     | 0.50              |
| 2:B:592:TYR:OH   | 2:B:619:ASP:CG   | 2.55                     | 0.50              |
| 3:M:356:LEU:CD2  | 3:M:358:ILE:HG13 | 2.41                     | 0.50              |
| 1:A:71:VAL:HG21  | 1:A:94:VAL:HG11  | 1.93                     | 0.50              |
| 1:A:147:LEU:HD22 | 1:A:166:LEU:CD2  | 2.41                     | 0.50              |
| 1:A:158:LEU:CG   | 1:A:162:ILE:HD11 | 2.41                     | 0.50              |
| 1:A:279:LEU:CD1  | 1:A:314:ALA:HB1  | 2.41                     | 0.50              |
| 1:A:401:VAL:HG23 | 1:A:418:ILE:N    | 2.27                     | 0.50              |
| 1:A:581:LEU:CD2  | 1:A:607:LEU:HD21 | 2.42                     | 0.50              |
| 2:B:171:GLY:HA2  | 2:B:207:VAL:CG1  | 2.40                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:196:LEU:HA   | 2:B:199:LEU:HD12 | 1.93                     | 0.50              |
| 2:B:242:SER:OG   | 3:M:98:ARG:NH2   | 2.45                     | 0.50              |
| 2:B:251:LEU:O    | 2:B:254:LYS:N    | 2.45                     | 0.50              |
| 2:B:292:GLU:CG   | 2:B:296:ASP:HB2  | 2.41                     | 0.50              |
| 2:B:292:GLU:HG2  | 2:B:296:ASP:CB   | 2.41                     | 0.50              |
| 2:B:352:ASN:HD22 | 3:M:70:ASN:HD22  | 1.59                     | 0.50              |
| 3:M:235:LEU:HD23 | 3:M:235:LEU:O    | 2.10                     | 0.50              |
| 3:M:374:TYR:CZ   | 3:M:390:ILE:HD13 | 2.47                     | 0.50              |
| 4:S:8:PHE:CE2    | 4:S:86:THR:N     | 2.74                     | 0.50              |
| 1:A:148:SER:O    | 1:A:151:SER:OG   | 2.25                     | 0.50              |
| 1:A:196:LEU:C    | 1:A:196:LEU:CD2  | 2.85                     | 0.50              |
| 1:A:428:MET:O    | 1:A:431:VAL:HB   | 2.12                     | 0.50              |
| 2:B:245:GLN:HG2  | 2:B:309:LEU:HD11 | 1.84                     | 0.50              |
| 2:B:469:ASP:OD1  | 2:B:506:ASN:CB   | 2.60                     | 0.50              |
| 3:M:44:ASP:HB2   | 3:M:50:TYR:HD2   | 1.77                     | 0.50              |
| 4:S:15:ARG:NH1   | 4:S:122:ILE:HD11 | 2.27                     | 0.50              |
| 1:A:186:PHE:HE2  | 1:A:187:LYS:HD3  | 1.77                     | 0.49              |
| 1:A:401:VAL:HG23 | 1:A:418:ILE:CA   | 2.42                     | 0.49              |
| 1:A:465:SER:H    | 2:B:1:MET:HE1    | 1.77                     | 0.49              |
| 2:B:147:MET:HB2  | 2:B:150:LEU:HG   | 1.92                     | 0.49              |
| 2:B:212:VAL:CG2  | 2:B:233:TYR:CE2  | 2.94                     | 0.49              |
| 2:B:563:PHE:CA   | 2:B:566:ALA:HB3  | 2.42                     | 0.49              |
| 3:M:212:ASN:CG   | 3:M:250:LEU:HD23 | 2.37                     | 0.49              |
| 3:M:233:LEU:HD22 | 3:M:323:MET:O    | 2.12                     | 0.49              |
| 3:M:245:ASP:O    | 3:M:246:VAL:CG2  | 2.60                     | 0.49              |
| 3:M:331:LEU:HD12 | 3:M:331:LEU:C    | 2.36                     | 0.49              |
| 4:S:93:GLU:HG2   | 4:S:98:ILE:HD11  | 1.94                     | 0.49              |
| 4:S:116:VAL:HG22 | 4:S:117:ASN:O    | 2.11                     | 0.49              |
| 1:A:64:LEU:CB    | 1:A:102:GLN:NE2  | 2.74                     | 0.49              |
| 1:A:92:LEU:HD21  | 1:A:124:ALA:HA   | 1.93                     | 0.49              |
| 1:A:395:PHE:CE2  | 1:A:420:ILE:HD13 | 2.48                     | 0.49              |
| 1:A:595:GLU:CD   | 2:B:473:ASN:OD1  | 2.55                     | 0.49              |
| 2:B:151:ALA:N    | 2:B:152:PRO:CD   | 2.75                     | 0.49              |
| 2:B:189:HIS:CE1  | 2:B:222:HIS:CG   | 3.01                     | 0.49              |
| 2:B:472:VAL:HG11 | 2:B:510:GLY:C    | 2.34                     | 0.49              |
| 2:B:511:ILE:O    | 2:B:512:VAL:C    | 2.48                     | 0.49              |
| 2:B:523:PHE:CZ   | 2:B:580:TYR:HD1  | 2.05                     | 0.49              |
| 3:M:288:ILE:CD1  | 3:M:300:LEU:CD2  | 2.90                     | 0.49              |
| 1:A:80:TYR:HB2   | 1:A:82:PHE:CE2   | 2.47                     | 0.49              |
| 1:A:179:LYS:NZ   | 4:S:141:VAL:HA   | 1.86                     | 0.49              |
| 1:A:253:ILE:HG23 | 1:A:281:LEU:HD13 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:292:TYR:O    | 1:A:295:VAL:HB   | 2.13                     | 0.49              |
| 1:A:446:ASP:O    | 1:A:447:PHE:C    | 2.51                     | 0.49              |
| 1:A:571:ARG:NH2  | 1:A:573:GLU:OE1  | 2.37                     | 0.49              |
| 2:B:167:ALA:CA   | 2:B:202:ASP:CG   | 2.83                     | 0.49              |
| 2:B:181:TYR:C    | 2:B:183:ALA:H    | 2.20                     | 0.49              |
| 2:B:253:ILE:CD1  | 2:B:324:ALA:HB2  | 2.43                     | 0.49              |
| 2:B:389:ILE:O    | 2:B:393:ILE:HG13 | 2.13                     | 0.49              |
| 3:M:290:PHE:CZ   | 3:M:297:PHE:CD1  | 3.00                     | 0.49              |
| 3:M:443:SER:CB   | 3:M:447:ILE:N    | 2.75                     | 0.49              |
| 4:S:102:ILE:O    | 4:S:105:PHE:HB3  | 2.13                     | 0.49              |
| 1:A:289:SER:HA   | 4:S:96:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:316:LEU:CD1  | 1:A:341:ILE:HG21 | 2.40                     | 0.49              |
| 1:A:581:LEU:HB3  | 1:A:607:LEU:HD13 | 1.95                     | 0.49              |
| 2:B:6:HIS:CB     | 3:M:25:PRO:C     | 2.85                     | 0.49              |
| 2:B:38:TYR:HD1   | 2:B:38:TYR:N     | 2.10                     | 0.49              |
| 2:B:234:CYS:HB3  | 2:B:301:LEU:CB   | 2.39                     | 0.49              |
| 2:B:589:SER:OG   | 2:B:618:PHE:CE2  | 2.53                     | 0.49              |
| 3:M:16:PHE:HE1   | 3:M:122:SER:CB   | 2.20                     | 0.49              |
| 3:M:74:TYR:OH    | 3:M:97:ASP:HB3   | 2.12                     | 0.49              |
| 4:S:53:THR:CG2   | 4:S:67:GLU:C     | 2.85                     | 0.49              |
| 1:A:465:SER:O    | 2:B:1:MET:HE3    | 2.12                     | 0.49              |
| 2:B:38:TYR:C     | 2:B:42:ILE:H     | 2.19                     | 0.49              |
| 2:B:139:LEU:HD21 | 2:B:173:VAL:CA   | 2.25                     | 0.49              |
| 2:B:168:MET:HA   | 2:B:207:VAL:HG22 | 1.94                     | 0.49              |
| 2:B:364:HIS:O    | 2:B:368:ILE:HG12 | 2.12                     | 0.49              |
| 2:B:537:PHE:CG   | 2:B:598:LEU:HB3  | 2.42                     | 0.49              |
| 3:M:222:PHE:CE1  | 3:M:240:ILE:HG21 | 2.47                     | 0.49              |
| 4:S:35:VAL:HB    | 4:S:77:TYR:CZ    | 2.46                     | 0.49              |
| 1:A:225:LEU:CD1  | 1:A:233:PHE:CE2  | 2.80                     | 0.49              |
| 1:A:371:ALA:O    | 1:A:374:LEU:N    | 2.45                     | 0.49              |
| 1:A:486:SER:O    | 1:A:487:MET:HB2  | 2.11                     | 0.49              |
| 1:A:529:GLY:CA   | 1:A:562:TRP:CZ2  | 2.96                     | 0.49              |
| 2:B:20:ARG:HH11  | 2:B:35:TYR:HE1   | 1.55                     | 0.49              |
| 2:B:29:LYS:HE2   | 2:B:30:LEU:CB    | 2.42                     | 0.49              |
| 2:B:118:LEU:O    | 2:B:121:ASN:N    | 2.44                     | 0.49              |
| 2:B:121:ASN:O    | 2:B:124:GLN:HB3  | 2.12                     | 0.49              |
| 2:B:162:VAL:C    | 2:B:164:ASP:N    | 2.70                     | 0.49              |
| 2:B:178:ILE:CD1  | 2:B:218:CYS:CB   | 2.89                     | 0.49              |
| 2:B:195:ILE:O    | 2:B:197:LYS:N    | 2.46                     | 0.49              |
| 2:B:237:ILE:O    | 2:B:239:GLN:N    | 2.44                     | 0.49              |
| 2:B:267:ASP:N    | 2:B:289:PRO:CB   | 2.63                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:328:LEU:O    | 2:B:329:ALA:C    | 2.47                     | 0.49              |
| 2:B:374:PHE:HB3  | 2:B:402:LEU:HD22 | 1.87                     | 0.49              |
| 2:B:433:VAL:HG21 | 2:B:471:TYR:CE1  | 2.47                     | 0.49              |
| 2:B:461:HIS:O    | 2:B:462:ASN:HB3  | 2.12                     | 0.49              |
| 2:B:585:GLY:O    | 2:B:589:SER:OG   | 2.30                     | 0.49              |
| 3:M:223:HIS:CD2  | 3:M:479:PHE:CD2  | 3.01                     | 0.49              |
| 3:M:250:LEU:HD13 | 3:M:254:PRO:CG   | 2.43                     | 0.49              |
| 3:M:280:ASP:N    | 3:M:280:ASP:OD1  | 2.45                     | 0.49              |
| 3:M:476:THR:OG1  | 3:M:477:GLY:N    | 2.46                     | 0.49              |
| 4:S:1:MET:H1     | 4:S:93:GLU:CD    | 2.09                     | 0.49              |
| 4:S:83:LEU:CD1   | 4:S:116:VAL:CG1  | 2.90                     | 0.49              |
| 1:A:535:ILE:O    | 1:A:536:MET:HG3  | 2.12                     | 0.49              |
| 1:A:566:PHE:CD1  | 1:A:567:GLN:N    | 2.81                     | 0.49              |
| 2:B:197:LYS:C    | 2:B:199:LEU:N    | 2.67                     | 0.49              |
| 2:B:305:SER:O    | 2:B:309:LEU:CD2  | 2.61                     | 0.49              |
| 2:B:316:THR:OG1  | 3:M:90:PHE:CZ    | 2.51                     | 0.49              |
| 2:B:367:SER:OG   | 2:B:401:THR:CG2  | 2.60                     | 0.49              |
| 2:B:371:GLN:HG2  | 2:B:401:THR:O    | 2.10                     | 0.49              |
| 3:M:69:ILE:HD12  | 3:M:93:LEU:HB3   | 1.95                     | 0.49              |
| 3:M:113:LYS:O    | 3:M:117:ASN:ND2  | 2.38                     | 0.49              |
| 3:M:221:THR:CA   | 3:M:474:THR:OG1  | 2.53                     | 0.49              |
| 3:M:235:LEU:CD2  | 3:M:307:SER:HA   | 2.42                     | 0.49              |
| 3:M:316:ARG:HG3  | 3:M:322:LEU:CD1  | 2.42                     | 0.49              |
| 3:M:338:PHE:CD2  | 3:M:415:ILE:HD11 | 2.48                     | 0.49              |
| 3:M:437:TYR:CE1  | 3:M:479:PHE:CD1  | 3.01                     | 0.49              |
| 4:S:53:THR:HG22  | 4:S:54:PRO:O     | 2.11                     | 0.49              |
| 1:A:179:LYS:HE3  | 4:S:140:MET:HG2  | 1.95                     | 0.49              |
| 2:B:78:ASP:OD1   | 2:B:80:GLN:HB2   | 2.13                     | 0.49              |
| 2:B:90:ILE:N     | 2:B:101:ILE:HD13 | 2.28                     | 0.49              |
| 2:B:215:TYR:HE2  | 2:B:229:HIS:ND1  | 2.10                     | 0.49              |
| 2:B:366:LEU:O    | 2:B:368:ILE:N    | 2.45                     | 0.49              |
| 2:B:427:ASN:HA   | 2:B:430:ILE:HD12 | 1.95                     | 0.49              |
| 2:B:479:VAL:CG1  | 2:B:486:HIS:ND1  | 2.15                     | 0.49              |
| 2:B:500:GLN:NE2  | 2:B:503:LEU:HD21 | 2.27                     | 0.49              |
| 2:B:534:ILE:CG1  | 2:B:595:VAL:HG23 | 2.42                     | 0.49              |
| 2:B:596:LEU:HD22 | 2:B:615:SER:CB   | 2.43                     | 0.49              |
| 3:M:7:ILE:HG13   | 3:M:16:PHE:HD2   | 1.78                     | 0.49              |
| 3:M:15:ILE:CG2   | 3:M:114:ILE:CG2  | 2.91                     | 0.49              |
| 3:M:300:LEU:O    | 3:M:300:LEU:HD12 | 2.13                     | 0.49              |
| 1:A:99:LYS:HG2   | 1:A:101:GLN:N    | 2.27                     | 0.49              |
| 1:A:400:VAL:O    | 1:A:403:LEU:HB2  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:548:GLN:CD   | 1:A:588:LEU:HD11 | 2.38                     | 0.49              |
| 2:B:10:SER:O     | 2:B:11:ALA:C     | 2.56                     | 0.49              |
| 2:B:83:PHE:CE1   | 2:B:105:LEU:HA   | 2.48                     | 0.49              |
| 2:B:133:GLU:O    | 2:B:168:MET:CE   | 2.60                     | 0.49              |
| 2:B:133:GLU:CB   | 2:B:168:MET:SD   | 3.01                     | 0.49              |
| 2:B:230:PHE:HB3  | 2:B:298:ASP:OD2  | 2.12                     | 0.49              |
| 2:B:237:ILE:CG2  | 2:B:305:SER:HB3  | 2.42                     | 0.49              |
| 2:B:530:LEU:CD2  | 2:B:591:MET:CB   | 2.89                     | 0.49              |
| 2:B:545:ARG:HH11 | 2:B:602:ASP:CG   | 2.21                     | 0.49              |
| 3:M:76:CYS:HB3   | 3:M:93:LEU:HD22  | 1.94                     | 0.49              |
| 3:M:219:LEU:CD2  | 3:M:473:LYS:HA   | 2.34                     | 0.49              |
| 3:M:304:VAL:HG21 | 3:M:309:GLN:CD   | 2.38                     | 0.49              |
| 1:A:114:PHE:CD1  | 1:A:114:PHE:C    | 2.90                     | 0.49              |
| 1:A:320:HIS:HB2  | 1:A:352:PHE:HE2  | 1.74                     | 0.49              |
| 1:A:488:ARG:CD   | 1:A:522:PHE:CE2  | 2.96                     | 0.49              |
| 2:B:106:LEU:HD11 | 2:B:144:ASP:HB3  | 1.89                     | 0.49              |
| 2:B:182:ARG:HD2  | 2:B:217:GLU:CG   | 2.42                     | 0.49              |
| 2:B:261:PRO:HB2  | 2:B:290:SER:OG   | 2.13                     | 0.49              |
| 2:B:276:SER:CB   | 2:B:289:PRO:HG3  | 2.43                     | 0.49              |
| 2:B:398:ILE:CG2  | 2:B:402:LEU:HD11 | 2.43                     | 0.49              |
| 2:B:400:SER:CA   | 2:B:439:CYS:SG   | 3.01                     | 0.49              |
| 2:B:463:LEU:HD13 | 2:B:467:VAL:CG1  | 2.43                     | 0.49              |
| 2:B:513:TRP:C    | 2:B:551:LEU:HD22 | 2.38                     | 0.49              |
| 2:B:546:CYS:N    | 2:B:607:ILE:CD1  | 2.76                     | 0.49              |
| 3:M:56:VAL:HB    | 3:M:64:LYS:HG3   | 1.93                     | 0.49              |
| 3:M:219:LEU:CB   | 3:M:472:TYR:C    | 2.86                     | 0.49              |
| 4:S:17:VAL:HG13  | 4:S:17:VAL:O     | 2.13                     | 0.49              |
| 2:B:102:HIS:HE2  | 2:B:138:ALA:CB   | 2.25                     | 0.48              |
| 2:B:256:CYS:HB3  | 2:B:328:LEU:CD2  | 2.42                     | 0.48              |
| 2:B:513:TRP:NE1  | 2:B:517:GLU:CG   | 2.76                     | 0.48              |
| 3:M:256:VAL:CG2  | 3:M:452:ILE:CG2  | 2.91                     | 0.48              |
| 1:A:309:PHE:CE1  | 1:A:348:PHE:CE2  | 3.00                     | 0.48              |
| 1:A:435:ILE:O    | 1:A:441:TYR:CE1  | 2.66                     | 0.48              |
| 2:B:37:TYR:HD2   | 2:B:38:TYR:CE1   | 2.29                     | 0.48              |
| 2:B:403:ILE:CB   | 2:B:408:VAL:HG22 | 2.31                     | 0.48              |
| 2:B:448:SER:OG   | 2:B:485:LYS:HE3  | 2.14                     | 0.48              |
| 2:B:490:ILE:CG2  | 2:B:515:PHE:CD2  | 2.96                     | 0.48              |
| 3:M:222:PHE:CD1  | 3:M:222:PHE:N    | 2.81                     | 0.48              |
| 3:M:223:HIS:CD2  | 3:M:479:PHE:CE2  | 3.01                     | 0.48              |
| 3:M:252:ASP:O    | 3:M:254:PRO:HD2  | 2.14                     | 0.48              |
| 4:S:112:CYS:HB2  | 4:S:113:PHE:CE1  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:TYR:OH   | 4:S:148:ARG:CB   | 2.45                     | 0.48              |
| 1:A:237:SER:N    | 1:A:238:PRO:CD   | 2.75                     | 0.48              |
| 1:A:356:ILE:HD13 | 1:A:374:LEU:HB3  | 1.94                     | 0.48              |
| 1:A:529:GLY:C    | 1:A:562:TRP:CH2  | 2.91                     | 0.48              |
| 2:B:133:GLU:HG2  | 2:B:168:MET:SD   | 2.53                     | 0.48              |
| 2:B:337:THR:OG1  | 2:B:373:LEU:HD13 | 2.13                     | 0.48              |
| 2:B:550:VAL:O    | 2:B:553:ALA:HB3  | 2.12                     | 0.48              |
| 3:M:54:SER:HB2   | 3:M:66:PHE:CD1   | 2.48                     | 0.48              |
| 3:M:100:LEU:C    | 3:M:103:TYR:O    | 2.56                     | 0.48              |
| 3:M:218:LEU:HD21 | 3:M:449:VAL:HG23 | 1.95                     | 0.48              |
| 3:M:222:PHE:C    | 3:M:479:PHE:CE2  | 2.78                     | 0.48              |
| 3:M:290:PHE:CZ   | 3:M:291:ILE:O    | 2.66                     | 0.48              |
| 3:M:323:MET:HE3  | 3:M:342:LEU:HB3  | 1.95                     | 0.48              |
| 1:A:179:LYS:NZ   | 4:S:141:VAL:CA   | 2.09                     | 0.48              |
| 1:A:226:SER:HB2  | 1:A:263:LEU:HD23 | 1.96                     | 0.48              |
| 1:A:433:ILE:HD11 | 1:A:473:ILE:HA   | 1.95                     | 0.48              |
| 2:B:136:CYS:CB   | 2:B:172:GLU:CG   | 2.84                     | 0.48              |
| 2:B:181:TYR:CD2  | 2:B:218:CYS:HA   | 2.48                     | 0.48              |
| 2:B:243:TRP:CH2  | 3:M:95:THR:HA    | 2.47                     | 0.48              |
| 2:B:280:PRO:HG2  | 2:B:283:TYR:HD1  | 1.63                     | 0.48              |
| 2:B:383:VAL:CG2  | 2:B:384:PHE:N    | 2.75                     | 0.48              |
| 3:M:56:VAL:H     | 3:M:64:LYS:CB    | 2.26                     | 0.48              |
| 3:M:100:LEU:HD23 | 3:M:124:ILE:CD1  | 2.44                     | 0.48              |
| 3:M:401:LYS:O    | 3:M:402:SER:C    | 2.54                     | 0.48              |
| 4:S:53:THR:HG21  | 4:S:68:VAL:CA    | 2.28                     | 0.48              |
| 1:A:509:PRO:HB3  | 1:A:547:VAL:HG23 | 1.93                     | 0.48              |
| 2:B:220:ALA:HA   | 2:B:258:GLN:HG3  | 1.95                     | 0.48              |
| 2:B:343:LEU:HD11 | 2:B:359:LEU:HD13 | 1.95                     | 0.48              |
| 2:B:343:LEU:HD12 | 2:B:359:LEU:CD1  | 2.43                     | 0.48              |
| 2:B:352:ASN:OD1  | 3:M:49:ASP:HA    | 2.12                     | 0.48              |
| 2:B:596:LEU:HD13 | 2:B:611:ALA:C    | 2.38                     | 0.48              |
| 3:M:84:LYS:O     | 3:M:88:ASP:CB    | 2.61                     | 0.48              |
| 3:M:244:VAL:O    | 3:M:299:LEU:CB   | 2.61                     | 0.48              |
| 4:S:89:VAL:CG1   | 4:S:98:ILE:HD12  | 2.43                     | 0.48              |
| 1:A:158:LEU:HD12 | 1:A:162:ILE:HG13 | 1.95                     | 0.48              |
| 1:A:595:GLU:CD   | 2:B:476:ARG:NH2  | 2.71                     | 0.48              |
| 2:B:39:SER:HG    | 2:B:40:GLN:N     | 2.12                     | 0.48              |
| 2:B:530:LEU:HD11 | 2:B:595:VAL:HG21 | 1.95                     | 0.48              |
| 2:B:540:GLU:OE1  | 2:B:548:ILE:HD11 | 2.13                     | 0.48              |
| 3:M:95:THR:CG2   | 3:M:137:SER:HA   | 2.43                     | 0.48              |
| 3:M:99:ILE:CG2   | 3:M:99:ILE:O     | 2.62                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:379:LEU:HB3  | 3:M:411:LEU:CD1  | 2.44                     | 0.48              |
| 1:A:174:ARG:HH22 | 4:S:148:ARG:HH22 | 1.51                     | 0.48              |
| 1:A:186:PHE:CE2  | 1:A:187:LYS:HD3  | 2.48                     | 0.48              |
| 2:B:51:LEU:HD11  | 2:B:66:ILE:CD1   | 2.44                     | 0.48              |
| 2:B:155:LEU:O    | 2:B:158:VAL:N    | 2.46                     | 0.48              |
| 2:B:175:LEU:HG   | 2:B:210:CYS:HB3  | 1.93                     | 0.48              |
| 2:B:193:LEU:HB3  | 2:B:225:LEU:CG   | 2.43                     | 0.48              |
| 2:B:461:HIS:HB2  | 2:B:463:LEU:CD2  | 2.44                     | 0.48              |
| 2:B:467:VAL:HG12 | 2:B:471:TYR:CD1  | 2.49                     | 0.48              |
| 2:B:537:PHE:CZ   | 2:B:545:ARG:HB3  | 2.48                     | 0.48              |
| 3:M:41:LEU:HB3   | 3:M:51:LEU:HA    | 1.96                     | 0.48              |
| 4:S:47:GLN:O     | 4:S:49:SER:N     | 2.44                     | 0.48              |
| 1:A:375:VAL:CG1  | 1:A:387:ILE:HG21 | 2.44                     | 0.48              |
| 1:A:384:LEU:CD1  | 1:A:385:LYS:N    | 2.77                     | 0.48              |
| 1:A:579:LYS:O    | 1:A:582:ILE:HB   | 2.14                     | 0.48              |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:CG   | 2.43                     | 0.48              |
| 2:B:13:ASP:O     | 2:B:16:LYS:N     | 2.47                     | 0.48              |
| 2:B:21:GLU:HA    | 2:B:24:ALA:HB2   | 1.86                     | 0.48              |
| 2:B:353:GLN:O    | 2:B:354:GLY:C    | 2.56                     | 0.48              |
| 2:B:538:SER:HB3  | 2:B:598:LEU:HD22 | 1.94                     | 0.48              |
| 3:M:104:PHE:CZ   | 3:M:120:ARG:HB2  | 2.49                     | 0.48              |
| 3:M:217:ASP:CB   | 3:M:470:ALA:C    | 2.87                     | 0.48              |
| 3:M:219:LEU:HD22 | 3:M:473:LYS:C    | 2.39                     | 0.48              |
| 3:M:240:ILE:HG22 | 3:M:444:ALA:CB   | 2.41                     | 0.48              |
| 3:M:242:GLY:N    | 3:M:444:ALA:CB   | 2.76                     | 0.48              |
| 3:M:290:PHE:HZ   | 3:M:293:PRO:CD   | 2.27                     | 0.48              |
| 1:A:300:LYS:O    | 1:A:301:GLY:C    | 2.55                     | 0.48              |
| 2:B:77:ILE:O     | 2:B:78:ASP:C     | 2.55                     | 0.48              |
| 2:B:219:TYR:CE2  | 2:B:226:LEU:CA   | 2.79                     | 0.48              |
| 2:B:483:PRO:HA   | 2:B:486:HIS:CB   | 2.43                     | 0.48              |
| 2:B:588:ILE:O    | 2:B:591:MET:HB2  | 2.14                     | 0.48              |
| 3:M:65:TYR:CE1   | 3:M:66:PHE:O     | 2.67                     | 0.48              |
| 3:M:245:ASP:CB   | 3:M:472:TYR:CE1  | 2.95                     | 0.48              |
| 3:M:356:LEU:HD11 | 3:M:437:TYR:CE2  | 2.49                     | 0.48              |
| 3:M:386:PHE:CB   | 3:M:397:TRP:CD1  | 2.97                     | 0.48              |
| 1:A:76:TYR:O     | 1:A:80:TYR:CD1   | 2.67                     | 0.48              |
| 1:A:121:LEU:HG   | 1:A:158:LEU:HD22 | 1.94                     | 0.48              |
| 1:A:516:ILE:HG12 | 1:A:551:LEU:HD13 | 1.96                     | 0.48              |
| 1:A:617:ASP:OD1  | 1:A:618:THR:N    | 2.45                     | 0.48              |
| 2:B:306:LEU:CD1  | 2:B:325:LEU:CD2  | 2.91                     | 0.48              |
| 2:B:341:GLU:CB   | 2:B:377:TYR:OH   | 2.60                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:508:ARG:HB3  | 2:B:544:THR:HG23 | 1.95                     | 0.48              |
| 2:B:587:ARG:O    | 2:B:591:MET:HG2  | 2.14                     | 0.48              |
| 3:M:212:ASN:HB3  | 3:M:250:LEU:HA   | 1.96                     | 0.48              |
| 3:M:435:LEU:O    | 3:M:479:PHE:CE2  | 2.60                     | 0.48              |
| 4:S:1:MET:SD     | 4:S:20:TYR:CD2   | 3.06                     | 0.48              |
| 1:A:156:PRO:HA   | 1:A:192:TYR:CD1  | 2.49                     | 0.47              |
| 1:A:438:ALA:O    | 1:A:441:TYR:HD1  | 1.96                     | 0.47              |
| 1:A:461:CYS:SG   | 1:A:464:ILE:HG22 | 2.54                     | 0.47              |
| 1:A:533:ILE:HG13 | 1:A:562:TRP:CH2  | 2.44                     | 0.47              |
| 2:B:108:PHE:CD2  | 2:B:112:ASP:HB3  | 2.49                     | 0.47              |
| 2:B:230:PHE:CZ   | 2:B:234:CYS:SG   | 3.06                     | 0.47              |
| 2:B:231:ARG:NH2  | 2:B:279:LEU:CD2  | 2.70                     | 0.47              |
| 2:B:237:ILE:HG21 | 2:B:305:SER:CB   | 2.43                     | 0.47              |
| 2:B:311:TYR:HD1  | 3:M:269:ILE:HD11 | 1.79                     | 0.47              |
| 2:B:367:SER:CB   | 2:B:401:THR:OG1  | 2.62                     | 0.47              |
| 2:B:578:PRO:CB   | 2:B:579:PRO:CD   | 2.92                     | 0.47              |
| 2:B:586:SER:O    | 2:B:590:GLN:HG3  | 2.13                     | 0.47              |
| 2:B:592:TYR:CG   | 2:B:593:ASN:N    | 2.82                     | 0.47              |
| 3:M:45:SER:HA    | 3:M:47:SER:N     | 2.28                     | 0.47              |
| 3:M:104:PHE:CD1  | 3:M:104:PHE:N    | 2.66                     | 0.47              |
| 3:M:290:PHE:HZ   | 3:M:293:PRO:CG   | 2.26                     | 0.47              |
| 4:S:16:LEU:HD12  | 4:S:17:VAL:N     | 2.29                     | 0.47              |
| 1:A:78:GLU:C     | 1:A:80:TYR:O     | 2.57                     | 0.47              |
| 1:A:289:SER:HA   | 4:S:96:LEU:CD1   | 2.42                     | 0.47              |
| 1:A:412:LYS:O    | 1:A:414:LYS:N    | 2.47                     | 0.47              |
| 2:B:486:HIS:CD2  | 2:B:518:ILE:CG1  | 2.97                     | 0.47              |
| 2:B:494:ALA:N    | 2:B:515:PHE:CZ   | 2.76                     | 0.47              |
| 2:B:500:GLN:OE1  | 2:B:503:LEU:HD21 | 2.14                     | 0.47              |
| 2:B:546:CYS:HB2  | 2:B:607:ILE:HG13 | 1.80                     | 0.47              |
| 3:M:309:GLN:O    | 3:M:313:SER:N    | 2.40                     | 0.47              |
| 3:M:386:PHE:CB   | 3:M:397:TRP:HD1  | 2.27                     | 0.47              |
| 4:S:58:LEU:HD13  | 4:S:69:ASN:N     | 2.28                     | 0.47              |
| 1:A:239:LEU:O    | 1:A:242:GLU:C    | 2.51                     | 0.47              |
| 1:A:395:PHE:CD2  | 1:A:428:MET:HE2  | 2.49                     | 0.47              |
| 1:A:504:ILE:O    | 1:A:505:ASN:O    | 2.33                     | 0.47              |
| 1:A:624:LEU:O    | 1:A:627:GLU:HB2  | 2.15                     | 0.47              |
| 2:B:74:ASP:O     | 2:B:77:ILE:CG1   | 2.62                     | 0.47              |
| 2:B:85:ASP:O     | 2:B:89:ASN:ND2   | 2.47                     | 0.47              |
| 2:B:120:ILE:HG13 | 2:B:150:LEU:HD13 | 1.96                     | 0.47              |
| 2:B:296:ASP:C    | 2:B:298:ASP:N    | 2.71                     | 0.47              |
| 2:B:475:ILE:CG2  | 2:B:489:ILE:CG2  | 2.90                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:490:ILE:HG23 | 2:B:515:PHE:CE2  | 2.47                     | 0.47              |
| 2:B:553:ALA:CB   | 2:B:614:ILE:CG2  | 2.92                     | 0.47              |
| 3:M:56:VAL:H     | 3:M:64:LYS:HG3   | 1.77                     | 0.47              |
| 3:M:121:ILE:HG23 | 3:M:125:PHE:CE1  | 2.49                     | 0.47              |
| 3:M:302:TYR:CD2  | 3:M:445:SER:CB   | 2.88                     | 0.47              |
| 3:M:320:ILE:CG2  | 3:M:439:TYR:OH   | 2.62                     | 0.47              |
| 3:M:410:VAL:HG11 | 3:M:412:ARG:CZ   | 2.45                     | 0.47              |
| 3:M:473:LYS:C    | 3:M:474:THR:CG2  | 2.87                     | 0.47              |
| 1:A:436:CYS:SG   | 1:A:450:TYR:CD2  | 3.03                     | 0.47              |
| 1:A:626:SER:O    | 1:A:630:PRO:HD2  | 2.15                     | 0.47              |
| 2:B:189:HIS:NE2  | 2:B:222:HIS:CG   | 2.82                     | 0.47              |
| 2:B:215:TYR:HD1  | 2:B:233:TYR:CZ   | 2.26                     | 0.47              |
| 2:B:490:ILE:CD1  | 2:B:518:ILE:CG2  | 2.87                     | 0.47              |
| 3:M:265:ASN:O    | 3:M:267:ILE:N    | 2.47                     | 0.47              |
| 3:M:317:MET:CB   | 3:M:320:ILE:O    | 2.60                     | 0.47              |
| 3:M:373:ALA:HB3  | 3:M:418:GLU:O    | 2.15                     | 0.47              |
| 4:S:8:PHE:CE2    | 4:S:84:TYR:O     | 2.67                     | 0.47              |
| 1:A:275:LEU:HA   | 1:A:278:ILE:CG1  | 2.45                     | 0.47              |
| 1:A:316:LEU:CD1  | 1:A:348:PHE:CE2  | 2.97                     | 0.47              |
| 1:A:356:ILE:HD11 | 1:A:374:LEU:HD23 | 1.95                     | 0.47              |
| 1:A:438:ALA:HB3  | 1:A:441:TYR:CE1  | 2.48                     | 0.47              |
| 1:A:595:GLU:HA   | 2:B:476:ARG:NH1  | 2.30                     | 0.47              |
| 2:B:95:THR:HG23  | 2:B:137:PHE:CE2  | 2.50                     | 0.47              |
| 2:B:196:LEU:HB2  | 2:B:229:HIS:CE1  | 2.48                     | 0.47              |
| 2:B:352:ASN:HD21 | 3:M:70:ASN:HB2   | 1.74                     | 0.47              |
| 2:B:546:CYS:O    | 2:B:549:LEU:HB3  | 2.14                     | 0.47              |
| 2:B:553:ALA:HA   | 2:B:614:ILE:HG23 | 1.96                     | 0.47              |
| 2:B:563:PHE:O    | 2:B:564:LYS:O    | 2.32                     | 0.47              |
| 3:M:214:LEU:H    | 3:M:466:LEU:HA   | 1.79                     | 0.47              |
| 3:M:325:LEU:HA   | 3:M:339:GLU:O    | 2.14                     | 0.47              |
| 3:M:376:ILE:HG22 | 3:M:379:LEU:CD1  | 2.45                     | 0.47              |
| 3:M:443:SER:HB3  | 3:M:447:ILE:CA   | 2.45                     | 0.47              |
| 1:A:92:LEU:HD13  | 1:A:123:LEU:HB3  | 1.96                     | 0.47              |
| 1:A:220:SER:HB3  | 4:S:140:MET:HE3  | 1.95                     | 0.47              |
| 1:A:316:LEU:O    | 1:A:319:LEU:HB2  | 2.14                     | 0.47              |
| 2:B:267:ASP:OD1  | 2:B:269:SER:HB2  | 2.14                     | 0.47              |
| 2:B:302:PHE:CE1  | 2:B:306:LEU:HD21 | 2.49                     | 0.47              |
| 2:B:343:LEU:HD23 | 2:B:363:ILE:CD1  | 2.32                     | 0.47              |
| 2:B:588:ILE:HG21 | 2:B:618:PHE:CE1  | 2.44                     | 0.47              |
| 3:M:62:VAL:HG12  | 3:M:64:LYS:HD3   | 1.97                     | 0.47              |
| 3:M:99:ILE:HD13  | 3:M:128:CYS:SG   | 2.55                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:220:GLU:OE1  | 3:M:222:PHE:CZ   | 2.68                     | 0.47              |
| 3:M:419:ASN:CG   | 3:M:424:PHE:CD2  | 2.93                     | 0.47              |
| 1:A:140:VAL:O    | 1:A:141:VAL:O    | 2.32                     | 0.47              |
| 1:A:166:LEU:HD12 | 1:A:185:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:170:LEU:HD13 | 1:A:181:ALA:HB3  | 1.96                     | 0.47              |
| 1:A:222:ILE:HG23 | 1:A:233:PHE:CD2  | 2.49                     | 0.47              |
| 1:A:253:ILE:HG12 | 1:A:281:LEU:HD13 | 1.97                     | 0.47              |
| 1:A:268:PRO:HA   | 1:A:271:ARG:HE   | 1.79                     | 0.47              |
| 1:A:275:LEU:CD1  | 1:A:308:ASP:CG   | 2.88                     | 0.47              |
| 1:A:397:ASP:O    | 1:A:418:ILE:CD1  | 2.63                     | 0.47              |
| 1:A:400:VAL:H    | 1:A:418:ILE:HG12 | 1.79                     | 0.47              |
| 1:A:429:VAL:CG1  | 1:A:469:LEU:CD1  | 2.91                     | 0.47              |
| 1:A:433:ILE:HG23 | 1:A:476:GLN:HB2  | 1.96                     | 0.47              |
| 1:A:438:ALA:O    | 1:A:440:ASN:N    | 2.35                     | 0.47              |
| 1:A:566:PHE:CZ   | 1:A:618:THR:O    | 2.57                     | 0.47              |
| 1:A:589:SER:C    | 1:A:597:GLN:HG3  | 2.34                     | 0.47              |
| 2:B:60:ARG:O     | 2:B:63:MET:N     | 2.45                     | 0.47              |
| 2:B:101:ILE:O    | 2:B:104:TYR:HB3  | 2.14                     | 0.47              |
| 2:B:155:LEU:CG   | 2:B:188:TYR:HD2  | 2.27                     | 0.47              |
| 2:B:260:LEU:HD22 | 2:B:291:TYR:OH   | 2.15                     | 0.47              |
| 2:B:343:LEU:CD1  | 2:B:359:LEU:CD1  | 2.92                     | 0.47              |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:CD1  | 2.44                     | 0.47              |
| 2:B:497:LEU:HB2  | 2:B:511:ILE:HG21 | 1.95                     | 0.47              |
| 3:M:20:LEU:C     | 3:M:21:GLY:O     | 2.50                     | 0.47              |
| 3:M:48:ASP:CA    | 3:M:75:TRP:CZ2   | 2.95                     | 0.47              |
| 3:M:111:ILE:HG13 | 3:M:112:LYS:N    | 2.29                     | 0.47              |
| 3:M:114:ILE:O    | 3:M:115:VAL:C    | 2.57                     | 0.47              |
| 4:S:83:LEU:HD11  | 4:S:116:VAL:HG13 | 1.95                     | 0.47              |
| 1:A:136:GLY:O    | 1:A:139:ASP:CA   | 2.62                     | 0.47              |
| 1:A:223:CYS:SG   | 1:A:259:LEU:HA   | 2.55                     | 0.47              |
| 1:A:244:LEU:HD13 | 1:A:256:LEU:CB   | 2.44                     | 0.47              |
| 1:A:421:PRO:HG2  | 1:A:424:TYR:CD1  | 2.49                     | 0.47              |
| 1:A:429:VAL:HG11 | 1:A:473:ILE:CG1  | 2.45                     | 0.47              |
| 1:A:637:GLU:HG3  | 2:B:516:GLY:O    | 2.14                     | 0.47              |
| 2:B:28:SER:N     | 2:B:32:GLU:CD    | 2.70                     | 0.47              |
| 2:B:303:LEU:HD13 | 2:B:333:GLN:HB3  | 1.95                     | 0.47              |
| 2:B:340:ILE:HG13 | 2:B:373:LEU:HB3  | 1.96                     | 0.47              |
| 2:B:418:TYR:CE1  | 2:B:419:VAL:HA   | 2.49                     | 0.47              |
| 2:B:534:ILE:HD11 | 2:B:591:MET:C    | 2.34                     | 0.47              |
| 2:B:592:TYR:HD2  | 2:B:618:PHE:CE2  | 2.29                     | 0.47              |
| 3:M:220:GLU:OE1  | 3:M:222:PHE:CE1  | 2.68                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:419:ASN:ND2  | 3:M:424:PHE:HD2  | 2.12                     | 0.47              |
| 1:A:180:LYS:HD3  | 4:S:137:GLN:HB2  | 1.97                     | 0.47              |
| 1:A:313:MET:HB2  | 1:A:348:PHE:CZ   | 2.50                     | 0.47              |
| 1:A:555:LEU:O    | 1:A:559:PHE:HD1  | 1.97                     | 0.47              |
| 1:A:589:SER:O    | 1:A:597:GLN:CD   | 2.57                     | 0.47              |
| 1:A:638:LEU:HA   | 2:B:520:SER:HB3  | 1.89                     | 0.47              |
| 2:B:2:VAL:HG12   | 2:B:6:HIS:CE1    | 2.49                     | 0.47              |
| 2:B:18:ILE:HB    | 2:B:23:ALA:CB    | 2.18                     | 0.47              |
| 2:B:278:PRO:CD   | 2:B:292:GLU:CG   | 2.69                     | 0.47              |
| 2:B:374:PHE:CD2  | 2:B:402:LEU:CG   | 2.93                     | 0.47              |
| 2:B:490:ILE:HG23 | 2:B:515:PHE:CD2  | 2.50                     | 0.47              |
| 2:B:569:THR:C    | 2:B:571:SER:N    | 2.57                     | 0.47              |
| 2:B:610:ARG:O    | 2:B:614:ILE:HG13 | 2.15                     | 0.47              |
| 3:M:242:GLY:HA2  | 3:M:444:ALA:HB2  | 1.94                     | 0.47              |
| 3:M:466:LEU:HD23 | 3:M:467:TYR:O    | 2.15                     | 0.47              |
| 1:A:150:LEU:O    | 1:A:153:ILE:N    | 2.47                     | 0.47              |
| 1:A:192:TYR:CE2  | 1:A:194:GLU:HB2  | 2.50                     | 0.47              |
| 1:A:370:LYS:C    | 1:A:374:LEU:HD13 | 2.40                     | 0.47              |
| 1:A:441:TYR:HB3  | 1:A:444:VAL:HG23 | 1.96                     | 0.47              |
| 1:A:446:ASP:CB   | 1:A:448:GLU:O    | 2.63                     | 0.47              |
| 1:A:605:GLU:OE2  | 1:A:632:PHE:CZ   | 2.68                     | 0.47              |
| 2:B:231:ARG:C    | 2:B:233:TYR:H    | 2.22                     | 0.47              |
| 3:M:273:HIS:CB   | 3:M:298:ARG:O    | 2.59                     | 0.47              |
| 3:M:376:ILE:CG2  | 3:M:379:LEU:HD11 | 2.45                     | 0.47              |
| 3:M:435:LEU:H    | 3:M:479:PHE:HB2  | 1.78                     | 0.47              |
| 4:S:38:LEU:CB    | 4:S:51:LEU:HD13  | 2.44                     | 0.47              |
| 1:A:278:ILE:O    | 1:A:280:GLU:N    | 2.44                     | 0.46              |
| 1:A:292:TYR:O    | 1:A:292:TYR:HD1  | 1.98                     | 0.46              |
| 1:A:404:GLN:C    | 2:B:7:ARG:NE     | 2.73                     | 0.46              |
| 1:A:436:CYS:SG   | 1:A:450:TYR:CD1  | 3.05                     | 0.46              |
| 1:A:449:TRP:O    | 1:A:453:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:602:GLU:CD   | 1:A:633:PHE:CE1  | 2.93                     | 0.46              |
| 1:A:605:GLU:CD   | 1:A:636:TYR:OH   | 2.57                     | 0.46              |
| 2:B:21:GLU:O     | 2:B:25:VAL:HG23  | 2.13                     | 0.46              |
| 2:B:127:LEU:HD22 | 2:B:157:THR:CG2  | 2.44                     | 0.46              |
| 2:B:127:LEU:O    | 2:B:135:ARG:HD3  | 2.15                     | 0.46              |
| 2:B:134:LEU:C    | 2:B:136:CYS:N    | 2.72                     | 0.46              |
| 2:B:340:ILE:HD11 | 2:B:366:LEU:HB3  | 1.97                     | 0.46              |
| 2:B:494:ALA:CA   | 2:B:515:PHE:CZ   | 2.98                     | 0.46              |
| 3:M:64:LYS:HB3   | 3:M:66:PHE:CE1   | 2.51                     | 0.46              |
| 3:M:224:VAL:CG1  | 3:M:226:PHE:CZ   | 2.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:319:SER:CA   | 3:M:343:ASN:O    | 2.63                     | 0.46              |
| 3:M:338:PHE:CE2  | 3:M:415:ILE:CD1  | 2.98                     | 0.46              |
| 4:S:8:PHE:HB3    | 4:S:36:TYR:CZ    | 2.50                     | 0.46              |
| 4:S:8:PHE:HA     | 4:S:13:GLN:O     | 2.16                     | 0.46              |
| 1:A:406:GLY:N    | 2:B:7:ARG:NH1    | 2.55                     | 0.46              |
| 1:A:435:ILE:O    | 1:A:441:TYR:CZ   | 2.68                     | 0.46              |
| 1:A:476:GLN:OE1  | 1:A:476:GLN:HA   | 2.15                     | 0.46              |
| 2:B:9:ALA:O      | 2:B:10:SER:C     | 2.58                     | 0.46              |
| 2:B:66:ILE:CG2   | 2:B:104:TYR:CE1  | 2.95                     | 0.46              |
| 2:B:215:TYR:CD1  | 2:B:233:TYR:CZ   | 2.98                     | 0.46              |
| 2:B:279:LEU:CG   | 2:B:288:TYR:HD1  | 2.22                     | 0.46              |
| 2:B:375:LEU:HB2  | 2:B:376:PRO:HD3  | 1.97                     | 0.46              |
| 2:B:397:GLN:HE21 | 2:B:431:MET:CE   | 2.27                     | 0.46              |
| 2:B:537:PHE:HE1  | 2:B:545:ARG:HB3  | 1.78                     | 0.46              |
| 3:M:217:ASP:HB3  | 3:M:470:ALA:C    | 2.41                     | 0.46              |
| 4:S:163:THR:C    | 4:S:163:THR:CB   | 2.79                     | 0.46              |
| 1:A:381:GLU:O    | 1:A:383:ASN:N    | 2.46                     | 0.46              |
| 1:A:559:PHE:CD1  | 1:A:581:LEU:HD22 | 2.47                     | 0.46              |
| 2:B:108:PHE:CD2  | 2:B:115:LEU:CB   | 2.98                     | 0.46              |
| 2:B:347:VAL:CG2  | 2:B:359:LEU:HD12 | 2.46                     | 0.46              |
| 2:B:435:SER:C    | 2:B:437:SER:N    | 2.73                     | 0.46              |
| 2:B:534:ILE:CD1  | 2:B:591:MET:C    | 2.77                     | 0.46              |
| 2:B:578:PRO:CD   | 2:B:581:TYR:HE1  | 2.26                     | 0.46              |
| 3:M:244:VAL:HG13 | 3:M:472:TYR:HE2  | 1.78                     | 0.46              |
| 3:M:245:ASP:C    | 3:M:246:VAL:HG23 | 2.40                     | 0.46              |
| 4:S:38:LEU:HB3   | 4:S:51:LEU:HD11  | 1.97                     | 0.46              |
| 1:A:77:LEU:O     | 1:A:82:PHE:CD2   | 2.69                     | 0.46              |
| 1:A:193:PRO:O    | 1:A:196:LEU:HB3  | 2.16                     | 0.46              |
| 1:A:429:VAL:HG11 | 1:A:469:LEU:CD1  | 2.44                     | 0.46              |
| 1:A:461:CYS:HB2  | 1:A:469:LEU:HD23 | 1.96                     | 0.46              |
| 1:A:528:ASN:C    | 1:A:530:ASN:N    | 2.71                     | 0.46              |
| 2:B:44:PRO:O     | 2:B:47:LEU:HB2   | 2.14                     | 0.46              |
| 2:B:227:HIS:HE1  | 2:B:292:GLU:HG2  | 1.73                     | 0.46              |
| 2:B:252:LEU:HB3  | 2:B:302:PHE:CD1  | 2.49                     | 0.46              |
| 2:B:306:LEU:HD12 | 2:B:325:LEU:HD21 | 1.98                     | 0.46              |
| 2:B:383:VAL:HG22 | 2:B:384:PHE:N    | 2.31                     | 0.46              |
| 2:B:383:VAL:HA   | 2:B:395:LYS:HE3  | 1.97                     | 0.46              |
| 3:M:134:PRO:O    | 3:M:136:VAL:HG23 | 2.14                     | 0.46              |
| 1:A:151:SER:C    | 1:A:153:ILE:N    | 2.68                     | 0.46              |
| 1:A:302:ASN:O    | 1:A:303:MET:C    | 2.55                     | 0.46              |
| 1:A:399:ASP:N    | 1:A:418:ILE:HD11 | 2.27                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:595:GLU:CG   | 2:B:476:ARG:HH22 | 2.29                     | 0.46              |
| 2:B:191:GLU:O    | 2:B:195:ILE:HG13 | 2.15                     | 0.46              |
| 2:B:276:SER:HB3  | 2:B:289:PRO:HG3  | 1.96                     | 0.46              |
| 2:B:334:MET:CE   | 2:B:339:PHE:CE1  | 2.98                     | 0.46              |
| 2:B:421:SER:C    | 2:B:422:ALA:O    | 2.50                     | 0.46              |
| 3:M:347:PHE:HE1  | 3:M:350:VAL:CG1  | 2.14                     | 0.46              |
| 3:M:347:PHE:CD2  | 3:M:350:VAL:O    | 2.68                     | 0.46              |
| 3:M:353:VAL:O    | 3:M:401:LYS:HB2  | 2.15                     | 0.46              |
| 1:A:182:ILE:HG23 | 1:A:221:VAL:HG21 | 1.97                     | 0.46              |
| 1:A:219:VAL:HG13 | 1:A:259:LEU:HD13 | 1.97                     | 0.46              |
| 2:B:18:ILE:CB    | 2:B:23:ALA:HB2   | 2.18                     | 0.46              |
| 2:B:212:VAL:CG2  | 2:B:233:TYR:CD2  | 2.99                     | 0.46              |
| 2:B:249:ILE:HD11 | 2:B:321:CYS:SG   | 2.55                     | 0.46              |
| 3:M:235:LEU:HD13 | 3:M:306:LEU:HB3  | 1.91                     | 0.46              |
| 3:M:270:PRO:HA   | 3:M:302:TYR:HD1  | 1.79                     | 0.46              |
| 3:M:435:LEU:HD12 | 3:M:435:LEU:N    | 2.31                     | 0.46              |
| 1:A:244:LEU:CB   | 1:A:256:LEU:HD13 | 2.46                     | 0.46              |
| 2:B:115:LEU:HD13 | 2:B:115:LEU:HA   | 1.83                     | 0.46              |
| 2:B:231:ARG:CD   | 2:B:297:PRO:HB2  | 2.45                     | 0.46              |
| 2:B:356:LYS:HE3  | 3:M:49:ASP:OD2   | 2.16                     | 0.46              |
| 2:B:508:ARG:HB2  | 2:B:544:THR:HG21 | 1.97                     | 0.46              |
| 2:B:568:VAL:C    | 2:B:571:SER:OG   | 2.59                     | 0.46              |
| 2:B:594:ALA:O    | 2:B:598:LEU:HG   | 2.15                     | 0.46              |
| 3:M:66:PHE:HB3   | 3:M:77:LEU:CD1   | 2.42                     | 0.46              |
| 3:M:256:VAL:O    | 3:M:289:THR:HA   | 2.16                     | 0.46              |
| 4:S:35:VAL:CG1   | 4:S:77:TYR:OH    | 2.63                     | 0.46              |
| 4:S:50:PHE:O     | 4:S:51:LEU:HD23  | 2.15                     | 0.46              |
| 1:A:151:SER:HB3  | 1:A:184:ALA:HA   | 1.98                     | 0.46              |
| 1:A:200:PHE:HZ   | 1:A:236:LEU:HD23 | 1.70                     | 0.46              |
| 1:A:280:GLU:O    | 1:A:283:GLU:HB3  | 2.16                     | 0.46              |
| 1:A:369:SER:CB   | 1:A:424:TYR:CE2  | 2.64                     | 0.46              |
| 2:B:20:ARG:HD2   | 2:B:21:GLU:CB    | 2.30                     | 0.46              |
| 2:B:108:PHE:C    | 2:B:110:GLU:N    | 2.64                     | 0.46              |
| 2:B:245:GLN:NE2  | 2:B:309:LEU:HD13 | 2.31                     | 0.46              |
| 2:B:296:ASP:C    | 2:B:298:ASP:H    | 2.22                     | 0.46              |
| 3:M:376:ILE:CD1  | 3:M:415:ILE:HG12 | 2.45                     | 0.46              |
| 4:S:65:ASN:O     | 4:S:67:GLU:CG    | 2.61                     | 0.46              |
| 1:A:261:THR:O    | 1:A:264:SER:OG   | 2.23                     | 0.46              |
| 1:A:381:GLU:CA   | 1:A:384:LEU:HD23 | 2.36                     | 0.46              |
| 2:B:155:LEU:HB2  | 2:B:188:TYR:CE2  | 2.51                     | 0.46              |
| 2:B:252:LEU:CG   | 2:B:302:PHE:CE1  | 2.95                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:310:ILE:HA   | 2:B:318:ILE:HG12 | 1.98                     | 0.46              |
| 2:B:340:ILE:HG13 | 2:B:373:LEU:CD2  | 2.43                     | 0.46              |
| 2:B:400:SER:HB2  | 2:B:439:CYS:SG   | 2.55                     | 0.46              |
| 2:B:527:PRO:HB2  | 2:B:587:ARG:HD2  | 1.98                     | 0.46              |
| 3:M:6:TYR:O      | 3:M:77:LEU:N     | 2.32                     | 0.46              |
| 3:M:51:LEU:HB3   | 3:M:68:VAL:HG21  | 1.98                     | 0.46              |
| 3:M:217:ASP:O    | 3:M:217:ASP:OD1  | 2.34                     | 0.46              |
| 3:M:240:ILE:HG21 | 3:M:444:ALA:C    | 2.40                     | 0.46              |
| 3:M:379:LEU:HD22 | 3:M:397:TRP:NE1  | 2.31                     | 0.46              |
| 3:M:443:SER:CB   | 3:M:447:ILE:C    | 2.88                     | 0.46              |
| 1:A:63:ASP:C     | 1:A:63:ASP:OD1   | 2.58                     | 0.46              |
| 1:A:163:ALA:CB   | 1:A:199:ASN:ND2  | 2.60                     | 0.46              |
| 2:B:90:ILE:HD11  | 2:B:123:LEU:HD21 | 1.97                     | 0.46              |
| 2:B:182:ARG:HD2  | 2:B:217:GLU:HB3  | 1.98                     | 0.46              |
| 2:B:237:ILE:HG23 | 2:B:238:LYS:N    | 2.30                     | 0.46              |
| 2:B:245:GLN:CB   | 2:B:309:LEU:HD12 | 2.45                     | 0.46              |
| 2:B:313:SER:O    | 2:B:315:PRO:HD3  | 2.15                     | 0.46              |
| 2:B:430:ILE:HG23 | 2:B:470:ALA:HB2  | 1.98                     | 0.46              |
| 3:M:249:TYR:CE1  | 3:M:467:TYR:CZ   | 3.04                     | 0.46              |
| 3:M:338:PHE:HE2  | 3:M:415:ILE:CG1  | 2.27                     | 0.46              |
| 3:M:340:LEU:HG   | 3:M:342:LEU:HD11 | 1.96                     | 0.46              |
| 3:M:379:LEU:HD23 | 3:M:411:LEU:CD2  | 2.45                     | 0.46              |
| 4:S:161:GLU:O    | 4:S:162:SER:C    | 2.56                     | 0.46              |
| 1:A:121:LEU:HD11 | 1:A:153:ILE:HG22 | 1.96                     | 0.45              |
| 1:A:154:ILE:HG21 | 1:A:191:GLN:HG3  | 1.85                     | 0.45              |
| 1:A:216:SER:HB2  | 1:A:252:ILE:CG1  | 2.39                     | 0.45              |
| 1:A:364:ASP:O    | 1:A:367:ILE:HB   | 2.16                     | 0.45              |
| 1:A:420:ILE:HA   | 1:A:421:PRO:HD3  | 1.80                     | 0.45              |
| 1:A:516:ILE:HG21 | 1:A:551:LEU:HA   | 1.97                     | 0.45              |
| 2:B:193:LEU:HD13 | 2:B:225:LEU:HD11 | 1.91                     | 0.45              |
| 2:B:250:GLU:O    | 2:B:253:ILE:HB   | 2.16                     | 0.45              |
| 2:B:271:GLU:O    | 2:B:272:GLY:C    | 2.52                     | 0.45              |
| 2:B:396:ILE:HG22 | 2:B:435:SER:OG   | 2.15                     | 0.45              |
| 2:B:467:VAL:HG12 | 2:B:471:TYR:HD1  | 1.81                     | 0.45              |
| 2:B:475:ILE:CG2  | 2:B:514:LEU:HD21 | 2.46                     | 0.45              |
| 2:B:478:LEU:O    | 2:B:480:GLN:N    | 2.49                     | 0.45              |
| 2:B:522:GLU:C    | 2:B:524:LYS:N    | 2.72                     | 0.45              |
| 3:M:262:THR:HG22 | 3:M:264:GLY:CA   | 2.46                     | 0.45              |
| 4:S:8:PHE:HE2    | 4:S:86:THR:H     | 1.63                     | 0.45              |
| 4:S:73:ILE:HG23  | 4:S:88:ILE:CG2   | 2.46                     | 0.45              |
| 4:S:113:PHE:CD1  | 4:S:113:PHE:N    | 2.84                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:329:ASN:O    | 1:A:333:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:404:GLN:N    | 2:B:3:ASP:OD2    | 2.42                     | 0.45              |
| 1:A:588:LEU:O    | 1:A:590:TYR:N    | 2.49                     | 0.45              |
| 1:A:601:VAL:O    | 1:A:602:GLU:O    | 2.34                     | 0.45              |
| 2:B:9:ALA:HA     | 2:B:12:LEU:HD12  | 1.99                     | 0.45              |
| 2:B:102:HIS:HB3  | 2:B:141:ALA:HB2  | 1.98                     | 0.45              |
| 2:B:226:LEU:CD2  | 2:B:255:TYR:HD1  | 1.99                     | 0.45              |
| 2:B:270:SER:C    | 2:B:273:SER:HB2  | 2.42                     | 0.45              |
| 2:B:280:PRO:CG   | 2:B:283:TYR:CE1  | 2.81                     | 0.45              |
| 1:A:203:PHE:HZ   | 1:A:221:VAL:HG11 | 1.78                     | 0.45              |
| 2:B:208:ILE:HD13 | 2:B:236:ILE:HD13 | 1.97                     | 0.45              |
| 3:M:16:PHE:HE2   | 3:M:125:PHE:CE2  | 2.34                     | 0.45              |
| 3:M:317:MET:SD   | 3:M:321:GLY:HA3  | 2.56                     | 0.45              |
| 3:M:449:VAL:CG1  | 3:M:452:ILE:HG13 | 2.46                     | 0.45              |
| 1:A:259:LEU:HD23 | 1:A:259:LEU:C    | 2.41                     | 0.45              |
| 1:A:581:LEU:CG   | 1:A:607:LEU:HD11 | 2.46                     | 0.45              |
| 1:A:638:LEU:CD2  | 2:B:558:TYR:O    | 2.65                     | 0.45              |
| 2:B:158:VAL:HG13 | 2:B:177:ILE:CG1  | 2.33                     | 0.45              |
| 2:B:189:HIS:CD2  | 2:B:193:LEU:HG   | 2.52                     | 0.45              |
| 2:B:191:GLU:C    | 2:B:193:LEU:H    | 2.24                     | 0.45              |
| 2:B:219:TYR:HD1  | 2:B:226:LEU:HD13 | 1.65                     | 0.45              |
| 2:B:252:LEU:C    | 2:B:302:PHE:CE2  | 2.95                     | 0.45              |
| 2:B:306:LEU:HD12 | 2:B:325:LEU:HD23 | 1.98                     | 0.45              |
| 2:B:553:ALA:CA   | 2:B:614:ILE:CG2  | 2.94                     | 0.45              |
| 3:M:243:ILE:HG21 | 3:M:298:ARG:HG2  | 1.98                     | 0.45              |
| 3:M:374:TYR:CE1  | 3:M:390:ILE:HD13 | 2.51                     | 0.45              |
| 1:A:97:SER:O     | 1:A:103:LYS:HE2  | 2.16                     | 0.45              |
| 1:A:313:MET:HB2  | 1:A:348:PHE:HZ   | 1.80                     | 0.45              |
| 1:A:373:GLU:CG   | 1:A:427:LYS:CE   | 2.90                     | 0.45              |
| 1:A:446:ASP:C    | 1:A:448:GLU:O    | 2.59                     | 0.45              |
| 2:B:527:PRO:CB   | 2:B:587:ARG:HG2  | 2.40                     | 0.45              |
| 2:B:537:PHE:C    | 2:B:539:ASN:N    | 2.75                     | 0.45              |
| 3:M:15:ILE:HG23  | 3:M:115:VAL:CG2  | 2.46                     | 0.45              |
| 3:M:45:SER:HA    | 3:M:47:SER:O     | 2.17                     | 0.45              |
| 3:M:242:GLY:O    | 3:M:302:TYR:N    | 2.47                     | 0.45              |
| 3:M:322:LEU:C    | 3:M:322:LEU:HD23 | 2.42                     | 0.45              |
| 3:M:353:VAL:O    | 3:M:401:LYS:CB   | 2.65                     | 0.45              |
| 1:A:158:LEU:CG   | 1:A:162:ILE:CD1  | 2.92                     | 0.45              |
| 1:A:244:LEU:CD2  | 1:A:277:LYS:HG3  | 2.47                     | 0.45              |
| 1:A:244:LEU:HB2  | 1:A:256:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:495:ILE:CG2  | 1:A:515:CYS:HB3  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:556:VAL:HG21 | 1:A:603:VAL:HG13 | 1.96                     | 0.45              |
| 2:B:74:ASP:O     | 2:B:77:ILE:CB    | 2.63                     | 0.45              |
| 2:B:102:HIS:ND1  | 2:B:137:PHE:CB   | 2.79                     | 0.45              |
| 2:B:143:SER:O    | 2:B:145:MET:N    | 2.50                     | 0.45              |
| 2:B:403:ILE:O    | 2:B:403:ILE:HG13 | 2.16                     | 0.45              |
| 2:B:526:CYS:HB2  | 2:B:555:LEU:HD11 | 1.97                     | 0.45              |
| 2:B:559:ASP:O    | 2:B:562:ASN:CA   | 2.64                     | 0.45              |
| 3:M:6:TYR:CD2    | 3:M:17:GLN:CG    | 3.00                     | 0.45              |
| 3:M:71:LYS:O     | 3:M:72:LEU:C     | 2.60                     | 0.45              |
| 4:S:7:ILE:HD13   | 4:S:16:LEU:HD23  | 1.99                     | 0.45              |
| 4:S:55:PRO:O     | 4:S:58:LEU:HB2   | 2.14                     | 0.45              |
| 1:A:114:PHE:CG   | 1:A:153:ILE:HG12 | 2.52                     | 0.45              |
| 1:A:241:TYR:CE1  | 1:A:277:LYS:CB   | 2.99                     | 0.45              |
| 1:A:289:SER:HB3  | 4:S:96:LEU:CB    | 2.28                     | 0.45              |
| 1:A:421:PRO:HD2  | 1:A:424:TYR:CG   | 2.51                     | 0.45              |
| 1:A:499:ILE:HD11 | 1:A:515:CYS:CB   | 2.46                     | 0.45              |
| 1:A:605:GLU:CG   | 1:A:632:PHE:CG   | 3.00                     | 0.45              |
| 2:B:2:VAL:CG1    | 2:B:6:HIS:CE1    | 3.00                     | 0.45              |
| 2:B:60:ARG:HD2   | 2:B:96:LYS:HG2   | 1.99                     | 0.45              |
| 2:B:139:LEU:HD23 | 2:B:172:GLU:O    | 2.17                     | 0.45              |
| 2:B:246:SER:HA   | 2:B:249:ILE:HD12 | 1.98                     | 0.45              |
| 2:B:292:GLU:CG   | 2:B:296:ASP:OD2  | 2.54                     | 0.45              |
| 2:B:458:MET:C    | 2:B:460:SER:N    | 2.73                     | 0.45              |
| 2:B:513:TRP:C    | 2:B:513:TRP:CD1  | 2.95                     | 0.45              |
| 3:M:64:LYS:NZ    | 3:M:79:SER:HB2   | 2.32                     | 0.45              |
| 3:M:103:TYR:O    | 3:M:104:PHE:CB   | 2.63                     | 0.45              |
| 1:A:258:LYS:HZ1  | 4:S:94:SER:HB3   | 1.31                     | 0.45              |
| 1:A:480:LEU:C    | 1:A:480:LEU:CD1  | 2.88                     | 0.45              |
| 2:B:90:ILE:HD11  | 2:B:123:LEU:HD23 | 1.97                     | 0.45              |
| 2:B:256:CYS:CB   | 2:B:328:LEU:HD23 | 2.46                     | 0.45              |
| 2:B:256:CYS:O    | 2:B:258:GLN:N    | 2.50                     | 0.45              |
| 2:B:266:VAL:HG13 | 2:B:291:TYR:H    | 1.82                     | 0.45              |
| 3:M:100:LEU:HD21 | 3:M:121:ILE:HG23 | 1.99                     | 0.45              |
| 3:M:128:CYS:O    | 3:M:130:GLU:O    | 2.35                     | 0.45              |
| 3:M:343:ASN:CG   | 3:M:408:VAL:HG11 | 2.41                     | 0.45              |
| 3:M:360:LEU:HD21 | 3:M:362:PHE:CE2  | 2.49                     | 0.45              |
| 3:M:455:VAL:O    | 3:M:455:VAL:HG12 | 2.16                     | 0.45              |
| 4:S:35:VAL:O     | 4:S:39:ILE:HG12  | 2.16                     | 0.45              |
| 4:S:54:PRO:O     | 4:S:69:ASN:HB2   | 2.17                     | 0.45              |
| 1:A:226:SER:O    | 1:A:230:PRO:HG3  | 2.17                     | 0.45              |
| 1:A:264:SER:HB3  | 1:A:271:ARG:HG3  | 1.92                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:413:SER:HB3  | 1:A:415:ARG:O    | 2.17                     | 0.45              |
| 1:A:629:LEU:C    | 1:A:629:LEU:HD23 | 2.42                     | 0.45              |
| 2:B:120:ILE:HG22 | 2:B:153:ILE:HG21 | 1.99                     | 0.45              |
| 2:B:311:TYR:CB   | 3:M:269:ILE:HD13 | 2.47                     | 0.45              |
| 2:B:430:ILE:HG13 | 2:B:467:VAL:HG22 | 1.99                     | 0.45              |
| 2:B:483:PRO:HB3  | 2:B:521:ILE:HG13 | 1.97                     | 0.45              |
| 2:B:494:ALA:CB   | 2:B:515:PHE:CZ   | 3.00                     | 0.45              |
| 2:B:500:GLN:OE1  | 2:B:503:LEU:HD11 | 2.17                     | 0.45              |
| 2:B:519:ALA:CB   | 2:B:555:LEU:CD1  | 2.92                     | 0.45              |
| 2:B:527:PRO:HG2  | 2:B:587:ARG:HG2  | 1.99                     | 0.45              |
| 2:B:544:THR:O    | 2:B:548:ILE:HG13 | 2.17                     | 0.45              |
| 3:M:134:PRO:O    | 3:M:136:VAL:HA   | 2.17                     | 0.45              |
| 3:M:256:VAL:CG2  | 3:M:452:ILE:HG22 | 2.47                     | 0.45              |
| 3:M:296:LYS:O    | 3:M:296:LYS:CG   | 2.65                     | 0.45              |
| 3:M:374:TYR:CE1  | 3:M:376:ILE:HG12 | 2.51                     | 0.45              |
| 1:A:271:ARG:HH11 | 1:A:303:MET:HA   | 1.81                     | 0.45              |
| 1:A:502:ASP:O    | 1:A:505:ASN:N    | 2.50                     | 0.45              |
| 2:B:24:ALA:CA    | 2:B:35:TYR:CE2   | 2.98                     | 0.45              |
| 2:B:37:TYR:O     | 2:B:42:ILE:N     | 2.50                     | 0.45              |
| 2:B:451:MET:HE2  | 2:B:489:ILE:CG1  | 2.46                     | 0.45              |
| 2:B:469:ASP:CG   | 2:B:506:ASN:HB2  | 2.42                     | 0.45              |
| 2:B:508:ARG:CB   | 2:B:544:THR:HG21 | 2.47                     | 0.45              |
| 2:B:549:LEU:C    | 2:B:551:LEU:N    | 2.74                     | 0.45              |
| 3:M:290:PHE:CZ   | 3:M:297:PHE:CE2  | 3.04                     | 0.45              |
| 3:M:323:MET:CG   | 3:M:342:LEU:HG   | 2.46                     | 0.45              |
| 3:M:325:LEU:HD23 | 3:M:325:LEU:C    | 2.42                     | 0.45              |
| 3:M:435:LEU:HB2  | 3:M:437:TYR:CE1  | 2.52                     | 0.45              |
| 1:A:121:LEU:CD1  | 1:A:155:THR:OG1  | 2.65                     | 0.44              |
| 1:A:179:LYS:HB2  | 4:S:142:ILE:CD1  | 2.23                     | 0.44              |
| 1:A:215:VAL:O    | 1:A:216:SER:O    | 2.35                     | 0.44              |
| 2:B:25:VAL:HG13  | 2:B:33:SER:CA    | 2.32                     | 0.44              |
| 2:B:174:ALA:HB1  | 2:B:211:ALA:CA   | 2.33                     | 0.44              |
| 2:B:279:LEU:HB3  | 2:B:280:PRO:HD2  | 1.98                     | 0.44              |
| 2:B:284:ASN:O    | 2:B:285:GLU:C    | 2.52                     | 0.44              |
| 2:B:291:TYR:CZ   | 2:B:293:VAL:CG1  | 3.00                     | 0.44              |
| 2:B:515:PHE:CD2  | 2:B:529:VAL:HG21 | 2.51                     | 0.44              |
| 3:M:64:LYS:HZ2   | 3:M:79:SER:CB    | 2.30                     | 0.44              |
| 4:S:98:ILE:HG22  | 4:S:102:ILE:HD11 | 1.98                     | 0.44              |
| 1:A:71:VAL:CG2   | 1:A:94:VAL:HG11  | 2.47                     | 0.44              |
| 1:A:85:ALA:HA    | 1:A:88:ASN:ND2   | 2.32                     | 0.44              |
| 1:A:100:LEU:C    | 1:A:100:LEU:HD12 | 2.42                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:338:PHE:HE2  | 1:A:352:PHE:CZ   | 2.36                     | 0.44              |
| 2:B:296:ASP:OD1  | 2:B:297:PRO:N    | 2.49                     | 0.44              |
| 2:B:534:ILE:HG12 | 2:B:595:VAL:HG23 | 1.98                     | 0.44              |
| 3:M:243:ILE:H    | 3:M:474:THR:HG21 | 1.81                     | 0.44              |
| 3:M:276:VAL:HG22 | 3:M:299:LEU:HD12 | 2.00                     | 0.44              |
| 3:M:316:ARG:O    | 3:M:318:ASN:N    | 2.51                     | 0.44              |
| 4:S:58:LEU:HD12  | 4:S:58:LEU:HA    | 1.81                     | 0.44              |
| 2:B:2:VAL:HG21   | 3:M:58:ARG:HD2   | 1.99                     | 0.44              |
| 2:B:120:ILE:CD1  | 2:B:142:LEU:CD2  | 2.95                     | 0.44              |
| 2:B:512:VAL:HB   | 2:B:551:LEU:CD1  | 2.48                     | 0.44              |
| 2:B:520:SER:C    | 2:B:523:PHE:HD2  | 2.25                     | 0.44              |
| 3:M:287:ASN:O    | 3:M:288:ILE:HG13 | 2.18                     | 0.44              |
| 3:M:473:LYS:O    | 3:M:474:THR:HG22 | 2.17                     | 0.44              |
| 4:S:4:ALA:CA     | 4:S:18:LYS:O     | 2.56                     | 0.44              |
| 4:S:122:ILE:O    | 4:S:123:PHE:C    | 2.61                     | 0.44              |
| 1:A:174:ARG:O    | 1:A:177:ILE:HB   | 2.18                     | 0.44              |
| 1:A:441:TYR:HB3  | 1:A:444:VAL:CG2  | 2.47                     | 0.44              |
| 1:A:563:CYS:CB   | 1:A:621:LEU:CD1  | 2.63                     | 0.44              |
| 1:A:586:GLU:N    | 1:A:604:LEU:HD12 | 2.32                     | 0.44              |
| 2:B:120:ILE:HG23 | 2:B:142:LEU:CD2  | 2.44                     | 0.44              |
| 2:B:374:PHE:CZ   | 2:B:381:PHE:HD1  | 2.29                     | 0.44              |
| 2:B:511:ILE:O    | 2:B:515:PHE:HD1  | 2.00                     | 0.44              |
| 2:B:591:MET:O    | 2:B:595:VAL:HG23 | 2.17                     | 0.44              |
| 2:B:592:TYR:OH   | 2:B:619:ASP:OD2  | 2.35                     | 0.44              |
| 3:M:56:VAL:N     | 3:M:64:LYS:HG3   | 2.32                     | 0.44              |
| 3:M:101:LEU:CD1  | 3:M:106:LYS:O    | 2.58                     | 0.44              |
| 3:M:213:GLU:HB3  | 3:M:467:TYR:CA   | 2.47                     | 0.44              |
| 3:M:304:VAL:HG21 | 3:M:309:GLN:NE2  | 2.32                     | 0.44              |
| 4:S:16:LEU:CD2   | 4:S:128:LEU:CD2  | 2.93                     | 0.44              |
| 4:S:17:VAL:HG22  | 4:S:19:PHE:CE2   | 2.51                     | 0.44              |
| 1:A:136:GLY:O    | 1:A:139:ASP:CB   | 2.65                     | 0.44              |
| 1:A:273:LYS:O    | 1:A:276:PRO:CD   | 2.60                     | 0.44              |
| 2:B:90:ILE:CD1   | 2:B:123:LEU:CD2  | 2.95                     | 0.44              |
| 2:B:177:ILE:HG21 | 2:B:196:LEU:CG   | 2.47                     | 0.44              |
| 2:B:208:ILE:O    | 2:B:212:VAL:HG23 | 2.17                     | 0.44              |
| 2:B:347:VAL:HG11 | 2:B:381:PHE:CE2  | 2.49                     | 0.44              |
| 2:B:419:VAL:O    | 2:B:420:ALA:C    | 2.58                     | 0.44              |
| 3:M:218:LEU:O    | 3:M:441:GLY:HA2  | 2.18                     | 0.44              |
| 4:S:135:ILE:O    | 4:S:140:MET:O    | 2.35                     | 0.44              |
| 1:A:190:LEU:HD13 | 1:A:224:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:226:SER:O    | 1:A:227:LYS:C    | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:150:LEU:O    | 2:B:154:ILE:HG13 | 2.18                     | 0.44              |
| 2:B:181:TYR:CB   | 2:B:218:CYS:SG   | 3.05                     | 0.44              |
| 2:B:223:LEU:CD1  | 2:B:258:GLN:HB2  | 2.39                     | 0.44              |
| 2:B:534:ILE:C    | 2:B:536:ASN:N    | 2.71                     | 0.44              |
| 3:M:220:GLU:HB2  | 3:M:222:PHE:HE1  | 1.82                     | 0.44              |
| 3:M:419:ASN:ND2  | 3:M:424:PHE:CD2  | 2.85                     | 0.44              |
| 1:A:313:MET:HG3  | 1:A:348:PHE:CE1  | 2.53                     | 0.44              |
| 1:A:585:PHE:HE2  | 1:A:603:VAL:CG1  | 2.29                     | 0.44              |
| 1:A:611:LEU:HD23 | 1:A:611:LEU:C    | 2.42                     | 0.44              |
| 2:B:108:PHE:CE2  | 2:B:115:LEU:HD23 | 2.53                     | 0.44              |
| 2:B:136:CYS:O    | 2:B:172:GLU:CB   | 2.64                     | 0.44              |
| 2:B:143:SER:CA   | 2:B:179:LYS:HB2  | 2.47                     | 0.44              |
| 2:B:170:ARG:O    | 2:B:171:GLY:C    | 2.55                     | 0.44              |
| 2:B:171:GLY:HA2  | 2:B:207:VAL:O    | 2.17                     | 0.44              |
| 2:B:212:VAL:HG13 | 2:B:248:LEU:HD23 | 1.99                     | 0.44              |
| 2:B:260:LEU:CD2  | 2:B:293:VAL:HG11 | 2.46                     | 0.44              |
| 2:B:278:PRO:HD3  | 2:B:290:SER:HA   | 1.98                     | 0.44              |
| 2:B:464:SER:O    | 2:B:468:LEU:HG   | 2.17                     | 0.44              |
| 2:B:512:VAL:HG21 | 2:B:548:ILE:CG1  | 2.48                     | 0.44              |
| 4:S:5:VAL:HG13   | 4:S:87:PHE:CD2   | 2.52                     | 0.44              |
| 4:S:53:THR:CG2   | 4:S:68:VAL:CA    | 2.94                     | 0.44              |
| 4:S:159:ALA:O    | 4:S:162:SER:N    | 2.46                     | 0.44              |
| 1:A:247:ILE:HG21 | 1:A:252:ILE:HB   | 2.00                     | 0.44              |
| 1:A:397:ASP:O    | 1:A:418:ILE:HD12 | 2.18                     | 0.44              |
| 1:A:402:ILE:O    | 1:A:403:LEU:C    | 2.56                     | 0.44              |
| 1:A:572:PHE:O    | 1:A:575:LYS:HB3  | 2.17                     | 0.44              |
| 2:B:261:PRO:HG2  | 2:B:292:GLU:HB2  | 1.99                     | 0.44              |
| 2:B:365:PHE:O    | 2:B:368:ILE:HB   | 2.18                     | 0.44              |
| 2:B:424:PHE:HA   | 2:B:425:PRO:HD3  | 1.58                     | 0.44              |
| 3:M:121:ILE:HG23 | 3:M:125:PHE:HE1  | 1.83                     | 0.44              |
| 3:M:262:THR:CG2  | 3:M:265:ASN:N    | 2.80                     | 0.44              |
| 2:B:2:VAL:HG12   | 2:B:6:HIS:NE2    | 2.32                     | 0.44              |
| 2:B:208:ILE:O    | 2:B:209:SER:C    | 2.59                     | 0.44              |
| 2:B:219:TYR:O    | 2:B:223:LEU:CG   | 2.65                     | 0.44              |
| 2:B:334:MET:O    | 2:B:336:ASN:O    | 2.36                     | 0.44              |
| 3:M:223:HIS:CB   | 3:M:477:GLY:O    | 2.66                     | 0.44              |
| 3:M:288:ILE:HD12 | 3:M:300:LEU:HD22 | 1.98                     | 0.44              |
| 3:M:290:PHE:CE2  | 3:M:297:PHE:CE2  | 3.05                     | 0.44              |
| 4:S:59:LEU:HD12  | 4:S:60:SER:O     | 2.18                     | 0.44              |
| 4:S:112:CYS:HB2  | 4:S:113:PHE:HD1  | 1.80                     | 0.44              |
| 4:S:131:VAL:CG2  | 4:S:153:VAL:CG2  | 2.89                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:399:ASP:OD2  | 1:A:403:LEU:HD12 | 2.18                     | 0.43              |
| 1:A:502:ASP:OD2  | 3:M:59:ASP:OD2   | 2.36                     | 0.43              |
| 1:A:610:SER:OG   | 1:A:625:LEU:HD13 | 2.18                     | 0.43              |
| 2:B:20:ARG:NH2   | 2:B:21:GLU:HG3   | 2.32                     | 0.43              |
| 2:B:512:VAL:O    | 2:B:515:PHE:HB2  | 2.18                     | 0.43              |
| 2:B:588:ILE:HG23 | 2:B:589:SER:N    | 2.33                     | 0.43              |
| 3:M:19:LEU:CD2   | 3:M:24:ALA:CB    | 2.95                     | 0.43              |
| 3:M:65:TYR:CZ    | 3:M:66:PHE:O     | 2.71                     | 0.43              |
| 3:M:224:VAL:CG2  | 3:M:306:LEU:CD1  | 2.95                     | 0.43              |
| 1:A:170:LEU:CD2  | 1:A:181:ALA:HB1  | 2.47                     | 0.43              |
| 1:A:394:GLN:O    | 1:A:397:ASP:N    | 2.52                     | 0.43              |
| 1:A:464:ILE:O    | 1:A:464:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:480:LEU:HD13 | 1:A:480:LEU:O    | 2.18                     | 0.43              |
| 1:A:594:PHE:HB3  | 2:B:476:ARG:HH21 | 1.83                     | 0.43              |
| 1:A:630:PRO:HG2  | 2:B:617:LEU:CG   | 2.42                     | 0.43              |
| 2:B:136:CYS:HA   | 2:B:172:GLU:CB   | 2.47                     | 0.43              |
| 2:B:195:ILE:C    | 2:B:197:LYS:H    | 2.26                     | 0.43              |
| 2:B:284:ASN:C    | 2:B:285:GLU:O    | 2.51                     | 0.43              |
| 2:B:493:LEU:CG   | 2:B:511:ILE:HG23 | 2.40                     | 0.43              |
| 3:M:16:PHE:CB    | 3:M:118:TYR:CD1  | 3.01                     | 0.43              |
| 3:M:270:PRO:N    | 3:M:302:TYR:CD1  | 2.85                     | 0.43              |
| 3:M:290:PHE:HZ   | 3:M:293:PRO:HD3  | 1.75                     | 0.43              |
| 3:M:317:MET:HB2  | 3:M:322:LEU:HB2  | 2.01                     | 0.43              |
| 1:A:72:LEU:O     | 1:A:76:TYR:CD1   | 2.72                     | 0.43              |
| 1:A:79:MET:O     | 4:S:25:LEU:CD1   | 2.66                     | 0.43              |
| 1:A:244:LEU:HD22 | 1:A:260:PHE:HE1  | 1.83                     | 0.43              |
| 1:A:261:THR:O    | 1:A:264:SER:N    | 2.50                     | 0.43              |
| 1:A:460:LEU:O    | 1:A:463:ASP:CB   | 2.65                     | 0.43              |
| 1:A:566:PHE:O    | 1:A:568:GLU:N    | 2.51                     | 0.43              |
| 1:A:594:PHE:C    | 2:B:476:ARG:HH21 | 2.23                     | 0.43              |
| 2:B:109:ALA:HA   | 2:B:116:THR:OG1  | 2.17                     | 0.43              |
| 2:B:178:ILE:CG1  | 2:B:214:ALA:O    | 2.58                     | 0.43              |
| 2:B:223:LEU:HD13 | 2:B:259:TYR:CA   | 2.41                     | 0.43              |
| 2:B:234:CYS:HB2  | 2:B:301:LEU:CB   | 2.48                     | 0.43              |
| 2:B:253:ILE:CG1  | 2:B:324:ALA:CB   | 2.96                     | 0.43              |
| 2:B:430:ILE:HG12 | 2:B:467:VAL:HA   | 2.01                     | 0.43              |
| 2:B:487:LEU:HD22 | 2:B:522:GLU:CB   | 2.42                     | 0.43              |
| 3:M:66:PHE:CD2   | 3:M:77:LEU:HD11  | 2.53                     | 0.43              |
| 3:M:215:TYR:HD2  | 3:M:470:ALA:N    | 2.16                     | 0.43              |
| 3:M:374:TYR:CD1  | 3:M:376:ILE:HD11 | 2.52                     | 0.43              |
| 1:A:194:GLU:O    | 1:A:197:ARG:N    | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:282:MET:O    | 1:A:284:SER:N    | 2.52                     | 0.43              |
| 1:A:402:ILE:HG21 | 1:A:421:PRO:HA   | 1.99                     | 0.43              |
| 1:A:447:PHE:O    | 1:A:450:TYR:HB3  | 2.18                     | 0.43              |
| 1:A:495:ILE:HG21 | 1:A:515:CYS:HB3  | 1.99                     | 0.43              |
| 2:B:20:ARG:HD2   | 2:B:21:GLU:N     | 2.33                     | 0.43              |
| 2:B:174:ALA:HB3  | 2:B:211:ALA:CA   | 2.44                     | 0.43              |
| 2:B:330:SER:O    | 2:B:331:PRO:C    | 2.62                     | 0.43              |
| 2:B:398:ILE:HG22 | 2:B:402:LEU:CD1  | 2.48                     | 0.43              |
| 2:B:554:LYS:O    | 2:B:557:SER:N    | 2.51                     | 0.43              |
| 3:M:63:TYR:CG    | 3:M:64:LYS:N     | 2.85                     | 0.43              |
| 3:M:374:TYR:CE1  | 3:M:390:ILE:CD1  | 3.01                     | 0.43              |
| 1:A:153:ILE:HB   | 1:A:158:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:157:SER:O    | 1:A:160:ARG:HB2  | 2.18                     | 0.43              |
| 1:A:432:ILE:O    | 1:A:435:ILE:HB   | 2.18                     | 0.43              |
| 2:B:16:LYS:HA    | 2:B:17:VAL:HA    | 1.83                     | 0.43              |
| 2:B:34:SER:O     | 2:B:37:TYR:HB3   | 2.18                     | 0.43              |
| 2:B:136:CYS:CA   | 2:B:172:GLU:CG   | 2.94                     | 0.43              |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:C    | 2.28                     | 0.43              |
| 2:B:281:ASP:OD1  | 2:B:287:GLU:CG   | 2.66                     | 0.43              |
| 3:M:51:LEU:CB    | 3:M:68:VAL:HG21  | 2.48                     | 0.43              |
| 3:M:243:ILE:CD1  | 3:M:301:GLU:HB3  | 2.47                     | 0.43              |
| 3:M:350:VAL:HA   | 3:M:442:GLN:CG   | 2.48                     | 0.43              |
| 4:S:14:PRO:CA    | 4:S:36:TYR:OH    | 2.65                     | 0.43              |
| 1:A:185:LEU:HB2  | 1:A:203:PHE:CE1  | 2.51                     | 0.43              |
| 1:A:241:TYR:CE1  | 1:A:277:LYS:HB2  | 2.54                     | 0.43              |
| 1:A:335:CYS:O    | 1:A:338:PHE:HB2  | 2.19                     | 0.43              |
| 1:A:384:LEU:HB2  | 1:A:441:TYR:HE2  | 1.83                     | 0.43              |
| 1:A:522:PHE:C    | 1:A:524:THR:N    | 2.75                     | 0.43              |
| 2:B:77:ILE:CG2   | 2:B:82:TYR:HE1   | 2.26                     | 0.43              |
| 2:B:90:ILE:HG13  | 2:B:98:LYS:HD3   | 2.01                     | 0.43              |
| 2:B:105:LEU:O    | 2:B:106:LEU:O    | 2.32                     | 0.43              |
| 2:B:418:TYR:OH   | 2:B:428:VAL:HG12 | 2.19                     | 0.43              |
| 2:B:522:GLU:O    | 2:B:522:GLU:CG   | 2.40                     | 0.43              |
| 2:B:549:LEU:CD1  | 2:B:614:ILE:HD12 | 2.49                     | 0.43              |
| 3:M:323:MET:HE1  | 3:M:342:LEU:HB3  | 1.95                     | 0.43              |
| 3:M:410:VAL:HG12 | 3:M:412:ARG:HG3  | 2.01                     | 0.43              |
| 4:S:25:LEU:O     | 4:S:28:GLN:HG3   | 2.18                     | 0.43              |
| 4:S:130:SER:OG   | 4:S:156:LEU:HD13 | 2.12                     | 0.43              |
| 1:A:111:SER:CB   | 1:A:152:THR:HG1  | 2.19                     | 0.43              |
| 1:A:275:LEU:HD21 | 1:A:311:THR:HG1  | 1.69                     | 0.43              |
| 1:A:295:VAL:HG12 | 1:A:337:LEU:HD22 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:36:THR:O     | 2:B:40:GLN:CB    | 2.66                     | 0.43              |
| 2:B:237:ILE:HG12 | 2:B:309:LEU:HD21 | 2.01                     | 0.43              |
| 2:B:337:THR:OG1  | 2:B:373:LEU:CD1  | 2.66                     | 0.43              |
| 2:B:457:HIS:O    | 2:B:458:MET:C    | 2.57                     | 0.43              |
| 2:B:475:ILE:CG2  | 2:B:514:LEU:CD2  | 2.97                     | 0.43              |
| 2:B:560:ILE:HA   | 2:B:564:LYS:H    | 1.82                     | 0.43              |
| 3:M:45:SER:HA    | 3:M:47:SER:H     | 1.83                     | 0.43              |
| 3:M:221:THR:HG22 | 3:M:223:HIS:CE1  | 2.54                     | 0.43              |
| 3:M:290:PHE:CB   | 3:M:299:LEU:CD1  | 2.95                     | 0.43              |
| 4:S:16:LEU:CD1   | 4:S:125:TRP:NE1  | 2.02                     | 0.43              |
| 1:A:256:LEU:O    | 1:A:260:PHE:CD1  | 2.71                     | 0.43              |
| 1:A:545:HIS:O    | 1:A:546:SER:O    | 2.37                     | 0.43              |
| 1:A:581:LEU:CG   | 1:A:607:LEU:CD1  | 2.97                     | 0.43              |
| 2:B:146:LYS:C    | 2:B:147:MET:HG2  | 2.44                     | 0.43              |
| 2:B:219:TYR:HD2  | 2:B:222:HIS:C    | 2.26                     | 0.43              |
| 2:B:291:TYR:HD2  | 2:B:294:VAL:HG12 | 1.84                     | 0.43              |
| 2:B:292:GLU:CG   | 2:B:296:ASP:CB   | 2.96                     | 0.43              |
| 2:B:334:MET:HE2  | 2:B:339:PHE:CE1  | 2.54                     | 0.43              |
| 2:B:343:LEU:HD23 | 2:B:366:LEU:HD12 | 2.00                     | 0.43              |
| 2:B:389:ILE:HG12 | 2:B:425:PRO:HG2  | 2.01                     | 0.43              |
| 2:B:418:TYR:CZ   | 2:B:432:ALA:HB2  | 2.53                     | 0.43              |
| 2:B:564:LYS:HG3  | 2:B:568:VAL:HG23 | 2.01                     | 0.43              |
| 2:B:585:GLY:O    | 2:B:589:SER:CB   | 2.66                     | 0.43              |
| 2:B:592:TYR:CE2  | 2:B:618:PHE:HD2  | 2.32                     | 0.43              |
| 3:M:271:SER:O    | 3:M:300:LEU:HA   | 2.19                     | 0.43              |
| 3:M:445:SER:HG   | 3:M:447:ILE:HG23 | 1.81                     | 0.43              |
| 1:A:251:TRP:CH2  | 4:S:96:LEU:O     | 2.72                     | 0.43              |
| 2:B:50:LEU:CD2   | 2:B:62:ALA:HB2   | 2.49                     | 0.43              |
| 2:B:127:LEU:CD2  | 2:B:157:THR:HG21 | 2.48                     | 0.43              |
| 2:B:148:SER:CB   | 2:B:183:ALA:HB1  | 2.48                     | 0.43              |
| 2:B:197:LYS:O    | 2:B:198:GLU:C    | 2.61                     | 0.43              |
| 2:B:354:GLY:O    | 2:B:358:MET:CG   | 2.46                     | 0.43              |
| 2:B:461:HIS:HB3  | 2:B:463:LEU:HD23 | 2.01                     | 0.43              |
| 3:M:100:LEU:HB3  | 3:M:109:LEU:HD22 | 2.01                     | 0.43              |
| 3:M:220:GLU:HA   | 3:M:474:THR:HG21 | 2.01                     | 0.43              |
| 3:M:246:VAL:HB   | 3:M:297:PHE:CE1  | 2.49                     | 0.43              |
| 3:M:253:ASN:OD1  | 3:M:292:PRO:HB2  | 2.19                     | 0.43              |
| 3:M:278:ILE:O    | 3:M:278:ILE:HG12 | 2.18                     | 0.43              |
| 3:M:324:SER:O    | 3:M:340:LEU:HA   | 2.19                     | 0.43              |
| 3:M:343:ASN:N    | 3:M:343:ASN:ND2  | 2.56                     | 0.43              |
| 3:M:364:VAL:HG12 | 3:M:372:ILE:CB   | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:407:THR:O    | 3:M:409:PRO:HD3  | 2.19                     | 0.43              |
| 1:A:270:LEU:CD1  | 1:A:274:LEU:HD23 | 2.49                     | 0.43              |
| 2:B:25:VAL:CG2   | 2:B:35:TYR:CB    | 2.96                     | 0.43              |
| 2:B:181:TYR:CD1  | 2:B:222:HIS:HD2  | 2.32                     | 0.43              |
| 2:B:196:LEU:O    | 2:B:199:LEU:HB2  | 2.19                     | 0.43              |
| 2:B:278:PRO:C    | 2:B:288:TYR:HB3  | 2.42                     | 0.43              |
| 2:B:518:ILE:O    | 2:B:518:ILE:CG1  | 2.67                     | 0.43              |
| 2:B:542:PRO:O    | 2:B:545:ARG:HB2  | 2.19                     | 0.43              |
| 3:M:96:ILE:CD1   | 3:M:125:PHE:HA   | 2.48                     | 0.43              |
| 3:M:317:MET:CB   | 3:M:322:LEU:H    | 2.31                     | 0.43              |
| 3:M:323:MET:CE   | 3:M:437:TYR:HE2  | 2.32                     | 0.43              |
| 3:M:327:PHE:CD2  | 3:M:430:LEU:HD22 | 2.54                     | 0.43              |
| 1:A:166:LEU:C    | 1:A:170:LEU:HD23 | 2.44                     | 0.42              |
| 2:B:70:MET:HE1   | 2:B:107:ARG:CG   | 2.43                     | 0.42              |
| 2:B:120:ILE:HD13 | 2:B:142:LEU:HD23 | 2.00                     | 0.42              |
| 2:B:214:ALA:C    | 2:B:216:LYS:H    | 2.27                     | 0.42              |
| 2:B:299:LEU:CD1  | 2:B:299:LEU:C    | 2.92                     | 0.42              |
| 2:B:310:ILE:HD11 | 2:B:321:CYS:CB   | 2.49                     | 0.42              |
| 2:B:345:ARG:HH12 | 3:M:305:ASP:CB   | 2.31                     | 0.42              |
| 2:B:398:ILE:HG22 | 2:B:402:LEU:HD11 | 2.01                     | 0.42              |
| 2:B:559:ASP:C    | 2:B:563:PHE:H    | 2.24                     | 0.42              |
| 3:M:6:TYR:HA     | 3:M:17:GLN:HA    | 2.00                     | 0.42              |
| 3:M:241:HIS:HB2  | 3:M:476:THR:HG22 | 1.95                     | 0.42              |
| 3:M:258:VAL:CG1  | 3:M:449:VAL:HG22 | 2.49                     | 0.42              |
| 3:M:280:ASP:OD1  | 3:M:282:VAL:HG23 | 2.19                     | 0.42              |
| 4:S:53:THR:HG21  | 4:S:69:ASN:N     | 2.34                     | 0.42              |
| 1:A:274:LEU:O    | 1:A:275:LEU:O    | 2.38                     | 0.42              |
| 1:A:401:VAL:HG23 | 1:A:418:ILE:H    | 1.85                     | 0.42              |
| 2:B:367:SER:CB   | 2:B:401:THR:HB   | 2.48                     | 0.42              |
| 2:B:426:GLU:O    | 2:B:429:VAL:HB   | 2.20                     | 0.42              |
| 2:B:512:VAL:CB   | 2:B:551:LEU:HD12 | 2.47                     | 0.42              |
| 2:B:572:GLU:C    | 2:B:574:ASN:H    | 2.27                     | 0.42              |
| 3:M:293:PRO:CA   | 3:M:294:ASP:O    | 2.66                     | 0.42              |
| 3:M:374:TYR:CE2  | 3:M:393:GLY:HA2  | 2.44                     | 0.42              |
| 4:S:53:THR:CG2   | 4:S:69:ASN:HB2   | 2.49                     | 0.42              |
| 4:S:57:LEU:N     | 4:S:58:LEU:O     | 2.46                     | 0.42              |
| 4:S:89:VAL:CG1   | 4:S:98:ILE:CD1   | 2.97                     | 0.42              |
| 1:A:92:LEU:HD21  | 1:A:124:ALA:CA   | 2.49                     | 0.42              |
| 1:A:154:ILE:HG22 | 1:A:191:GLN:CG   | 2.45                     | 0.42              |
| 1:A:176:TYR:CZ   | 4:S:143:GLU:CD   | 2.93                     | 0.42              |
| 1:A:189:PHE:CD2  | 1:A:225:LEU:HD21 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:250:ASN:OD1  | 1:A:285:THR:CG2  | 2.68                     | 0.42              |
| 1:A:251:TRP:HA   | 1:A:254:ILE:HD12 | 2.02                     | 0.42              |
| 1:A:350:SER:O    | 1:A:352:PHE:N    | 2.51                     | 0.42              |
| 1:A:427:LYS:O    | 1:A:431:VAL:HG23 | 2.18                     | 0.42              |
| 2:B:13:ASP:O     | 2:B:16:LYS:O     | 2.38                     | 0.42              |
| 2:B:123:LEU:CD1  | 2:B:142:LEU:HD23 | 2.35                     | 0.42              |
| 2:B:181:TYR:HE1  | 2:B:222:HIS:HE2  | 1.66                     | 0.42              |
| 2:B:340:ILE:CB   | 2:B:373:LEU:HG   | 2.49                     | 0.42              |
| 2:B:537:PHE:CZ   | 2:B:599:ALA:HA   | 2.54                     | 0.42              |
| 3:M:368:ASP:O    | 3:M:371:GLU:HB2  | 2.19                     | 0.42              |
| 4:S:89:VAL:HG11  | 4:S:98:ILE:CG2   | 2.50                     | 0.42              |
| 1:A:186:PHE:HD1  | 1:A:221:VAL:HA   | 1.84                     | 0.42              |
| 1:A:206:LYS:C    | 1:A:208:ASP:N    | 2.75                     | 0.42              |
| 1:A:356:ILE:CD1  | 1:A:374:LEU:HD23 | 2.49                     | 0.42              |
| 1:A:366:SER:O    | 1:A:370:LYS:CG   | 2.56                     | 0.42              |
| 1:A:528:ASN:O    | 1:A:529:GLY:O    | 2.34                     | 0.42              |
| 1:A:634:ASN:ND2  | 2:B:554:LYS:O    | 2.52                     | 0.42              |
| 1:A:634:ASN:HB3  | 2:B:558:TYR:CD1  | 2.53                     | 0.42              |
| 2:B:158:VAL:HG12 | 2:B:177:ILE:HD11 | 2.00                     | 0.42              |
| 2:B:219:TYR:CD2  | 2:B:222:HIS:O    | 2.72                     | 0.42              |
| 2:B:227:HIS:O    | 2:B:228:GLY:C    | 2.60                     | 0.42              |
| 2:B:256:CYS:CB   | 2:B:328:LEU:HD21 | 2.43                     | 0.42              |
| 2:B:383:VAL:HG22 | 2:B:384:PHE:C    | 2.45                     | 0.42              |
| 2:B:434:LYS:O    | 2:B:437:SER:HB3  | 2.19                     | 0.42              |
| 2:B:580:TYR:CB   | 2:B:582:ASP:CG   | 2.89                     | 0.42              |
| 3:M:117:ASN:O    | 3:M:120:ARG:N    | 2.52                     | 0.42              |
| 3:M:226:PHE:CD2  | 3:M:235:LEU:HA   | 2.55                     | 0.42              |
| 3:M:269:ILE:C    | 3:M:302:TYR:CD1  | 2.97                     | 0.42              |
| 3:M:288:ILE:HD12 | 3:M:300:LEU:HD23 | 2.02                     | 0.42              |
| 4:S:55:PRO:CG    | 4:S:71:GLU:HG2   | 2.49                     | 0.42              |
| 1:A:121:LEU:HD13 | 1:A:155:THR:CB   | 2.49                     | 0.42              |
| 1:A:186:PHE:HB2  | 1:A:221:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:192:TYR:CD2  | 1:A:192:TYR:O    | 2.72                     | 0.42              |
| 1:A:260:PHE:O    | 1:A:261:THR:O    | 2.29                     | 0.42              |
| 1:A:372:ILE:O    | 1:A:375:VAL:HB   | 2.20                     | 0.42              |
| 1:A:403:LEU:CD2  | 1:A:422:GLU:HG3  | 2.34                     | 0.42              |
| 1:A:536:MET:HB3  | 1:A:555:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:554:ALA:O    | 1:A:557:LYS:N    | 2.49                     | 0.42              |
| 1:A:588:LEU:C    | 1:A:590:TYR:N    | 2.75                     | 0.42              |
| 2:B:334:MET:O    | 2:B:336:ASN:N    | 2.49                     | 0.42              |
| 2:B:527:PRO:CG   | 2:B:587:ARG:HG2  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:531:ARG:HG3  | 2:B:591:MET:HE1  | 2.01                     | 0.42              |
| 2:B:574:ASN:C    | 2:B:576:GLN:N    | 2.74                     | 0.42              |
| 3:M:57:GLY:O     | 3:M:58:ARG:HG3   | 2.20                     | 0.42              |
| 1:A:83:ASP:OD2   | 1:A:85:ALA:N     | 2.52                     | 0.42              |
| 1:A:402:ILE:C    | 1:A:404:GLN:N    | 2.76                     | 0.42              |
| 2:B:101:ILE:O    | 2:B:105:LEU:HD13 | 2.20                     | 0.42              |
| 2:B:102:HIS:CB   | 2:B:141:ALA:HB2  | 2.50                     | 0.42              |
| 2:B:279:LEU:CD1  | 2:B:285:GLU:HG2  | 2.41                     | 0.42              |
| 2:B:343:LEU:HD22 | 2:B:366:LEU:HD11 | 1.99                     | 0.42              |
| 3:M:347:PHE:O    | 3:M:350:VAL:N    | 2.49                     | 0.42              |
| 3:M:355:ASP:O    | 3:M:356:LEU:C    | 2.60                     | 0.42              |
| 4:S:152:SER:O    | 4:S:155:GLU:HB2  | 2.20                     | 0.42              |
| 1:A:250:ASN:O    | 1:A:254:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:282:MET:HE1  | 1:A:315:CYS:HA   | 2.02                     | 0.42              |
| 1:A:537:THR:O    | 1:A:540:ILE:HG22 | 2.20                     | 0.42              |
| 1:A:556:VAL:HG21 | 1:A:603:VAL:CG2  | 2.49                     | 0.42              |
| 1:A:582:ILE:CD1  | 1:A:608:ARG:HA   | 2.50                     | 0.42              |
| 2:B:18:ILE:HD13  | 2:B:18:ILE:N     | 2.32                     | 0.42              |
| 2:B:63:MET:SD    | 2:B:101:ILE:HA   | 2.59                     | 0.42              |
| 2:B:106:LEU:CG   | 2:B:144:ASP:HB3  | 2.49                     | 0.42              |
| 2:B:162:VAL:CG2  | 2:B:199:LEU:HG   | 2.45                     | 0.42              |
| 2:B:302:PHE:HE1  | 2:B:306:LEU:HD21 | 1.84                     | 0.42              |
| 2:B:304:GLN:O    | 2:B:307:ASN:HB2  | 2.20                     | 0.42              |
| 2:B:367:SER:CB   | 2:B:401:THR:CB   | 2.98                     | 0.42              |
| 2:B:538:SER:HB3  | 2:B:598:LEU:CD2  | 2.50                     | 0.42              |
| 2:B:566:ALA:HB1  | 2:B:581:TYR:HB3  | 2.00                     | 0.42              |
| 3:M:223:HIS:HB2  | 3:M:476:THR:OG1  | 2.19                     | 0.42              |
| 3:M:234:ARG:O    | 3:M:235:LEU:C    | 2.60                     | 0.42              |
| 3:M:290:PHE:CZ   | 3:M:297:PHE:CG   | 3.08                     | 0.42              |
| 3:M:323:MET:HE2  | 3:M:437:TYR:HE2  | 1.84                     | 0.42              |
| 1:A:154:ILE:HB   | 1:A:191:GLN:CG   | 2.31                     | 0.42              |
| 1:A:224:GLU:O    | 1:A:227:LYS:N    | 2.48                     | 0.42              |
| 1:A:589:SER:HB2  | 1:A:601:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:606:PHE:CD1  | 1:A:629:LEU:HG   | 2.54                     | 0.42              |
| 1:A:637:GLU:O    | 2:B:517:GLU:HA   | 2.19                     | 0.42              |
| 2:B:178:ILE:HD11 | 2:B:215:TYR:N    | 2.35                     | 0.42              |
| 2:B:227:HIS:O    | 2:B:230:PHE:N    | 2.51                     | 0.42              |
| 2:B:345:ARG:O    | 2:B:349:MET:HG3  | 2.20                     | 0.42              |
| 2:B:374:PHE:HA   | 2:B:377:TYR:HD1  | 1.85                     | 0.42              |
| 2:B:400:SER:CB   | 2:B:439:CYS:SG   | 3.08                     | 0.42              |
| 2:B:494:ALA:HB2  | 2:B:515:PHE:HE2  | 1.79                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:19:LEU:HD11  | 3:M:24:ALA:HB2   | 2.01                     | 0.42              |
| 3:M:65:TYR:CE1   | 3:M:86:PRO:HB3   | 2.50                     | 0.42              |
| 3:M:111:ILE:CG1  | 3:M:112:LYS:N    | 2.82                     | 0.42              |
| 3:M:223:HIS:CD2  | 3:M:478:ASN:CB   | 3.03                     | 0.42              |
| 3:M:245:ASP:O    | 3:M:472:TYR:HE1  | 1.90                     | 0.42              |
| 4:S:53:THR:CB    | 4:S:68:VAL:CA    | 2.96                     | 0.42              |
| 1:A:153:ILE:CG2  | 1:A:158:LEU:CD2  | 2.97                     | 0.42              |
| 1:A:298:ILE:HG13 | 1:A:311:THR:HG22 | 2.01                     | 0.42              |
| 1:A:359:LEU:HB3  | 1:A:367:ILE:CG2  | 2.49                     | 0.42              |
| 1:A:369:SER:CB   | 1:A:424:TYR:HE2  | 2.21                     | 0.42              |
| 1:A:555:LEU:HD12 | 1:A:581:LEU:HD11 | 2.00                     | 0.42              |
| 1:A:566:PHE:CD1  | 1:A:570:LYS:HA   | 2.55                     | 0.42              |
| 2:B:98:LYS:HD2   | 2:B:102:HIS:NE2  | 2.35                     | 0.42              |
| 2:B:215:TYR:CE2  | 2:B:229:HIS:ND1  | 2.86                     | 0.42              |
| 2:B:230:PHE:HD2  | 2:B:298:ASP:CA   | 2.32                     | 0.42              |
| 2:B:241:ASP:CG   | 3:M:274:ASP:CG   | 2.88                     | 0.42              |
| 2:B:493:LEU:HD11 | 2:B:511:ILE:HG12 | 2.01                     | 0.42              |
| 2:B:533:LEU:O    | 2:B:536:ASN:N    | 2.46                     | 0.42              |
| 3:M:54:SER:H     | 3:M:66:PHE:HD1   | 1.67                     | 0.42              |
| 3:M:222:PHE:HB2  | 3:M:479:PHE:CE1  | 2.54                     | 0.42              |
| 3:M:364:VAL:HG12 | 3:M:372:ILE:HG13 | 2.01                     | 0.42              |
| 3:M:461:GLY:O    | 3:M:462:LYS:C    | 2.52                     | 0.42              |
| 4:S:32:LEU:C     | 4:S:35:VAL:HG22  | 2.43                     | 0.42              |
| 4:S:135:ILE:CG2  | 4:S:141:VAL:HG22 | 2.44                     | 0.42              |
| 1:A:121:LEU:CD1  | 1:A:155:THR:H    | 2.26                     | 0.42              |
| 1:A:584:PHE:O    | 1:A:587:ASN:N    | 2.53                     | 0.42              |
| 2:B:50:LEU:HD23  | 2:B:62:ALA:CA    | 2.50                     | 0.42              |
| 2:B:82:TYR:HB2   | 2:B:104:TYR:OH   | 2.19                     | 0.42              |
| 2:B:94:ASP:OD1   | 2:B:95:THR:N     | 2.53                     | 0.42              |
| 2:B:127:LEU:CD1  | 2:B:157:THR:OG1  | 2.68                     | 0.42              |
| 2:B:174:ALA:C    | 2:B:214:ALA:HB2  | 2.45                     | 0.42              |
| 2:B:408:VAL:HG11 | 2:B:446:TRP:CG   | 2.55                     | 0.42              |
| 2:B:589:SER:C    | 2:B:591:MET:N    | 2.77                     | 0.42              |
| 3:M:323:MET:HG2  | 3:M:437:TYR:OH   | 2.20                     | 0.42              |
| 3:M:362:PHE:O    | 3:M:364:VAL:N    | 2.48                     | 0.42              |
| 4:S:57:LEU:C     | 4:S:67:GLU:O     | 2.62                     | 0.42              |
| 4:S:58:LEU:HD12  | 4:S:68:VAL:HG13  | 2.02                     | 0.42              |
| 1:A:197:ARG:O    | 1:A:198:ASP:C    | 2.61                     | 0.41              |
| 1:A:390:THR:O    | 1:A:394:GLN:HG2  | 2.20                     | 0.41              |
| 1:A:456:ASP:O    | 1:A:459:MET:N    | 2.49                     | 0.41              |
| 1:A:570:LYS:HB3  | 1:A:618:THR:HG22 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:602:GLU:CD   | 2:B:513:TRP:HH2  | 2.27                     | 0.41              |
| 2:B:104:TYR:O    | 2:B:107:ARG:CB   | 2.65                     | 0.41              |
| 2:B:159:LYS:HA   | 2:B:195:ILE:HD13 | 2.02                     | 0.41              |
| 2:B:234:CYS:CB   | 2:B:301:LEU:HB2  | 2.50                     | 0.41              |
| 2:B:340:ILE:CG1  | 2:B:373:LEU:CG   | 2.97                     | 0.41              |
| 2:B:381:PHE:O    | 2:B:382:TYR:C    | 2.58                     | 0.41              |
| 2:B:513:TRP:HE1  | 2:B:517:GLU:CG   | 2.33                     | 0.41              |
| 2:B:537:PHE:HA   | 2:B:540:GLU:CD   | 2.44                     | 0.41              |
| 2:B:563:PHE:CE2  | 2:B:584:SER:CA   | 3.03                     | 0.41              |
| 3:M:64:LYS:CE    | 3:M:79:SER:HB2   | 2.50                     | 0.41              |
| 3:M:262:THR:HG22 | 3:M:264:GLY:H    | 1.81                     | 0.41              |
| 3:M:263:MET:HG2  | 3:M:263:MET:O    | 2.20                     | 0.41              |
| 3:M:471:LYS:C    | 3:M:472:TYR:HD1  | 2.28                     | 0.41              |
| 4:S:7:ILE:HG23   | 4:S:85:PHE:CD2   | 2.54                     | 0.41              |
| 4:S:55:PRO:HB3   | 4:S:71:GLU:HG2   | 2.02                     | 0.41              |
| 4:S:58:LEU:HD22  | 4:S:70:ASN:HA    | 2.02                     | 0.41              |
| 4:S:130:SER:HB2  | 4:S:156:LEU:CD1  | 2.50                     | 0.41              |
| 1:A:189:PHE:C    | 1:A:191:GLN:N    | 2.78                     | 0.41              |
| 1:A:223:CYS:HB2  | 1:A:259:LEU:CG   | 2.50                     | 0.41              |
| 1:A:316:LEU:O    | 1:A:319:LEU:N    | 2.53                     | 0.41              |
| 1:A:438:ALA:HB3  | 1:A:441:TYR:HE1  | 1.86                     | 0.41              |
| 2:B:117:LEU:HD23 | 2:B:150:LEU:HD23 | 2.02                     | 0.41              |
| 2:B:137:PHE:N    | 2:B:172:GLU:HG3  | 2.31                     | 0.41              |
| 2:B:329:ALA:HB2  | 2:B:334:MET:HG2  | 2.02                     | 0.41              |
| 2:B:451:MET:HG3  | 2:B:489:ILE:HD13 | 2.01                     | 0.41              |
| 2:B:486:HIS:CD2  | 2:B:490:ILE:HG12 | 2.55                     | 0.41              |
| 2:B:490:ILE:CG1  | 2:B:518:ILE:HG12 | 2.47                     | 0.41              |
| 3:M:15:ILE:HG21  | 3:M:114:ILE:CG2  | 2.50                     | 0.41              |
| 3:M:104:PHE:CD2  | 3:M:109:LEU:HD21 | 2.56                     | 0.41              |
| 3:M:356:LEU:C    | 3:M:356:LEU:CD2  | 2.90                     | 0.41              |
| 3:M:432:THR:O    | 3:M:432:THR:HG23 | 2.19                     | 0.41              |
| 4:S:71:GLU:O     | 4:S:72:ASP:C     | 2.63                     | 0.41              |
| 1:A:322:PHE:CB   | 1:A:330:LEU:HD21 | 2.49                     | 0.41              |
| 1:A:514:GLU:HA   | 1:A:514:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:548:GLN:NE2  | 1:A:588:LEU:HD11 | 2.36                     | 0.41              |
| 2:B:95:THR:HG22  | 2:B:137:PHE:HE2  | 1.84                     | 0.41              |
| 2:B:117:LEU:O    | 2:B:120:ILE:HB   | 2.20                     | 0.41              |
| 2:B:234:CYS:HB2  | 2:B:301:LEU:HB3  | 2.02                     | 0.41              |
| 2:B:308:CYS:C    | 2:B:311:TYR:H    | 2.28                     | 0.41              |
| 2:B:396:ILE:HD13 | 2:B:432:ALA:HB2  | 2.02                     | 0.41              |
| 3:M:6:TYR:CA     | 3:M:16:PHE:O     | 2.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:65:TYR:CE2   | 3:M:86:PRO:HA    | 2.55                     | 0.41              |
| 3:M:72:LEU:O     | 3:M:109:LEU:O    | 2.38                     | 0.41              |
| 3:M:221:THR:HG21 | 3:M:475:GLN:HA   | 2.02                     | 0.41              |
| 3:M:262:THR:C    | 3:M:264:GLY:N    | 2.74                     | 0.41              |
| 3:M:374:TYR:HE1  | 3:M:376:ILE:HG12 | 1.85                     | 0.41              |
| 3:M:405:THR:CG2  | 3:M:406:GLY:N    | 2.77                     | 0.41              |
| 3:M:443:SER:CA   | 3:M:447:ILE:HG13 | 2.50                     | 0.41              |
| 3:M:447:ILE:O    | 3:M:448:TYR:C    | 2.60                     | 0.41              |
| 4:S:53:THR:C     | 4:S:69:ASN:CG    | 2.88                     | 0.41              |
| 4:S:87:PHE:CD1   | 4:S:87:PHE:N     | 2.89                     | 0.41              |
| 4:S:135:ILE:HG23 | 4:S:141:VAL:CG1  | 2.49                     | 0.41              |
| 1:A:166:LEU:CD2  | 1:A:184:ALA:HB3  | 2.50                     | 0.41              |
| 1:A:395:PHE:O    | 1:A:396:VAL:C    | 2.56                     | 0.41              |
| 1:A:408:ILE:HG21 | 4:S:64:ASN:O     | 2.19                     | 0.41              |
| 1:A:609:LEU:HD21 | 1:A:628:VAL:CG2  | 2.37                     | 0.41              |
| 2:B:108:PHE:HE2  | 2:B:112:ASP:CB   | 2.32                     | 0.41              |
| 2:B:277:CYS:HB2  | 2:B:296:ASP:H    | 1.84                     | 0.41              |
| 2:B:464:SER:OG   | 2:B:467:VAL:HG23 | 2.20                     | 0.41              |
| 2:B:508:ARG:O    | 2:B:512:VAL:CG2  | 2.54                     | 0.41              |
| 2:B:513:TRP:NE1  | 2:B:517:GLU:HG3  | 2.35                     | 0.41              |
| 2:B:569:THR:HA   | 2:B:571:SER:H    | 1.85                     | 0.41              |
| 3:M:19:LEU:HD21  | 3:M:24:ALA:HB3   | 2.02                     | 0.41              |
| 3:M:221:THR:HG23 | 3:M:437:TYR:O    | 2.20                     | 0.41              |
| 3:M:304:VAL:HG11 | 3:M:445:SER:HA   | 2.02                     | 0.41              |
| 4:S:58:LEU:O     | 4:S:59:LEU:C     | 2.59                     | 0.41              |
| 4:S:64:ASN:O     | 4:S:66:ASP:N     | 2.53                     | 0.41              |
| 4:S:87:PHE:CE2   | 4:S:102:ILE:HG12 | 2.56                     | 0.41              |
| 1:A:251:TRP:HZ3  | 4:S:96:LEU:C     | 2.28                     | 0.41              |
| 1:A:275:LEU:HD11 | 1:A:311:THR:OG1  | 2.21                     | 0.41              |
| 2:B:63:MET:HE1   | 2:B:104:TYR:CG   | 2.56                     | 0.41              |
| 2:B:124:GLN:CA   | 2:B:127:LEU:HD12 | 2.36                     | 0.41              |
| 2:B:132:SER:O    | 2:B:136:CYS:SG   | 2.77                     | 0.41              |
| 2:B:136:CYS:CA   | 2:B:172:GLU:CB   | 2.99                     | 0.41              |
| 2:B:276:SER:OG   | 2:B:289:PRO:CD   | 2.69                     | 0.41              |
| 2:B:293:VAL:HA   | 2:B:299:LEU:CB   | 2.48                     | 0.41              |
| 2:B:296:ASP:O    | 2:B:298:ASP:N    | 2.53                     | 0.41              |
| 2:B:398:ILE:O    | 2:B:399:LEU:C    | 2.63                     | 0.41              |
| 2:B:534:ILE:HG23 | 2:B:598:LEU:HD12 | 2.02                     | 0.41              |
| 2:B:617:LEU:O    | 2:B:618:PHE:C    | 2.60                     | 0.41              |
| 3:M:18:TYR:CD1   | 3:M:19:LEU:N     | 2.89                     | 0.41              |
| 3:M:214:LEU:C    | 3:M:214:LEU:CD2  | 2.80                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:79:MET:HG2   | 1:A:112:GLN:OE1  | 2.21                     | 0.41              |
| 1:A:222:ILE:HG21 | 1:A:240:LEU:CD1  | 2.30                     | 0.41              |
| 1:A:244:LEU:CD1  | 1:A:281:LEU:HD13 | 2.34                     | 0.41              |
| 1:A:450:TYR:O    | 1:A:454:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:637:GLU:HG2  | 2:B:554:LYS:HB3  | 1.95                     | 0.41              |
| 2:B:74:ASP:O     | 2:B:77:ILE:HG12  | 2.21                     | 0.41              |
| 2:B:246:SER:OG   | 2:B:317:VAL:HG22 | 2.20                     | 0.41              |
| 2:B:374:PHE:CG   | 2:B:374:PHE:O    | 2.74                     | 0.41              |
| 2:B:421:SER:O    | 2:B:422:ALA:C    | 2.59                     | 0.41              |
| 2:B:433:VAL:CG2  | 2:B:471:TYR:CZ   | 3.03                     | 0.41              |
| 2:B:436:LEU:HD12 | 2:B:454:LEU:HD21 | 2.02                     | 0.41              |
| 2:B:522:GLU:C    | 2:B:524:LYS:H    | 2.28                     | 0.41              |
| 3:M:7:ILE:HD11   | 3:M:121:ILE:HG21 | 2.02                     | 0.41              |
| 3:M:107:ASP:C    | 3:M:108:LYS:HG3  | 2.45                     | 0.41              |
| 1:A:231:GLN:N    | 1:A:232:PRO:CD   | 2.84                     | 0.41              |
| 1:A:330:LEU:O    | 1:A:330:LEU:HD12 | 2.21                     | 0.41              |
| 1:A:356:ILE:O    | 1:A:359:LEU:N    | 2.52                     | 0.41              |
| 1:A:401:VAL:O    | 1:A:404:GLN:N    | 2.38                     | 0.41              |
| 1:A:464:ILE:O    | 1:A:464:ILE:HG23 | 2.20                     | 0.41              |
| 1:A:564:ASN:OD1  | 1:A:622:PRO:HB3  | 2.20                     | 0.41              |
| 1:A:582:ILE:HD11 | 1:A:608:ARG:HA   | 2.02                     | 0.41              |
| 2:B:100:LEU:O    | 2:B:103:LEU:HB2  | 2.21                     | 0.41              |
| 2:B:142:LEU:O    | 2:B:143:SER:C    | 2.47                     | 0.41              |
| 2:B:267:ASP:N    | 2:B:289:PRO:HB3  | 2.33                     | 0.41              |
| 2:B:366:LEU:C    | 2:B:368:ILE:N    | 2.74                     | 0.41              |
| 2:B:387:ASP:CB   | 2:B:388:PRO:HD2  | 2.50                     | 0.41              |
| 2:B:505:ASP:CA   | 2:B:544:THR:OG1  | 2.63                     | 0.41              |
| 3:M:45:SER:HB3   | 3:M:51:LEU:HD12  | 2.01                     | 0.41              |
| 3:M:117:ASN:O    | 3:M:120:ARG:HB2  | 2.21                     | 0.41              |
| 3:M:240:ILE:HB   | 3:M:304:VAL:CG1  | 2.51                     | 0.41              |
| 3:M:270:PRO:N    | 3:M:302:TYR:CE1  | 2.89                     | 0.41              |
| 4:S:43:ASN:O     | 4:S:45:ASP:N     | 2.51                     | 0.41              |
| 1:A:219:VAL:O    | 1:A:259:LEU:CD1  | 2.69                     | 0.41              |
| 1:A:244:LEU:O    | 1:A:246:THR:N    | 2.53                     | 0.41              |
| 1:A:279:LEU:HA   | 1:A:282:MET:HG2  | 2.03                     | 0.41              |
| 1:A:289:SER:CB   | 4:S:96:LEU:HB3   | 2.51                     | 0.41              |
| 1:A:393:LYS:O    | 1:A:394:GLN:C    | 2.61                     | 0.41              |
| 1:A:405:THR:N    | 2:B:7:ARG:NE     | 2.49                     | 0.41              |
| 1:A:426:ILE:CD1  | 1:A:466:ASP:OD2  | 2.67                     | 0.41              |
| 2:B:102:HIS:CD2  | 2:B:123:LEU:HD21 | 2.56                     | 0.41              |
| 2:B:175:LEU:HA   | 2:B:214:ALA:HB2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:181:TYR:CD2  | 2:B:218:CYS:C    | 2.93                     | 0.41              |
| 2:B:264:THR:O    | 2:B:265:VAL:C    | 2.60                     | 0.41              |
| 2:B:346:THR:HG22 | 2:B:350:THR:HG23 | 2.02                     | 0.41              |
| 2:B:398:ILE:C    | 2:B:400:SER:N    | 2.77                     | 0.41              |
| 2:B:422:ALA:HB2  | 2:B:424:PHE:CE1  | 2.44                     | 0.41              |
| 2:B:433:VAL:HG21 | 2:B:471:TYR:CD1  | 2.56                     | 0.41              |
| 2:B:436:LEU:O    | 2:B:450:VAL:HG11 | 2.21                     | 0.41              |
| 3:M:222:PHE:HB2  | 3:M:479:PHE:HZ   | 1.85                     | 0.41              |
| 3:M:327:PHE:HE1  | 3:M:336:ASP:CG   | 2.28                     | 0.41              |
| 1:A:64:LEU:HA    | 1:A:102:GLN:NE2  | 2.33                     | 0.41              |
| 1:A:401:VAL:HG21 | 1:A:419:ILE:HB   | 2.03                     | 0.41              |
| 1:A:581:LEU:CD1  | 1:A:585:PHE:CZ   | 3.03                     | 0.41              |
| 1:A:581:LEU:CG   | 1:A:585:PHE:CE2  | 3.02                     | 0.41              |
| 1:A:595:GLU:OE2  | 2:B:473:ASN:OD1  | 2.39                     | 0.41              |
| 2:B:30:LEU:C     | 2:B:32:GLU:N     | 2.79                     | 0.41              |
| 2:B:102:HIS:CE1  | 2:B:137:PHE:CB   | 3.04                     | 0.41              |
| 2:B:142:LEU:HB3  | 2:B:154:ILE:HG12 | 2.02                     | 0.41              |
| 2:B:162:VAL:HG11 | 2:B:195:ILE:HG23 | 2.02                     | 0.41              |
| 2:B:178:ILE:CD1  | 2:B:214:ALA:O    | 2.68                     | 0.41              |
| 2:B:178:ILE:HG21 | 2:B:217:GLU:HB2  | 1.82                     | 0.41              |
| 2:B:277:CYS:HB2  | 2:B:295:ASN:HB2  | 2.02                     | 0.41              |
| 2:B:278:PRO:CD   | 2:B:292:GLU:HG3  | 2.42                     | 0.41              |
| 2:B:279:LEU:HD12 | 2:B:285:GLU:CB   | 2.51                     | 0.41              |
| 2:B:307:ASN:O    | 2:B:308:CYS:C    | 2.63                     | 0.41              |
| 2:B:355:ASN:O    | 2:B:359:LEU:CD2  | 2.69                     | 0.41              |
| 2:B:408:VAL:HB   | 2:B:446:TRP:CD1  | 2.55                     | 0.41              |
| 2:B:537:PHE:CE2  | 2:B:598:LEU:C    | 2.99                     | 0.41              |
| 2:B:549:LEU:CG   | 2:B:611:ALA:HA   | 2.50                     | 0.41              |
| 2:B:556:LEU:HD11 | 2:B:592:TYR:HB2  | 2.02                     | 0.41              |
| 3:M:6:TYR:CD2    | 3:M:17:GLN:HG2   | 2.56                     | 0.41              |
| 3:M:134:PRO:O    | 3:M:136:VAL:HG22 | 2.20                     | 0.41              |
| 3:M:222:PHE:N    | 3:M:222:PHE:HD1  | 2.19                     | 0.41              |
| 3:M:343:ASN:CG   | 3:M:408:VAL:CG1  | 2.94                     | 0.41              |
| 3:M:356:LEU:HD12 | 3:M:437:TYR:CD2  | 2.56                     | 0.41              |
| 4:S:15:ARG:CZ    | 4:S:122:ILE:HD11 | 2.50                     | 0.41              |
| 4:S:125:TRP:O    | 4:S:129:GLU:HG3  | 2.21                     | 0.41              |
| 1:A:253:ILE:CD1  | 1:A:285:THR:CG2  | 2.99                     | 0.41              |
| 1:A:313:MET:HG3  | 1:A:348:PHE:HE1  | 1.86                     | 0.41              |
| 1:A:585:PHE:CD2  | 1:A:603:VAL:CG1  | 3.01                     | 0.41              |
| 2:B:4:SER:O      | 2:B:8:ILE:HD12   | 2.21                     | 0.41              |
| 2:B:92:THR:HG22  | 2:B:93:ASN:N     | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:172:GLU:O    | 2:B:175:LEU:N    | 2.54                     | 0.41              |
| 2:B:230:PHE:CD2  | 2:B:298:ASP:CA   | 3.04                     | 0.41              |
| 3:M:99:ILE:HG21  | 3:M:124:ILE:HG21 | 1.85                     | 0.41              |
| 3:M:213:GLU:HB3  | 3:M:467:TYR:HA   | 2.03                     | 0.41              |
| 3:M:229:LYS:HG2  | 3:M:230:LYS:HG3  | 2.02                     | 0.41              |
| 3:M:355:ASP:OD2  | 3:M:357:LYS:CE   | 2.65                     | 0.41              |
| 1:A:104:ARG:HG3  | 1:A:145:ILE:HD12 | 2.03                     | 0.40              |
| 1:A:190:LEU:HD11 | 1:A:228:LYS:CE   | 2.48                     | 0.40              |
| 2:B:52:ASN:O     | 2:B:53:SER:C     | 2.63                     | 0.40              |
| 2:B:62:ALA:O     | 2:B:66:ILE:HD12  | 2.21                     | 0.40              |
| 2:B:378:THR:C    | 2:B:380:LYS:N    | 2.79                     | 0.40              |
| 2:B:563:PHE:O    | 2:B:566:ALA:N    | 2.54                     | 0.40              |
| 3:M:219:LEU:HB2  | 3:M:472:TYR:C    | 2.46                     | 0.40              |
| 3:M:304:VAL:O    | 3:M:304:VAL:HG13 | 2.21                     | 0.40              |
| 3:M:353:VAL:HG22 | 3:M:354:ASP:O    | 2.21                     | 0.40              |
| 4:S:4:ALA:CB     | 4:S:19:PHE:CD2   | 3.03                     | 0.40              |
| 4:S:133:GLU:C    | 4:S:135:ILE:N    | 2.76                     | 0.40              |
| 1:A:320:HIS:ND1  | 1:A:352:PHE:HD2  | 2.18                     | 0.40              |
| 1:A:398:GLU:C    | 1:A:418:ILE:HG13 | 2.47                     | 0.40              |
| 2:B:119:SER:O    | 2:B:123:LEU:HG   | 2.21                     | 0.40              |
| 2:B:127:LEU:CB   | 2:B:161:LEU:HD11 | 2.43                     | 0.40              |
| 2:B:127:LEU:O    | 2:B:135:ARG:CD   | 2.69                     | 0.40              |
| 2:B:167:ALA:CB   | 2:B:202:ASP:CG   | 2.94                     | 0.40              |
| 2:B:182:ARG:HD2  | 2:B:217:GLU:HG3  | 2.03                     | 0.40              |
| 2:B:325:LEU:CD1  | 2:B:339:PHE:CD2  | 2.99                     | 0.40              |
| 2:B:490:ILE:HG13 | 2:B:518:ILE:CB   | 2.50                     | 0.40              |
| 2:B:523:PHE:CZ   | 2:B:580:TYR:CD2  | 3.01                     | 0.40              |
| 2:B:556:LEU:CD2  | 2:B:588:ILE:HG13 | 2.34                     | 0.40              |
| 2:B:589:SER:HA   | 2:B:618:PHE:CE2  | 2.55                     | 0.40              |
| 3:M:219:LEU:HB3  | 3:M:472:TYR:C    | 2.45                     | 0.40              |
| 3:M:226:PHE:HB2  | 3:M:481:VAL:HG22 | 2.03                     | 0.40              |
| 3:M:386:PHE:HB3  | 3:M:397:TRP:HD1  | 1.83                     | 0.40              |
| 4:S:3:HIS:CE1    | 4:S:90:ASP:HB3   | 2.56                     | 0.40              |
| 1:A:135:ASP:O    | 1:A:136:GLY:C    | 2.50                     | 0.40              |
| 1:A:170:LEU:HD13 | 1:A:170:LEU:HA   | 1.82                     | 0.40              |
| 1:A:292:TYR:HE1  | 1:A:296:ASN:HB2  | 1.83                     | 0.40              |
| 1:A:319:LEU:HD13 | 1:A:337:LEU:HB2  | 2.03                     | 0.40              |
| 1:A:429:VAL:HG11 | 1:A:473:ILE:CD1  | 2.49                     | 0.40              |
| 1:A:617:ASP:CG   | 1:A:618:THR:N    | 2.80                     | 0.40              |
| 1:A:634:ASN:HD22 | 2:B:554:LYS:HA   | 1.82                     | 0.40              |
| 2:B:25:VAL:O     | 2:B:32:GLU:O     | 2.40                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:136:CYS:SG   | 2:B:168:MET:CG   | 3.01                     | 0.40              |
| 2:B:136:CYS:CA   | 2:B:172:GLU:HB2  | 2.51                     | 0.40              |
| 2:B:200:MET:HE2  | 2:B:229:HIS:HA   | 1.68                     | 0.40              |
| 2:B:371:GLN:C    | 2:B:373:LEU:H    | 2.27                     | 0.40              |
| 2:B:527:PRO:CG   | 2:B:587:ARG:CG   | 2.98                     | 0.40              |
| 2:B:546:CYS:HA   | 2:B:607:ILE:CB   | 2.51                     | 0.40              |
| 2:B:570:GLY:O    | 2:B:571:SER:C    | 2.50                     | 0.40              |
| 3:M:216:VAL:O    | 3:M:216:VAL:CG2  | 2.69                     | 0.40              |
| 3:M:234:ARG:O    | 3:M:236:LEU:N    | 2.54                     | 0.40              |
| 3:M:319:SER:HB3  | 3:M:344:ILE:HA   | 2.03                     | 0.40              |
| 3:M:347:PHE:O    | 3:M:349:LYS:N    | 2.52                     | 0.40              |
| 1:A:174:ARG:HA   | 1:A:175:PRO:HD2  | 1.67                     | 0.40              |
| 1:A:182:ILE:CG2  | 1:A:221:VAL:CG2  | 2.88                     | 0.40              |
| 1:A:255:ARG:O    | 1:A:258:LYS:N    | 2.55                     | 0.40              |
| 2:B:80:GLN:C     | 2:B:83:PHE:H     | 2.29                     | 0.40              |
| 2:B:90:ILE:HD13  | 2:B:123:LEU:HD23 | 2.03                     | 0.40              |
| 2:B:105:LEU:C    | 2:B:145:MET:HE1  | 2.47                     | 0.40              |
| 2:B:196:LEU:HB3  | 2:B:215:TYR:HE2  | 1.70                     | 0.40              |
| 2:B:262:LYS:O    | 2:B:263:PRO:C    | 2.51                     | 0.40              |
| 2:B:378:THR:CG2  | 2:B:379:LYS:H    | 2.34                     | 0.40              |
| 2:B:397:GLN:NE2  | 2:B:431:MET:CE   | 2.84                     | 0.40              |
| 2:B:433:VAL:CG1  | 2:B:471:TYR:HA   | 2.43                     | 0.40              |
| 2:B:537:PHE:C    | 2:B:539:ASN:H    | 2.29                     | 0.40              |
| 3:M:222:PHE:CB   | 3:M:479:PHE:CZ   | 3.04                     | 0.40              |
| 3:M:262:THR:HG23 | 3:M:265:ASN:O    | 2.21                     | 0.40              |
| 3:M:293:PRO:CB   | 3:M:294:ASP:O    | 2.68                     | 0.40              |
| 4:S:35:VAL:HG12  | 4:S:77:TYR:OH    | 2.20                     | 0.40              |
| 1:A:93:GLU:O     | 1:A:96:SER:OG    | 2.29                     | 0.40              |
| 1:A:373:GLU:HG2  | 1:A:427:LYS:NZ   | 2.36                     | 0.40              |
| 1:A:563:CYS:O    | 1:A:566:PHE:CE2  | 2.74                     | 0.40              |
| 2:B:148:SER:HB3  | 2:B:183:ALA:HB1  | 2.03                     | 0.40              |
| 2:B:158:VAL:HA   | 2:B:173:VAL:HG13 | 2.02                     | 0.40              |
| 2:B:181:TYR:O    | 2:B:183:ALA:CA   | 2.61                     | 0.40              |
| 2:B:343:LEU:O    | 2:B:347:VAL:HG23 | 2.21                     | 0.40              |
| 2:B:447:GLU:O    | 2:B:450:VAL:HB   | 2.21                     | 0.40              |
| 2:B:467:VAL:CG1  | 2:B:471:TYR:CE1  | 3.04                     | 0.40              |
| 2:B:477:MET:O    | 2:B:480:GLN:N    | 2.54                     | 0.40              |
| 2:B:549:LEU:O    | 2:B:552:SER:N    | 2.54                     | 0.40              |
| 3:M:63:TYR:N     | 3:M:81:SER:O     | 2.52                     | 0.40              |
| 3:M:64:LYS:HE3   | 3:M:79:SER:HB2   | 2.04                     | 0.40              |
| 3:M:122:SER:O    | 3:M:125:PHE:HB2  | 2.21                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:M:136:VAL:CG1 | 3:M:137:SER:N   | 2.83                     | 0.40              |
| 3:M:250:LEU:CD1 | 3:M:254:PRO:HG2 | 2.52                     | 0.40              |
| 4:S:60:SER:O    | 4:S:66:ASP:CB   | 2.70                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 574/964 (60%)   | 547 (95%)  | 16 (3%)  | 11 (2%)  | 6           | 32 |
| 2   | B     | 619/809 (76%)   | 521 (84%)  | 64 (10%) | 34 (6%)  | 1           | 15 |
| 3   | M     | 391/483 (81%)   | 331 (85%)  | 44 (11%) | 16 (4%)  | 2           | 18 |
| 4   | S     | 166/194 (86%)   | 157 (95%)  | 6 (4%)   | 3 (2%)   | 6           | 34 |
| All | All   | 1750/2450 (71%) | 1556 (89%) | 130 (7%) | 64 (4%)  | 4           | 20 |

All (64) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 267 | GLU  |
| 1   | A     | 278 | ILE  |
| 1   | A     | 305 | GLU  |
| 1   | A     | 449 | TRP  |
| 2   | B     | 13  | ASP  |
| 2   | B     | 18  | ILE  |
| 2   | B     | 19  | THR  |
| 2   | B     | 200 | MET  |
| 2   | B     | 228 | GLY  |
| 2   | B     | 558 | TYR  |
| 2   | B     | 560 | ILE  |
| 2   | B     | 564 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 565 | GLN  |
| 3   | M     | 104 | PHE  |
| 3   | M     | 106 | LYS  |
| 3   | M     | 280 | ASP  |
| 3   | M     | 429 | ASP  |
| 3   | M     | 447 | ILE  |
| 4   | S     | 72  | ASP  |
| 1   | A     | 174 | ARG  |
| 1   | A     | 536 | MET  |
| 1   | A     | 571 | ARG  |
| 2   | B     | 29  | LYS  |
| 2   | B     | 78  | ASP  |
| 2   | B     | 177 | ILE  |
| 2   | B     | 179 | LYS  |
| 2   | B     | 194 | ASP  |
| 2   | B     | 215 | TYR  |
| 2   | B     | 313 | SER  |
| 2   | B     | 432 | ALA  |
| 2   | B     | 561 | ASP  |
| 2   | B     | 568 | VAL  |
| 3   | M     | 355 | ASP  |
| 3   | M     | 405 | THR  |
| 4   | S     | 65  | ASN  |
| 1   | A     | 507 | GLN  |
| 2   | B     | 14  | THR  |
| 2   | B     | 42  | ILE  |
| 2   | B     | 43  | ASN  |
| 2   | B     | 196 | LEU  |
| 2   | B     | 199 | LEU  |
| 2   | B     | 227 | HIS  |
| 2   | B     | 232 | ARG  |
| 2   | B     | 242 | SER  |
| 2   | B     | 573 | GLU  |
| 3   | M     | 316 | ARG  |
| 3   | M     | 352 | GLN  |
| 2   | B     | 274 | PRO  |
| 2   | B     | 578 | PRO  |
| 3   | M     | 45  | SER  |
| 3   | M     | 254 | PRO  |
| 3   | M     | 363 | ASN  |
| 4   | S     | 164 | ASP  |
| 1   | A     | 279 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 306 | GLU  |
| 2   | B     | 9   | ALA  |
| 2   | B     | 182 | ARG  |
| 2   | B     | 198 | GLU  |
| 2   | B     | 296 | ASP  |
| 3   | M     | 81  | SER  |
| 3   | M     | 84  | LYS  |
| 3   | M     | 346 | ASN  |
| 1   | A     | 116 | LYS  |
| 3   | M     | 321 | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 536/898 (60%)   | 527 (98%)  | 9 (2%)   | 53          | 69 |
| 2   | B     | 565/738 (77%)   | 551 (98%)  | 14 (2%)  | 42          | 63 |
| 3   | M     | 360/441 (82%)   | 351 (98%)  | 9 (2%)   | 42          | 63 |
| 4   | S     | 159/175 (91%)   | 156 (98%)  | 3 (2%)   | 50          | 67 |
| All | All   | 1620/2252 (72%) | 1585 (98%) | 35 (2%)  | 45          | 64 |

All (35) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 170 | LEU  |
| 1   | A     | 175 | PRO  |
| 1   | A     | 186 | PHE  |
| 1   | A     | 196 | LEU  |
| 1   | A     | 241 | TYR  |
| 1   | A     | 292 | TYR  |
| 1   | A     | 418 | ILE  |
| 1   | A     | 484 | VAL  |
| 1   | A     | 509 | PRO  |
| 2   | B     | 1   | MET  |
| 2   | B     | 4   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 10  | SER  |
| 2   | B     | 12  | LEU  |
| 2   | B     | 14  | THR  |
| 2   | B     | 16  | LYS  |
| 2   | B     | 19  | THR  |
| 2   | B     | 29  | LYS  |
| 2   | B     | 30  | LEU  |
| 2   | B     | 42  | ILE  |
| 2   | B     | 115 | LEU  |
| 2   | B     | 418 | TYR  |
| 2   | B     | 518 | ILE  |
| 2   | B     | 592 | TYR  |
| 3   | M     | 6   | TYR  |
| 3   | M     | 118 | TYR  |
| 3   | M     | 214 | LEU  |
| 3   | M     | 293 | PRO  |
| 3   | M     | 343 | ASN  |
| 3   | M     | 379 | LEU  |
| 3   | M     | 437 | TYR  |
| 3   | M     | 472 | TYR  |
| 3   | M     | 479 | PHE  |
| 4   | S     | 8   | PHE  |
| 4   | S     | 38  | LEU  |
| 4   | S     | 113 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 88  | ASN  |
| 1   | A     | 102 | GLN  |
| 1   | A     | 199 | ASN  |
| 1   | A     | 476 | GLN  |
| 1   | A     | 634 | ASN  |
| 2   | B     | 41  | ASN  |
| 2   | B     | 102 | HIS  |
| 2   | B     | 222 | HIS  |
| 2   | B     | 333 | GLN  |
| 2   | B     | 352 | ASN  |
| 2   | B     | 371 | GLN  |
| 2   | B     | 397 | GLN  |
| 2   | B     | 407 | ASN  |
| 2   | B     | 441 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 449 | HIS  |
| 2   | B     | 486 | HIS  |
| 2   | B     | 574 | ASN  |
| 3   | M     | 17  | GLN  |
| 3   | M     | 70  | ASN  |
| 3   | M     | 309 | GLN  |
| 3   | M     | 343 | ASN  |
| 3   | M     | 346 | ASN  |
| 4   | S     | 61  | ASN  |
| 4   | S     | 70  | ASN  |
| 4   | S     | 126 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | M     | 30               |

*Continued on next page...*

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 4   | S     | 8                |
| 2   | B     | 6                |
| 1   | A     | 4                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | S     | 68:VAL    | C      | 69:ASN    | N      | 1.67         |
| 1     | A     | 466:ASP   | C      | 467:LYS   | N      | 1.20         |
| 1     | M     | 23:THR    | C      | 24:ALA    | N      | 1.20         |
| 1     | M     | 65:TYR    | C      | 66:PHE    | N      | 1.20         |
| 1     | M     | 252:ASP   | C      | 253:ASN   | N      | 1.20         |
| 1     | M     | 288:ILE   | C      | 289:THR   | N      | 1.20         |
| 1     | S     | 60:SER    | C      | 61:ASN    | N      | 1.20         |
| 1     | A     | 378:ILE   | C      | 379:VAL   | N      | 1.19         |
| 1     | B     | 184:GLY   | C      | 185:LYS   | N      | 1.19         |
| 1     | B     | 259:TYR   | C      | 260:LEU   | N      | 1.19         |
| 1     | B     | 334:MET   | C      | 335:LYS   | N      | 1.19         |
| 1     | M     | 6:TYR     | C      | 7:ILE     | N      | 1.19         |
| 1     | M     | 82:LYS    | C      | 83:SER    | N      | 1.19         |
| 1     | S     | 62:GLU    | C      | 63:ASN    | N      | 1.19         |
| 1     | S     | 114:THR   | C      | 115:GLU   | N      | 1.19         |
| 1     | A     | 289:SER   | C      | 290:VAL   | N      | 1.18         |
| 1     | A     | 439:ASP   | C      | 440:ASN   | N      | 1.18         |
| 1     | M     | 64:LYS    | C      | 65:TYR    | N      | 1.18         |
| 1     | M     | 70:ASN    | C      | 71:LYS    | N      | 1.18         |
| 1     | M     | 379:LEU   | C      | 380:ARG   | N      | 1.18         |
| 1     | S     | 70:ASN    | C      | 71:GLU    | N      | 1.18         |
| 1     | M     | 136:VAL   | C      | 137:SER   | N      | 1.17         |
| 1     | M     | 403:THR   | C      | 404:ALA   | N      | 1.17         |
| 1     | M     | 450:GLU   | C      | 451:ALA   | N      | 1.17         |
| 1     | M     | 453:ASP   | C      | 454:ILE   | N      | 1.17         |
| 1     | S     | 6:LEU     | C      | 7:ILE     | N      | 1.17         |
| 1     | S     | 22:PRO    | C      | 23:VAL    | N      | 1.17         |
| 1     | M     | 62:VAL    | C      | 63:TYR    | N      | 1.16         |
| 1     | M     | 134:PRO   | C      | 135:ASN   | N      | 1.16         |
| 1     | M     | 279:ASN   | C      | 280:ASP   | N      | 1.16         |
| 1     | M     | 319:SER   | C      | 320:ILE   | N      | 1.16         |
| 1     | M     | 352:GLN   | C      | 353:VAL   | N      | 1.16         |
| 1     | M     | 61:GLU    | C      | 62:VAL    | N      | 1.15         |
| 1     | B     | 581:TYR   | C      | 582:ASP   | N      | 1.14         |
| 1     | M     | 106:LYS   | C      | 107:ASP   | N      | 1.14         |
| 1     | M     | 351:SER   | C      | 352:GLN   | N      | 1.14         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 284:ASN   | C      | 285:GLU   | N      | 1.13         |
| 1     | B     | 293:VAL   | C      | 294:VAL   | N      | 1.13         |
| 1     | M     | 20:LEU    | C      | 21:GLY    | N      | 1.13         |
| 1     | M     | 21:GLY    | C      | 22:ALA    | N      | 1.13         |
| 1     | M     | 52:ASP    | C      | 53:HIS    | N      | 1.13         |
| 1     | M     | 130:GLU   | C      | 131:ALA   | N      | 1.12         |
| 1     | M     | 80:THR    | C      | 81:SER    | N      | 1.11         |
| 1     | M     | 105:ASP   | C      | 106:LYS   | N      | 1.10         |
| 1     | M     | 81:SER    | C      | 82:LYS    | N      | 1.08         |
| 1     | M     | 3:LEU     | C      | 4:SER     | N      | 1.07         |
| 1     | S     | 48:SER    | C      | 49:SER    | N      | 1.04         |
| 1     | M     | 135:ASN   | C      | 136:VAL   | N      | 0.94         |

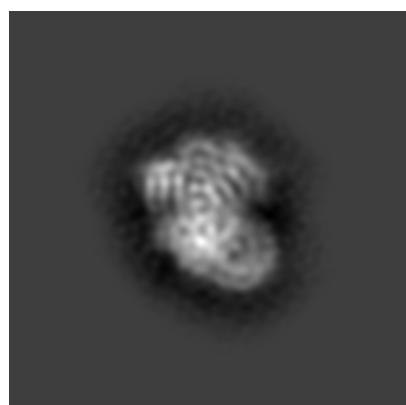
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13188. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

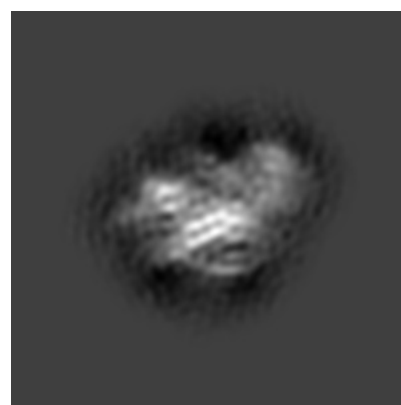
#### 6.1.1 Primary map



X



Y

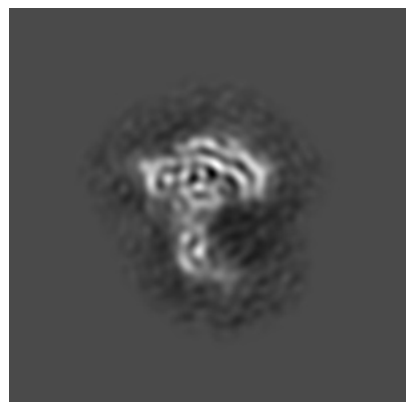


Z

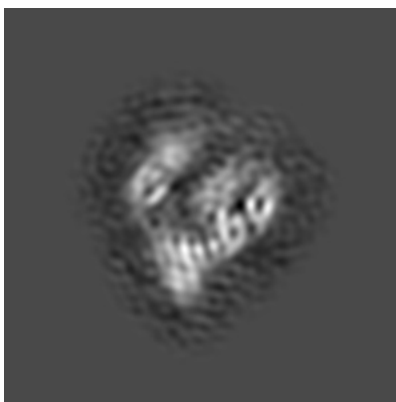
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

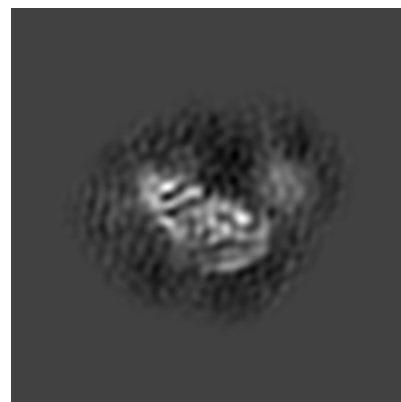
#### 6.2.1 Primary map



X Index: 132



Y Index: 132

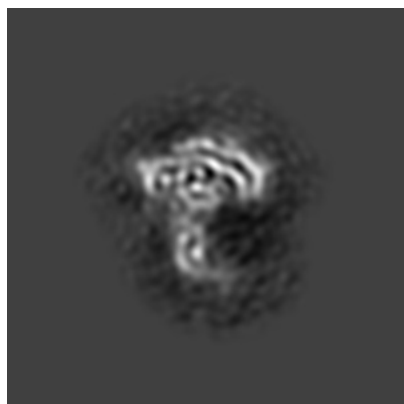


Z Index: 132

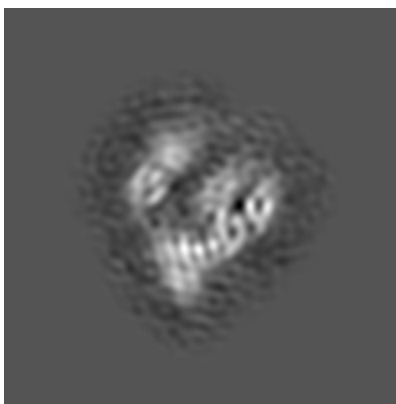
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 131



Y Index: 133



Z Index: 111

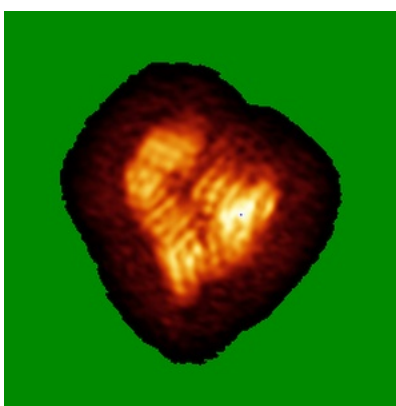
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X



Y

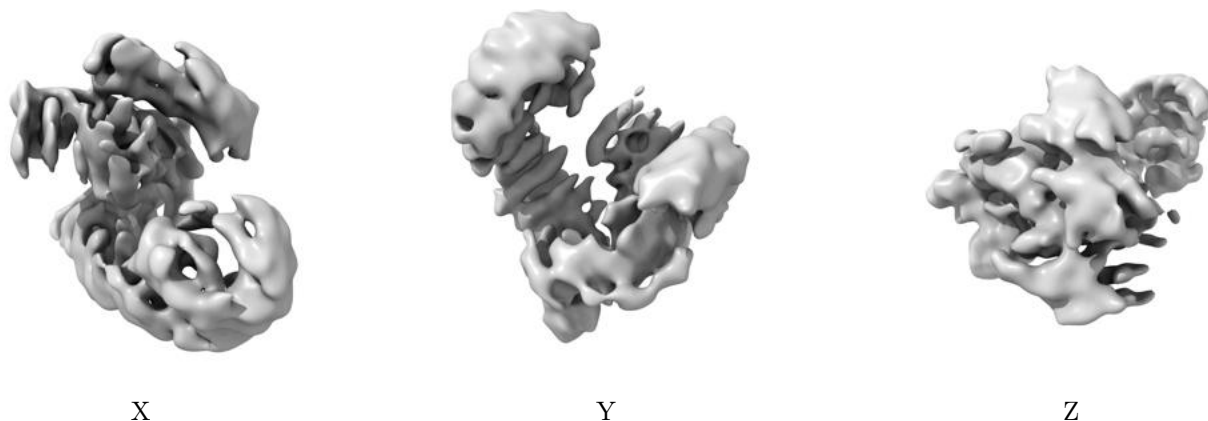


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

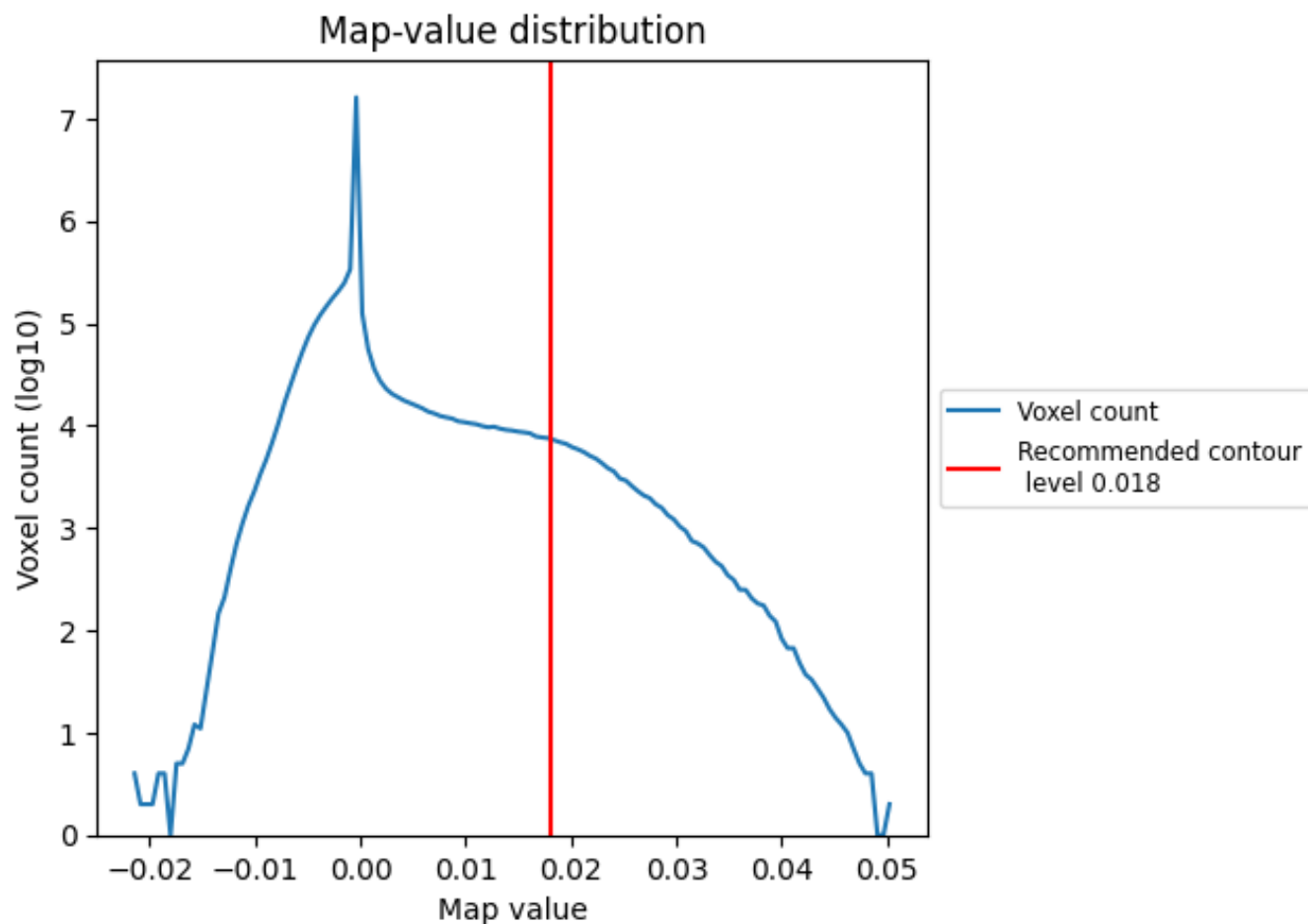
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

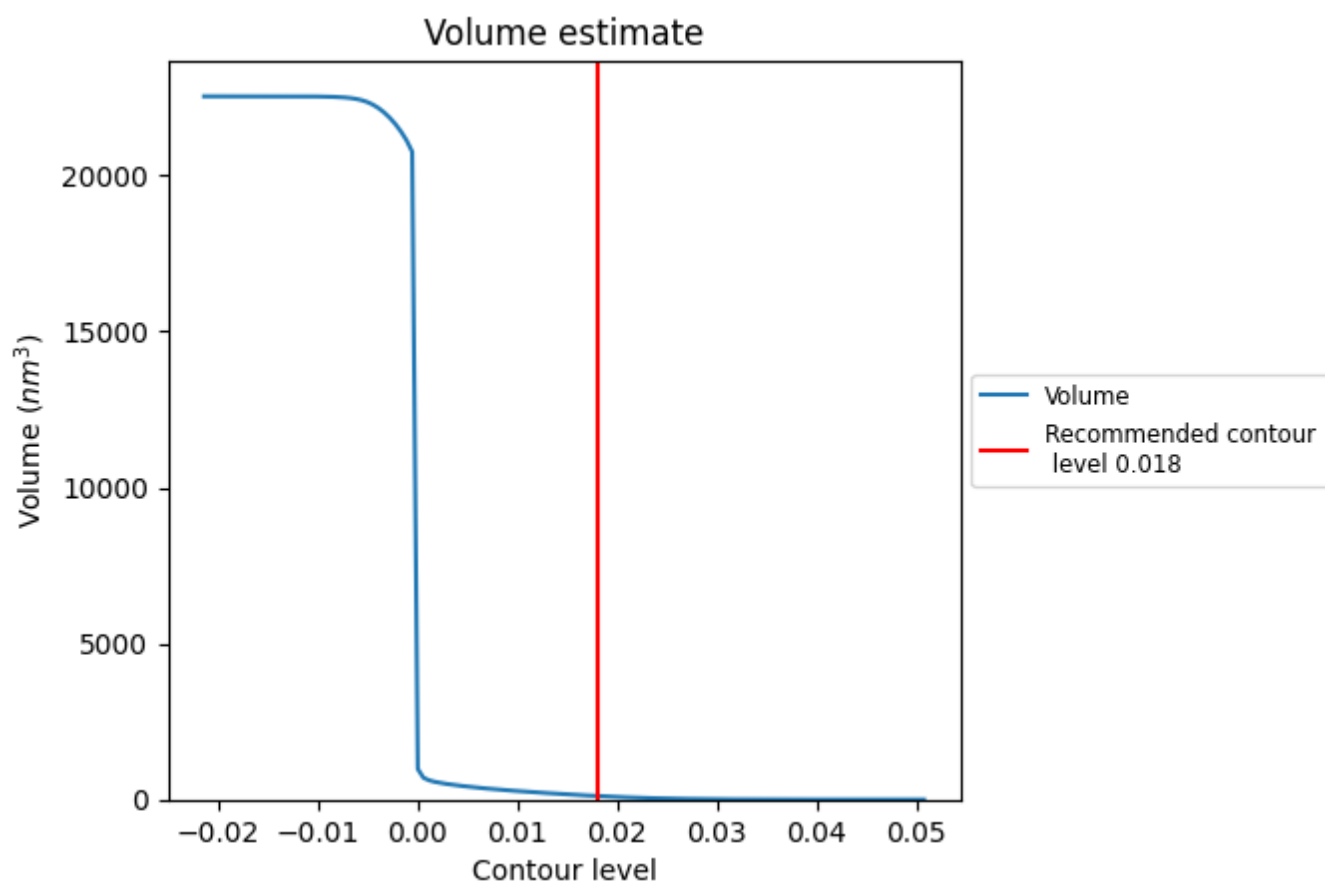
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

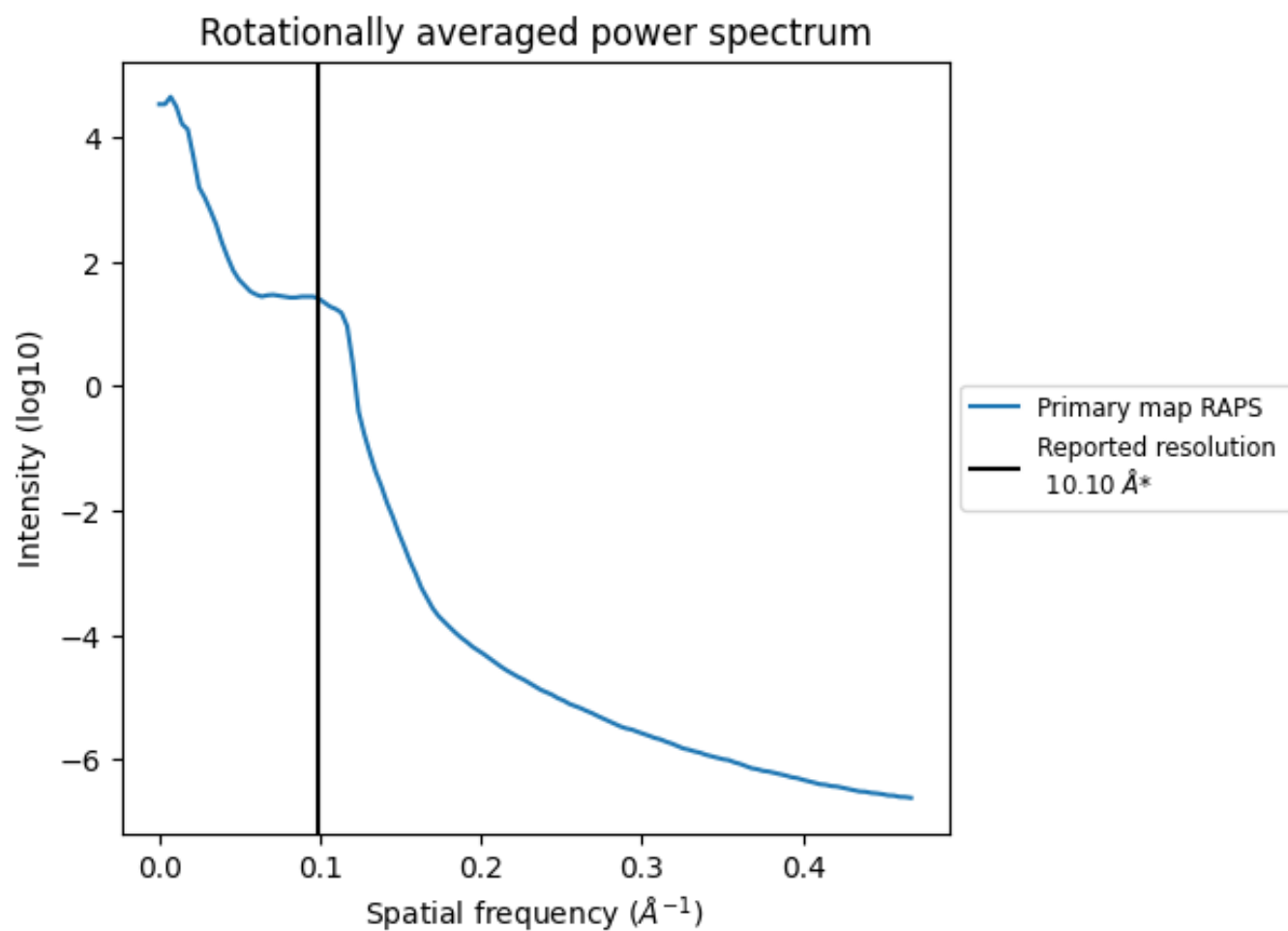
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm<sup>3</sup>; this corresponds to an approximate mass of 104 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.099 Å<sup>-1</sup>

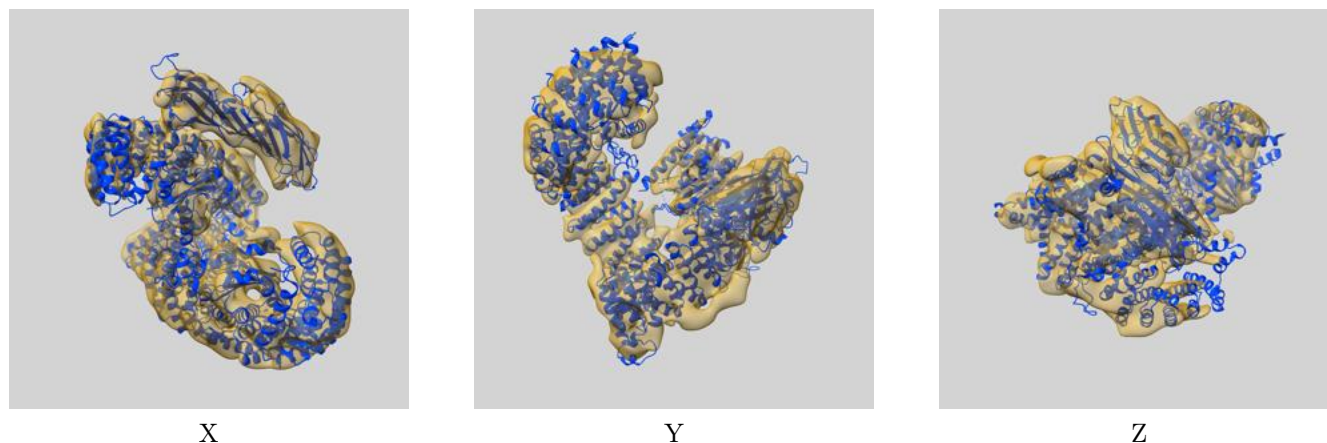
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

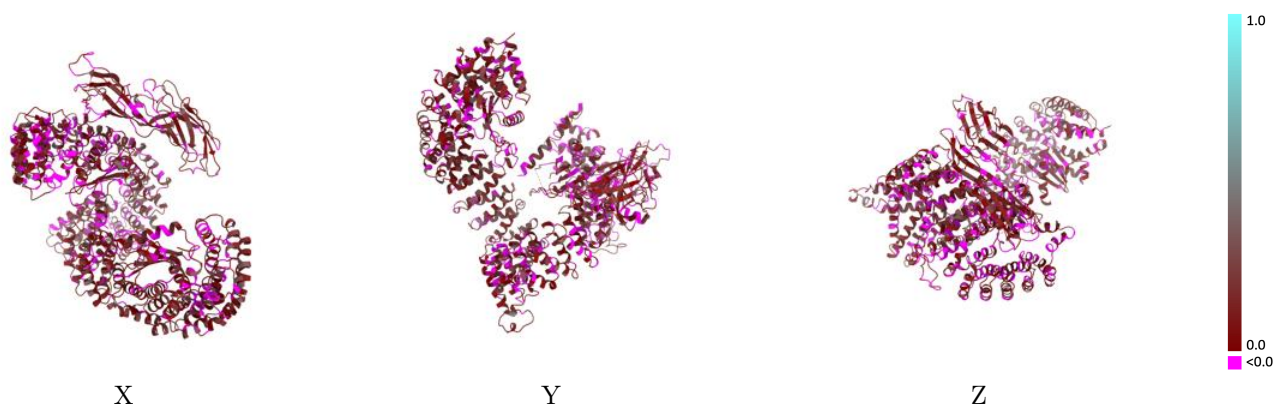
This section contains information regarding the fit between EMDB map EMD-13188 and PDB model 7P3Y. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



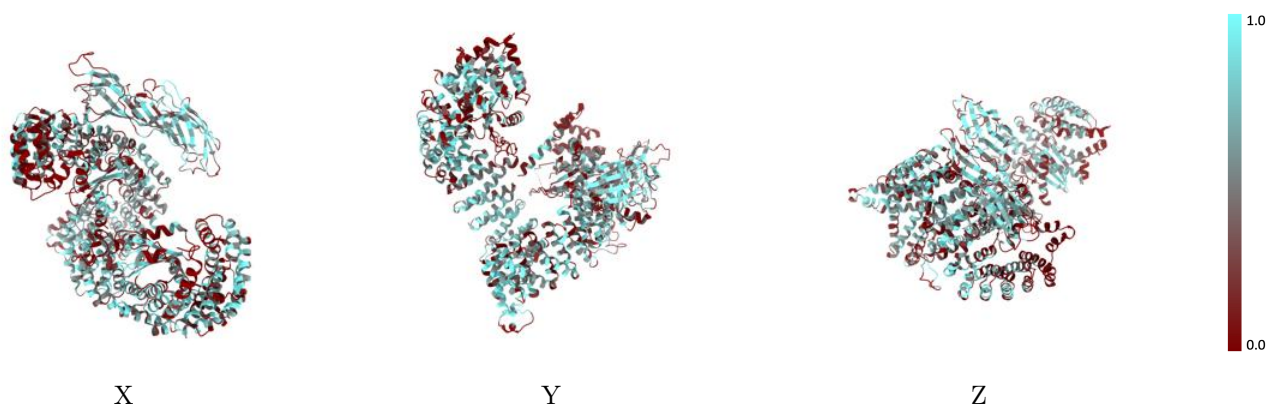
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



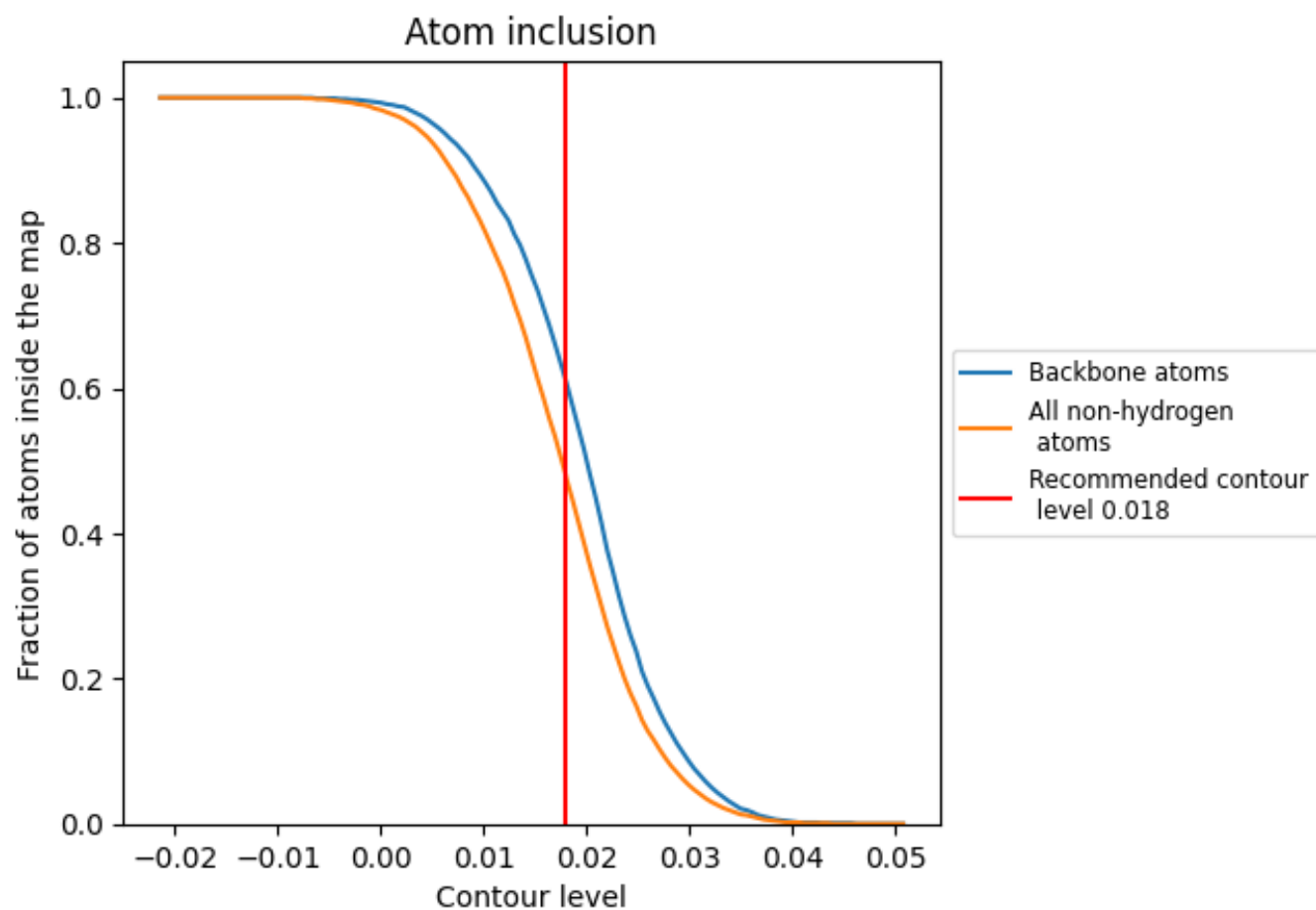
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.4800 | <div></div> 0.0930 |
| A     | <div></div> 0.5230 | <div></div> 0.1180 |
| B     | <div></div> 0.4750 | <div></div> 0.0770 |
| M     | <div></div> 0.4780 | <div></div> 0.0870 |
| S     | <div></div> 0.3550 | <div></div> 0.0780 |

