



## Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 06:47 PM UTC

PDB ID : 1O1B / pdb\_00001o1b  
EMDB ID : EMD-1001  
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM  
TOMOGRAMS OF INSECT FLIGHT MUSCLE  
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.  
Deposited on : 2002-11-15  
Resolution : 70.00 Å (reported)  
Based on initial models : 2MYS, 1ATN

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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

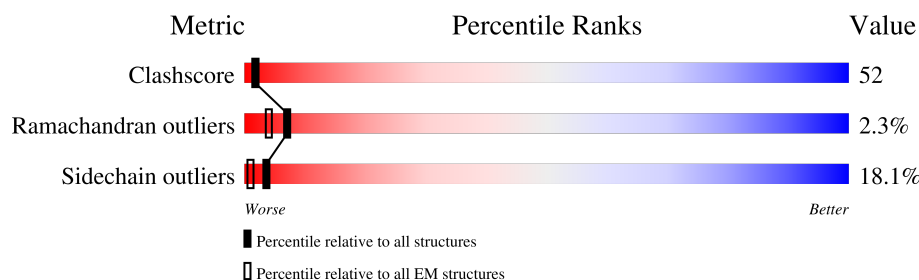
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 70.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 229148                   | 23984                    |
| Ramachandran outliers | 224038                   | 23583                    |
| Sidechain outliers    | 223484                   | 23102                    |

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     | 840    | <div> <div>100%</div> <div>25% 49% 22% .</div> </div> |
| 1   | D     | 840    | <div> <div>100%</div> <div>25% 49% 23% .</div> </div> |
| 1   | G     | 840    | <div> <div>100%</div> <div>24% 49% 22% .</div> </div> |
| 1   | J     | 840    | <div> <div>99%</div> <div>24% 49% 23% .</div> </div>  |
| 2   | B     | 145    | <div> <div>100%</div> <div>66% 25% 7% .</div> </div>  |
| 2   | E     | 145    | <div> <div>100%</div> <div>63% 28% 6% .</div> </div>  |
| 2   | H     | 145    | <div> <div>100%</div> <div>62% 29% 6% .</div> </div>  |
| 2   | K     | 145    | <div> <div>92%</div> <div>64% 26% 7% .</div> </div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 147    |                  |
| 3   | F     | 147    |                  |
| 3   | I     | 147    |                  |
| 3   | L     | 147    |                  |
| 4   | 0     | 375    |                  |
| 4   | 1     | 375    |                  |
| 4   | 2     | 375    |                  |
| 4   | 3     | 375    |                  |
| 4   | 4     | 375    |                  |
| 4   | 5     | 375    |                  |
| 4   | 7     | 375    |                  |
| 4   | 8     | 375    |                  |
| 4   | 9     | 375    |                  |
| 4   | V     | 375    |                  |
| 4   | W     | 375    |                  |
| 4   | X     | 375    |                  |
| 4   | Y     | 375    |                  |
| 4   | Z     | 375    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1   | MLY  | A     | 505 | -         | -        | X       | -                |
| 1   | MLY  | A     | 553 | -         | -        | X       | -                |
| 1   | MLY  | A     | 764 | -         | -        | X       | -                |
| 1   | MLY  | A     | 768 | -         | -        | X       | -                |
| 1   | MLY  | A     | 839 | -         | -        | X       | -                |
| 1   | MLY  | D     | 553 | -         | -        | X       | -                |
| 1   | MLY  | D     | 768 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1   | MLY  | D     | 782 | -         | -        | X       | -                |
| 1   | MLY  | D     | 839 | -         | -        | X       | -                |
| 1   | MLY  | G     | 553 | -         | -        | X       | -                |
| 1   | MLY  | G     | 764 | -         | -        | X       | -                |
| 1   | MLY  | G     | 768 | -         | -        | X       | -                |
| 1   | MLY  | G     | 84  | -         | -        | X       | -                |
| 1   | MLY  | J     | 553 | -         | -        | X       | -                |
| 1   | MLY  | J     | 764 | -         | -        | X       | -                |
| 1   | MLY  | J     | 768 | -         | -        | X       | -                |
| 1   | MLY  | J     | 84  | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 76872 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 SKELETAL MUSCLE MYOSIN II.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | D     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | G     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | J     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | E     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | H     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | K     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | F     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | I     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | L     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |

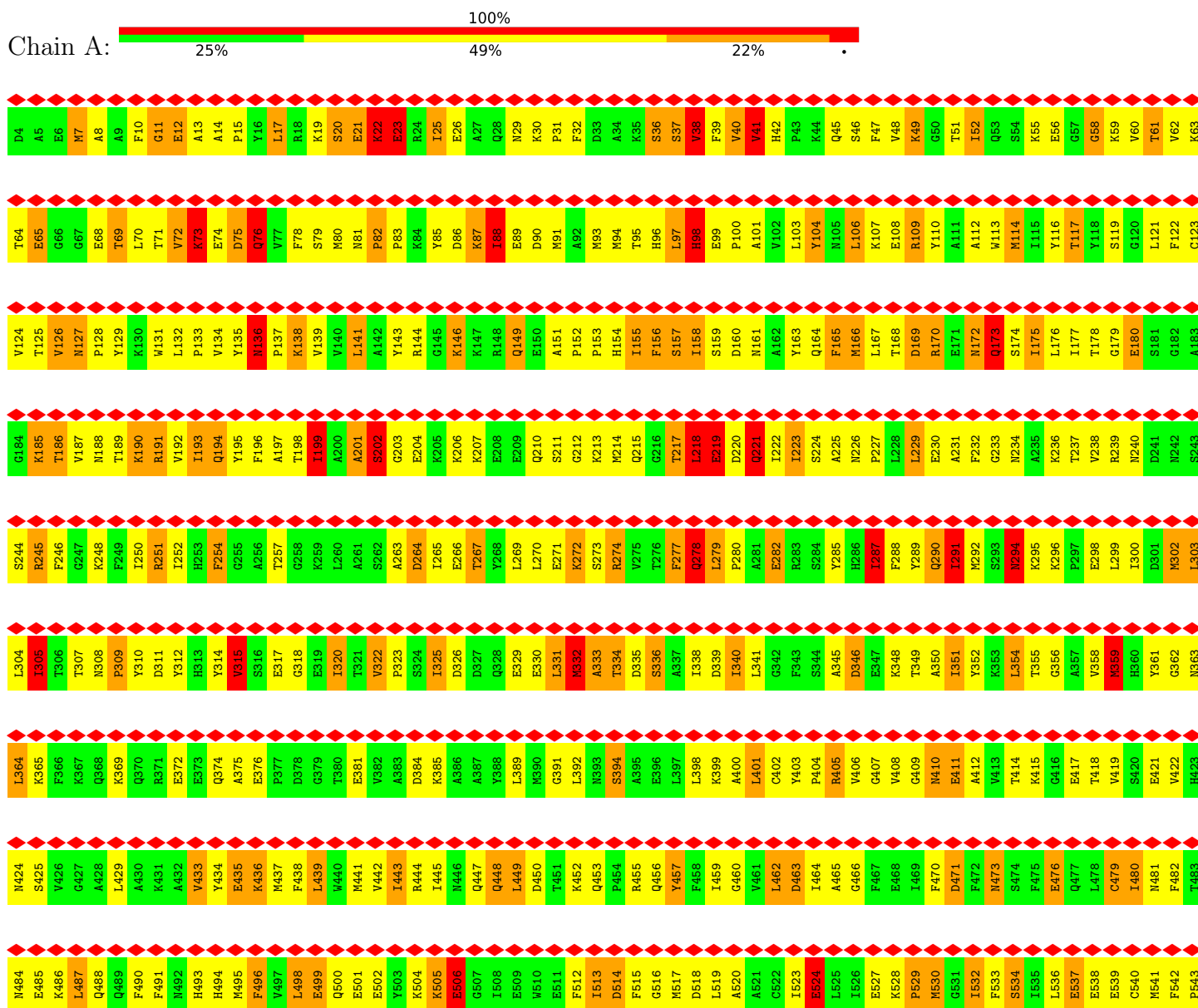
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

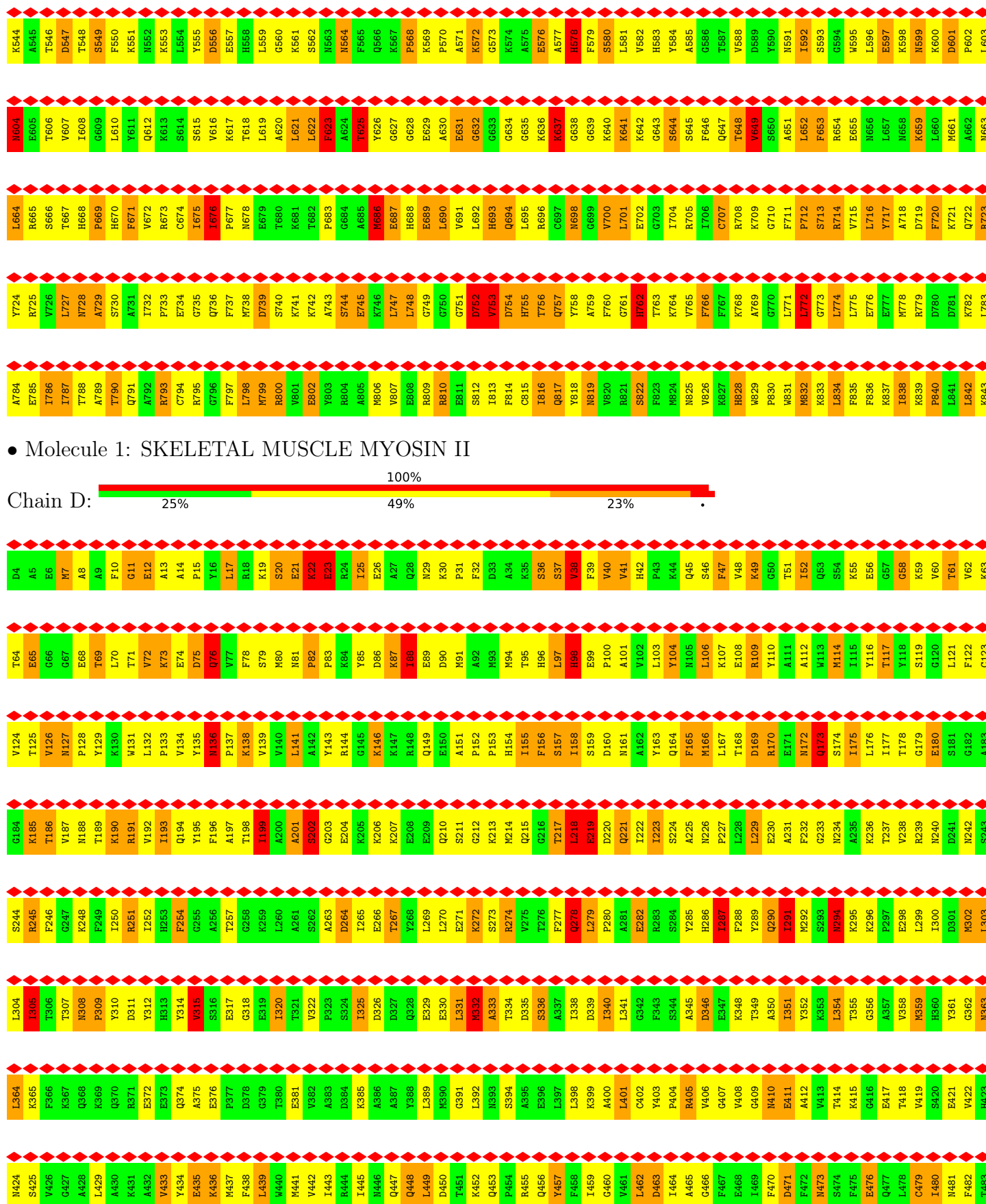
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 0     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 1     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 2     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 3     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 4     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 5     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 7     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 8     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 9     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | V     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | W     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | X     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | Y     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | Z     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |

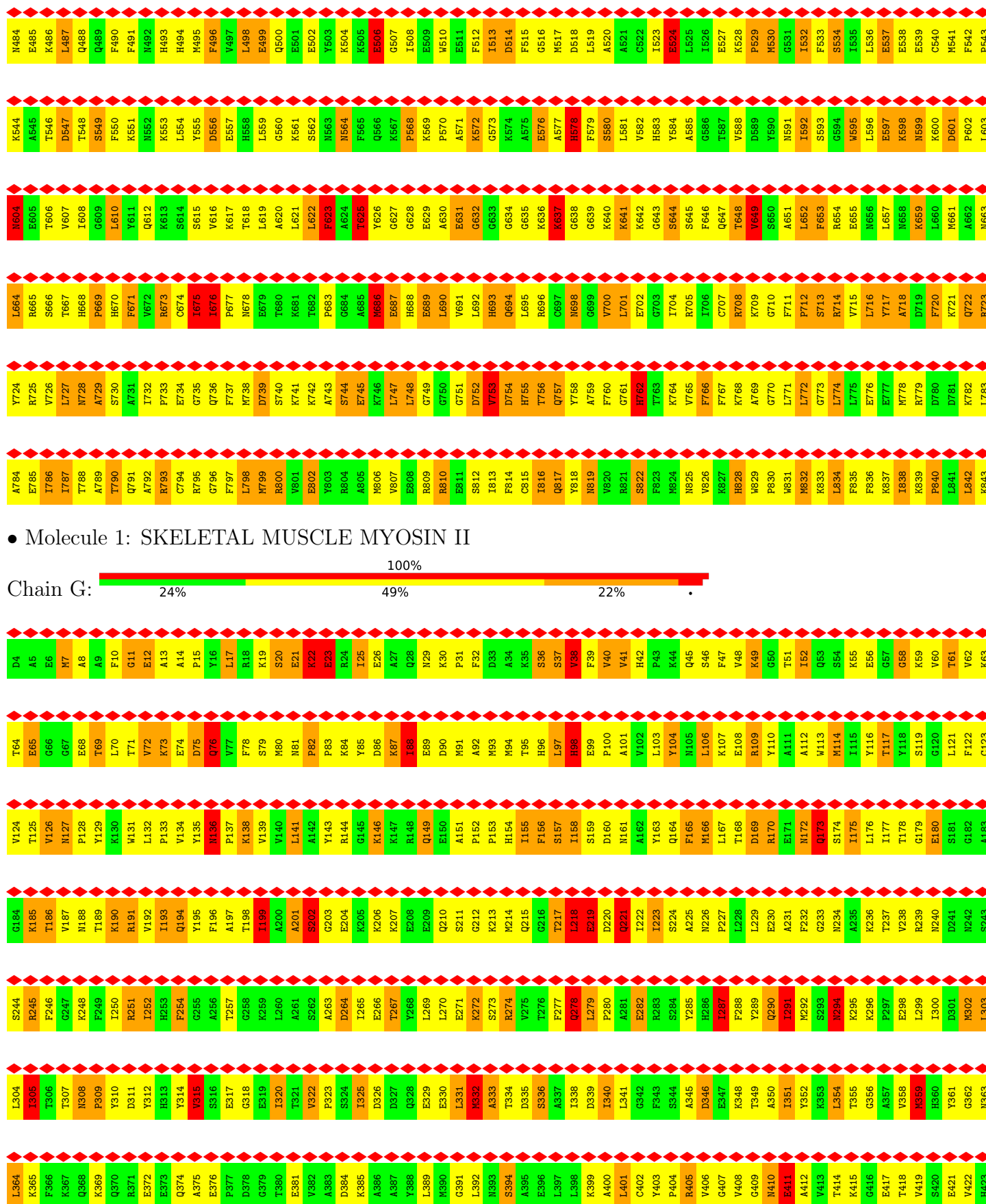
### 3 Residue-property plots

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.

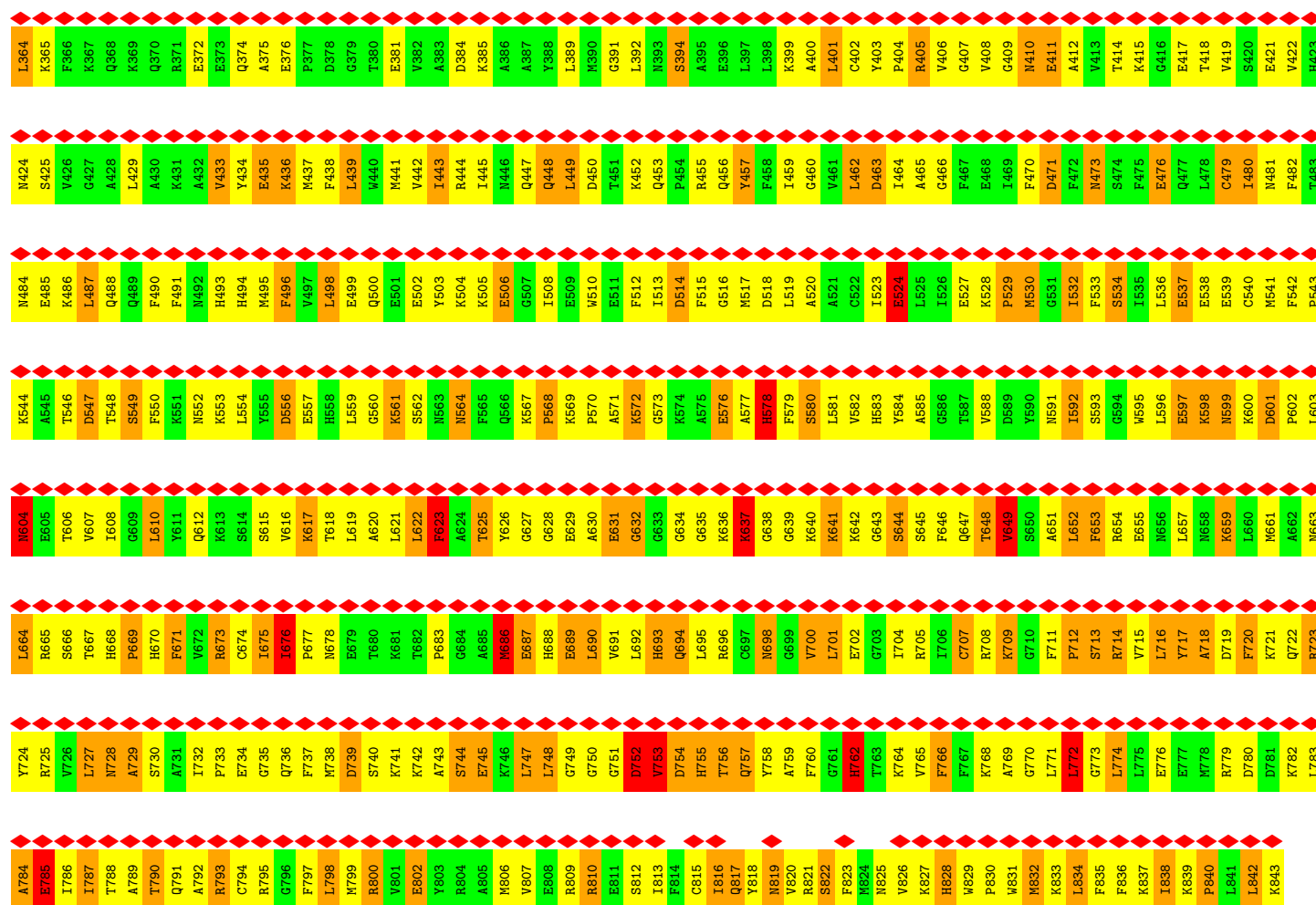
#### • Molecule 1: SKELETAL MUSCLE MYOSIN II



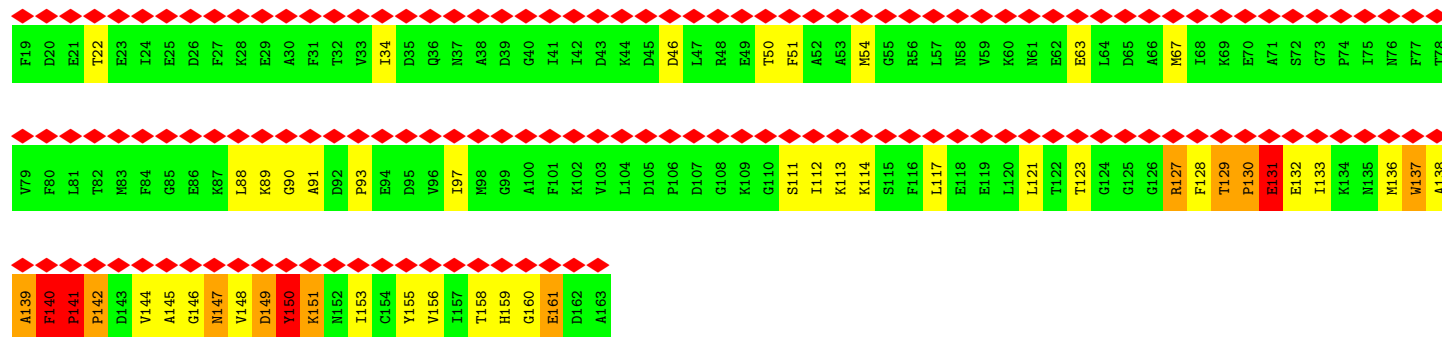






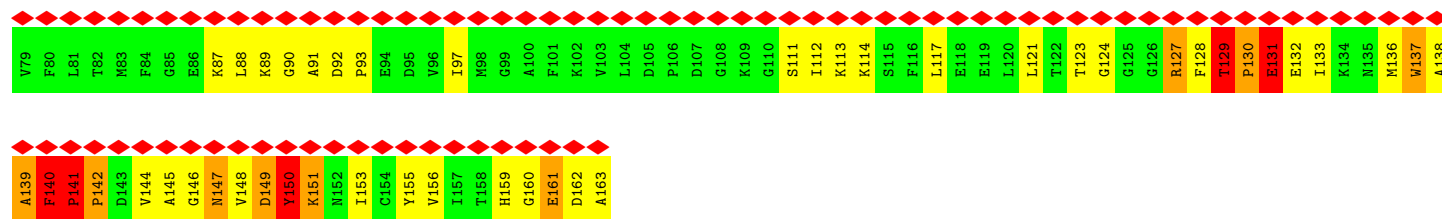


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

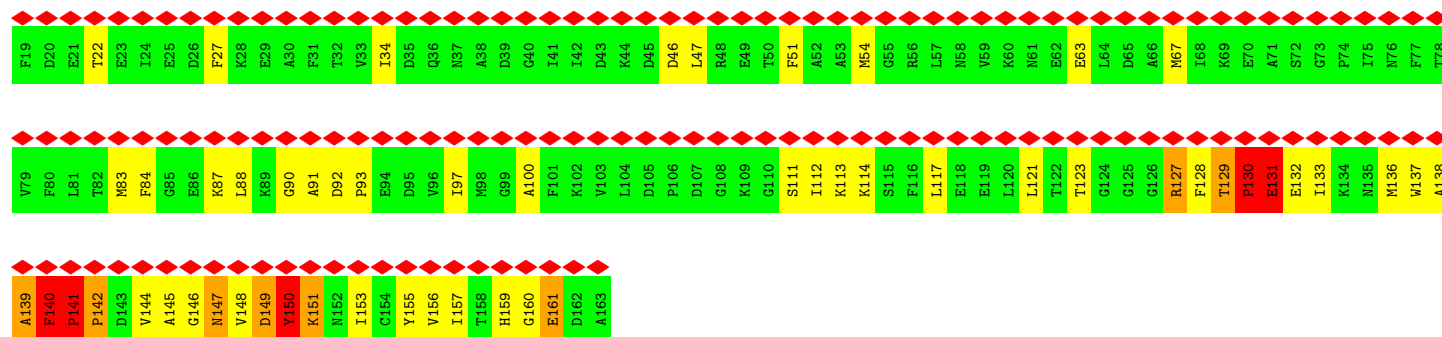


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN





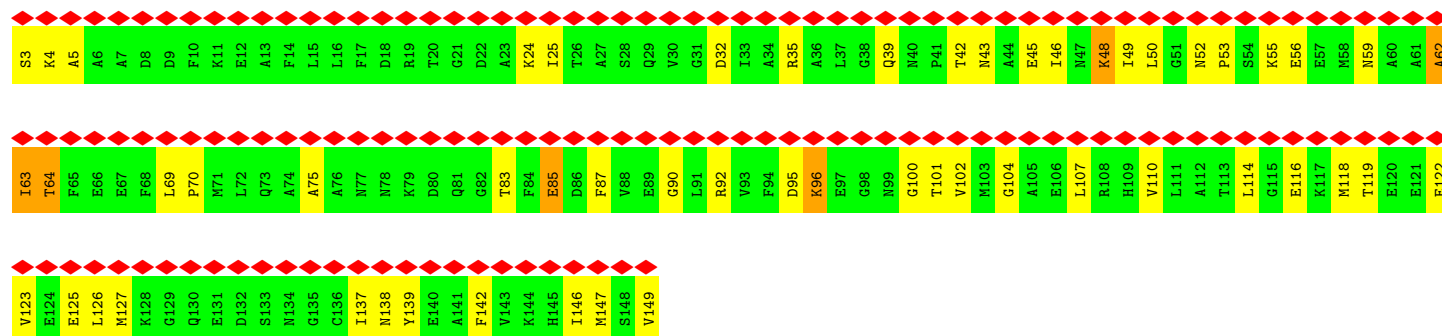
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



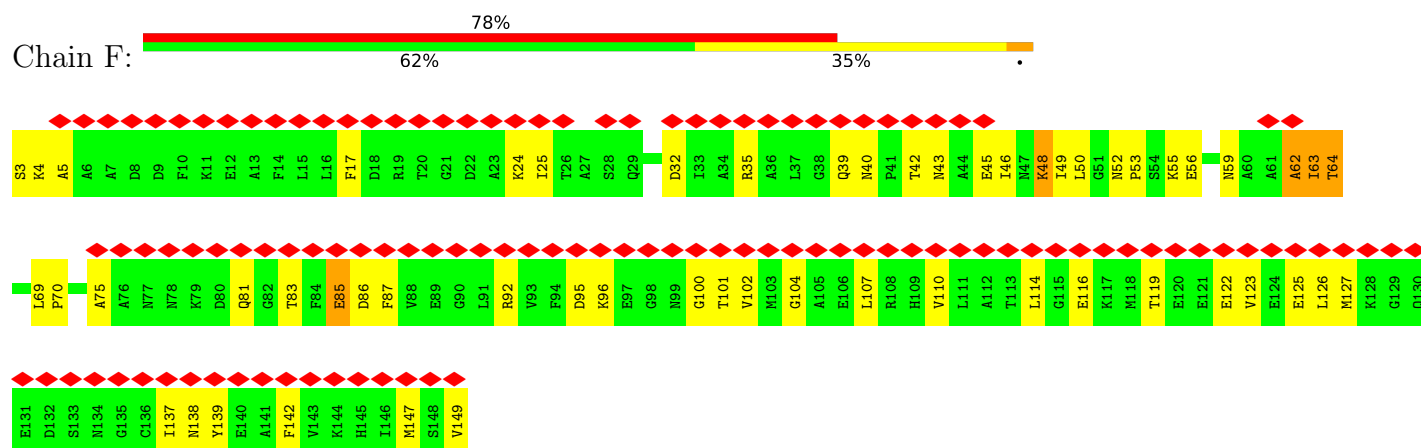
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



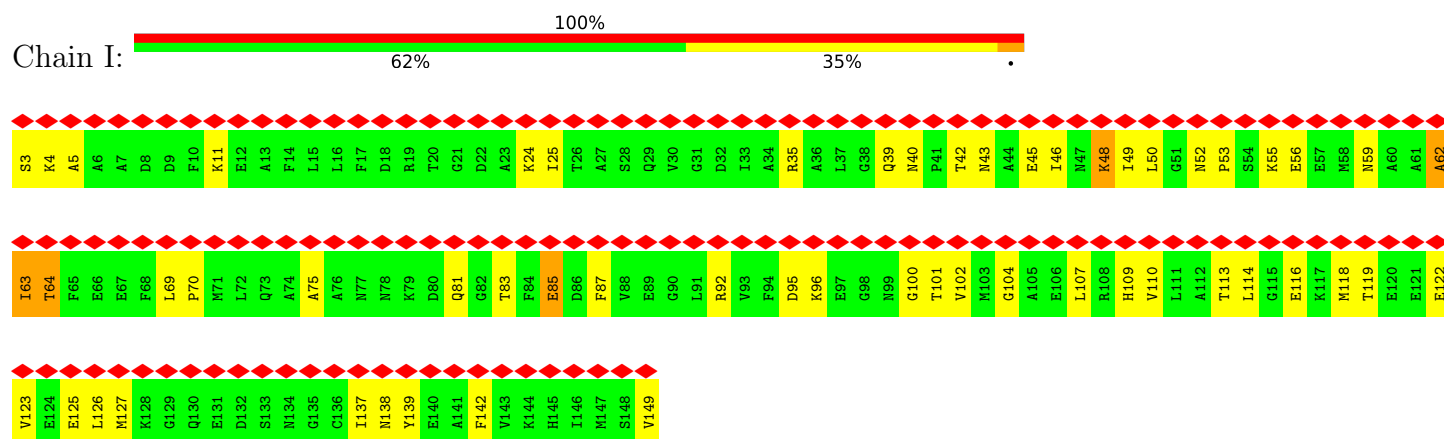
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



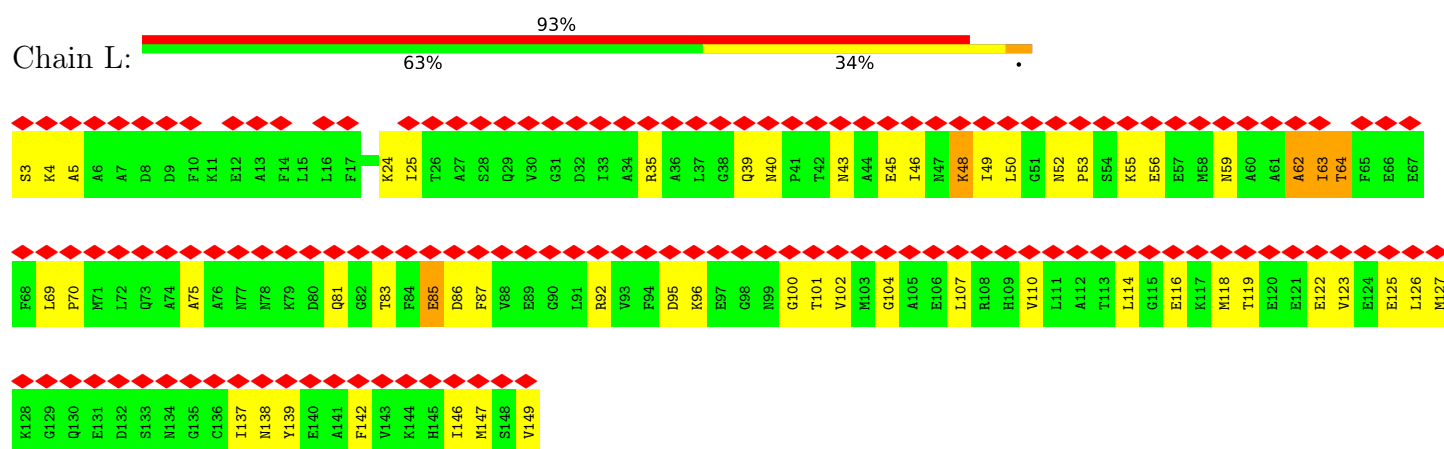
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



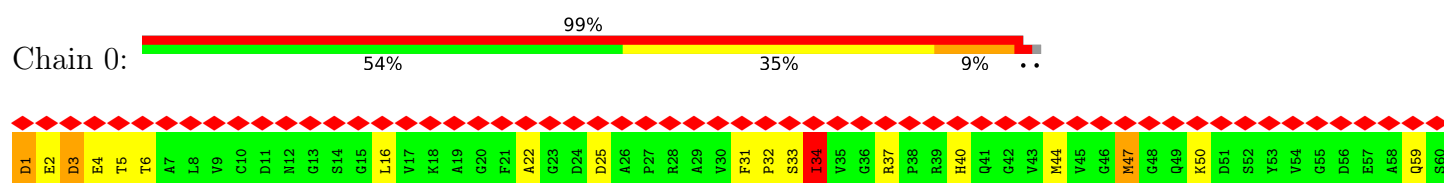
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

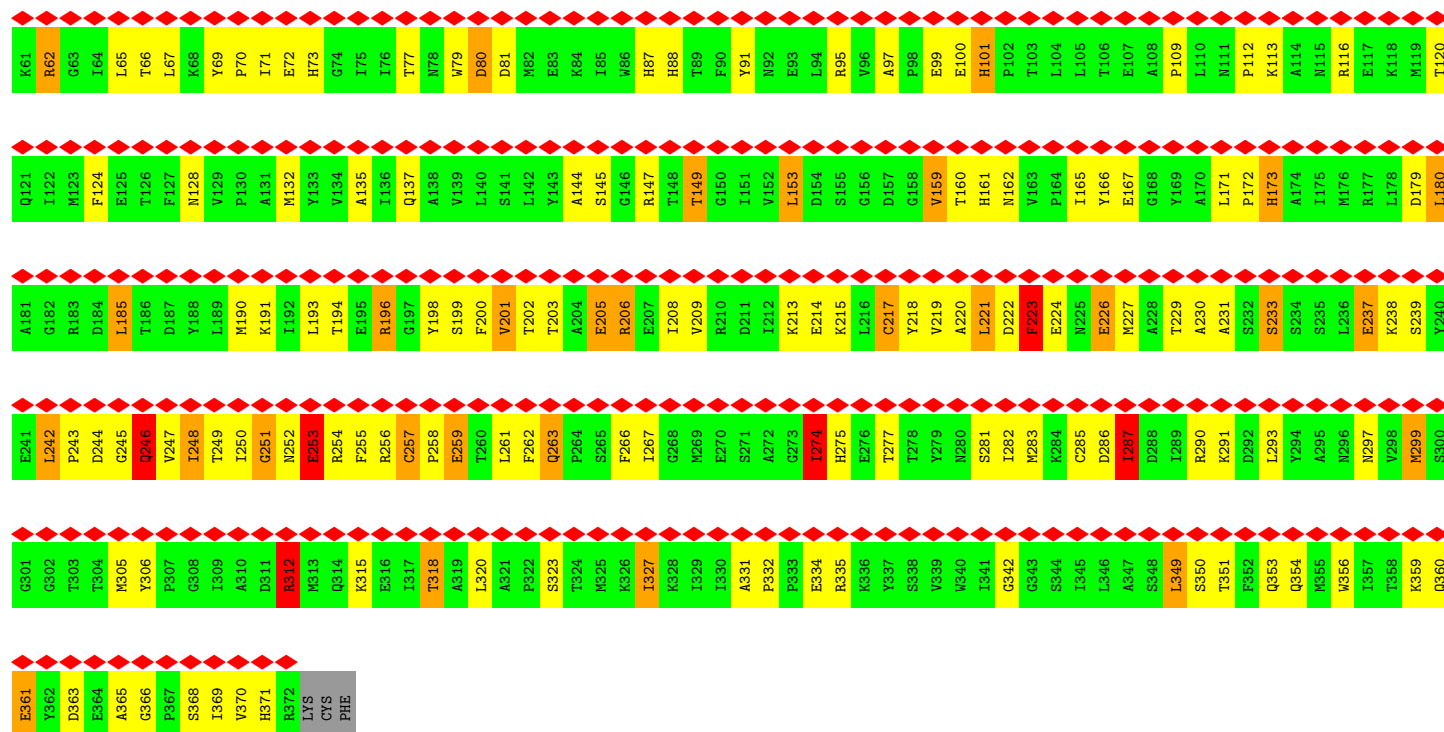


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

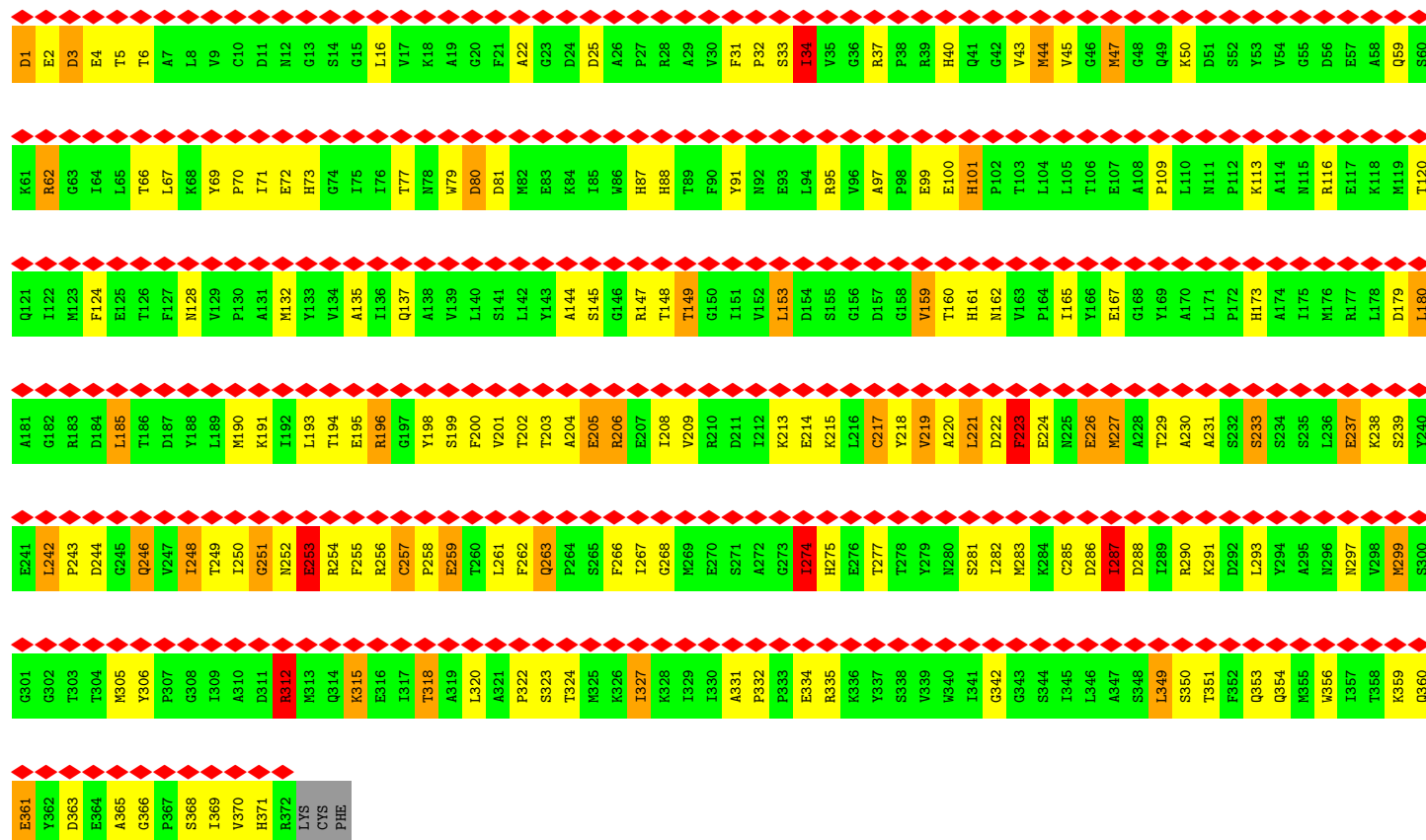


- Molecule 4: SKELETAL MUSCLE ACTIN





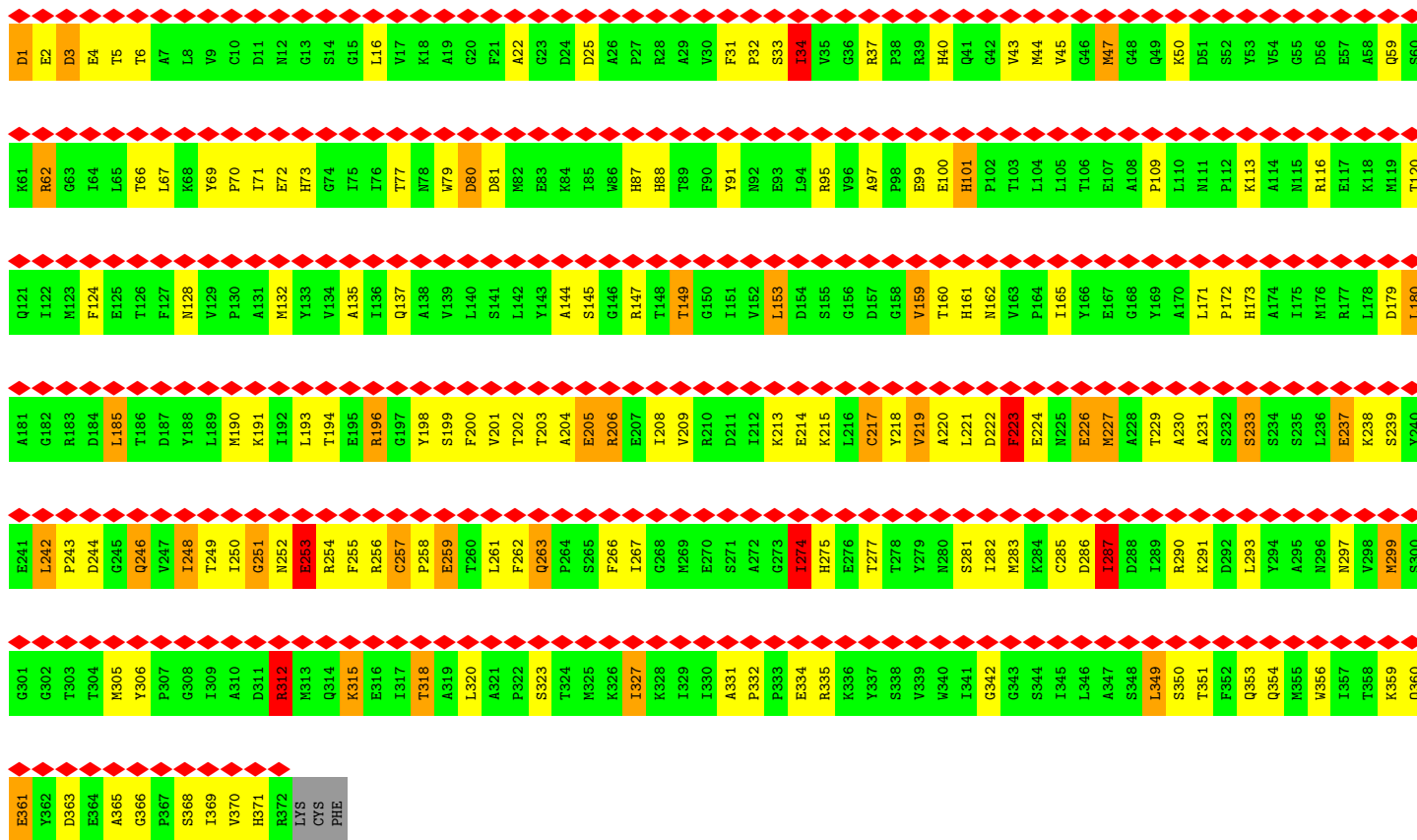
• Molecule 4: SKELETAL MUSCLE ACTIN



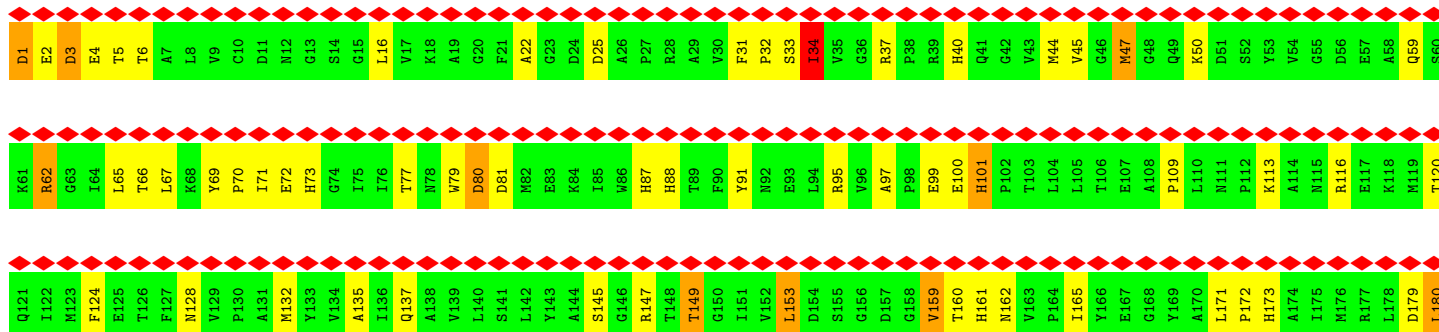


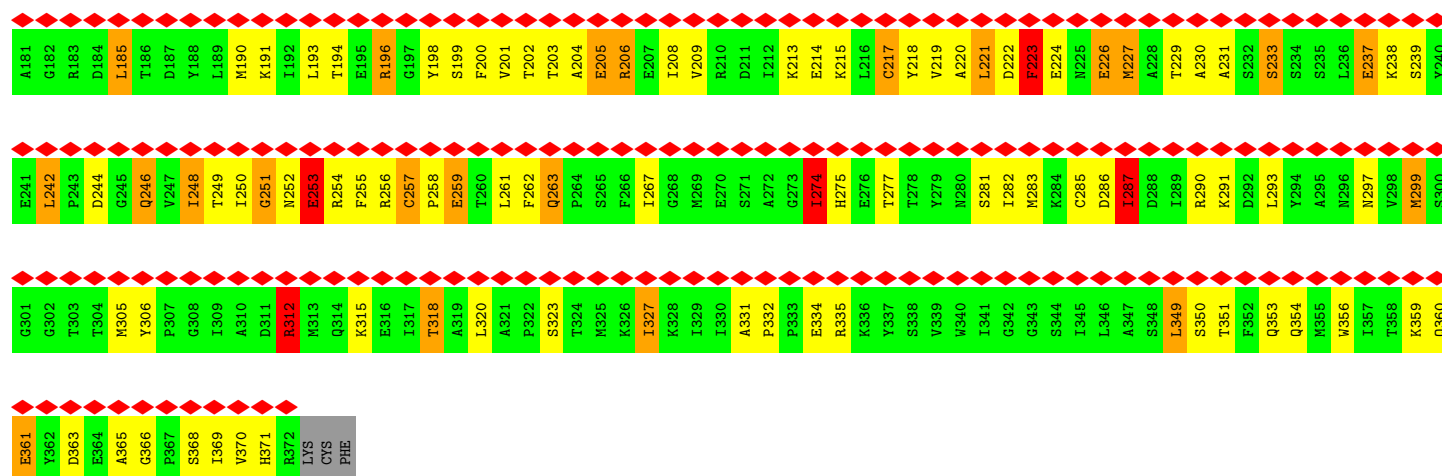


• Molecule 4: SKELETAL MUSCLE ACTIN

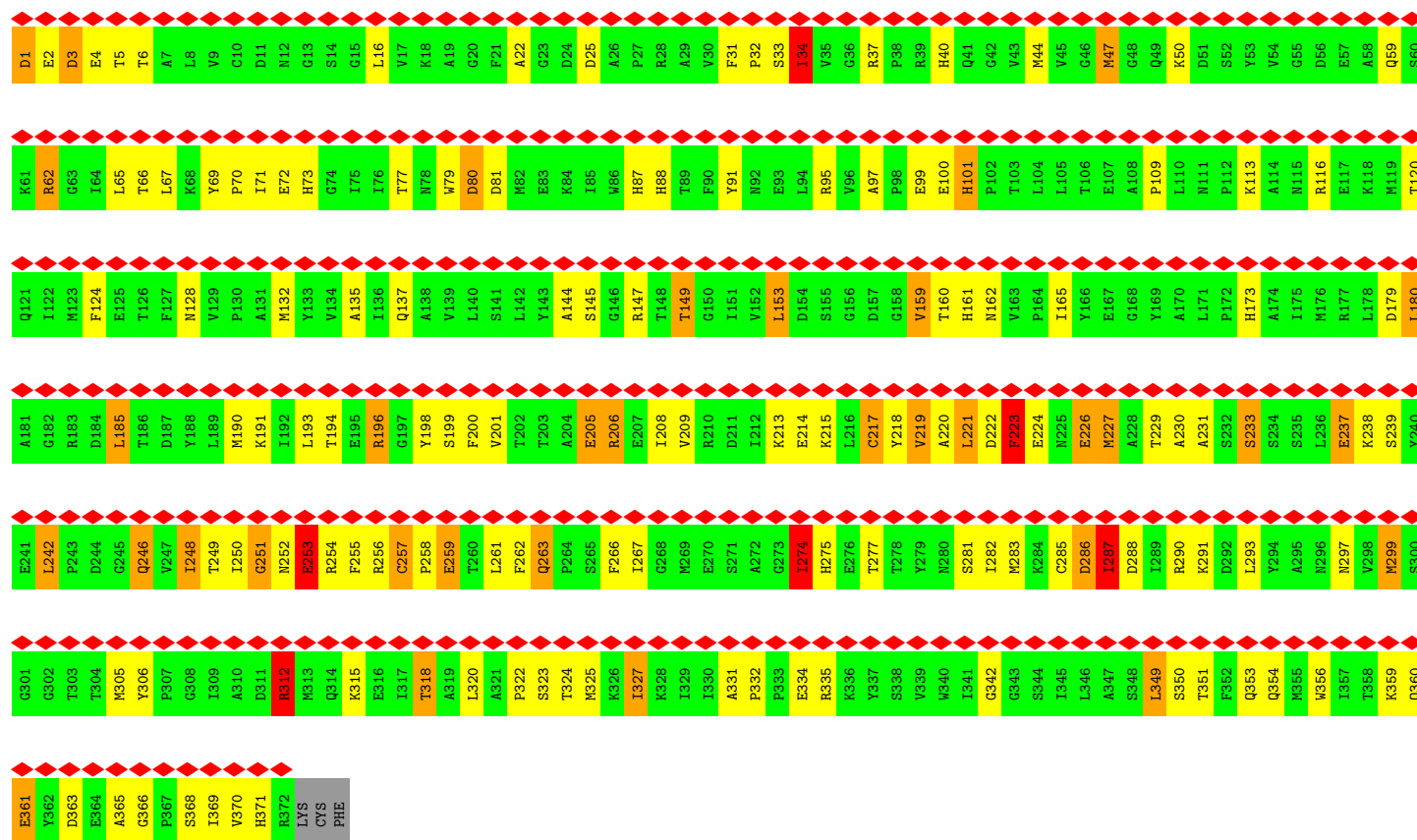


• Molecule 4: SKELETAL MUSCLE ACTIN

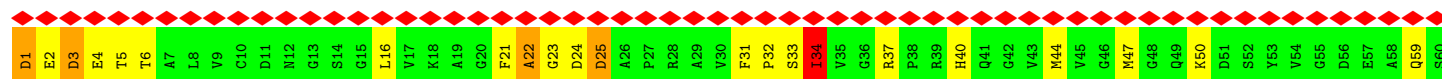


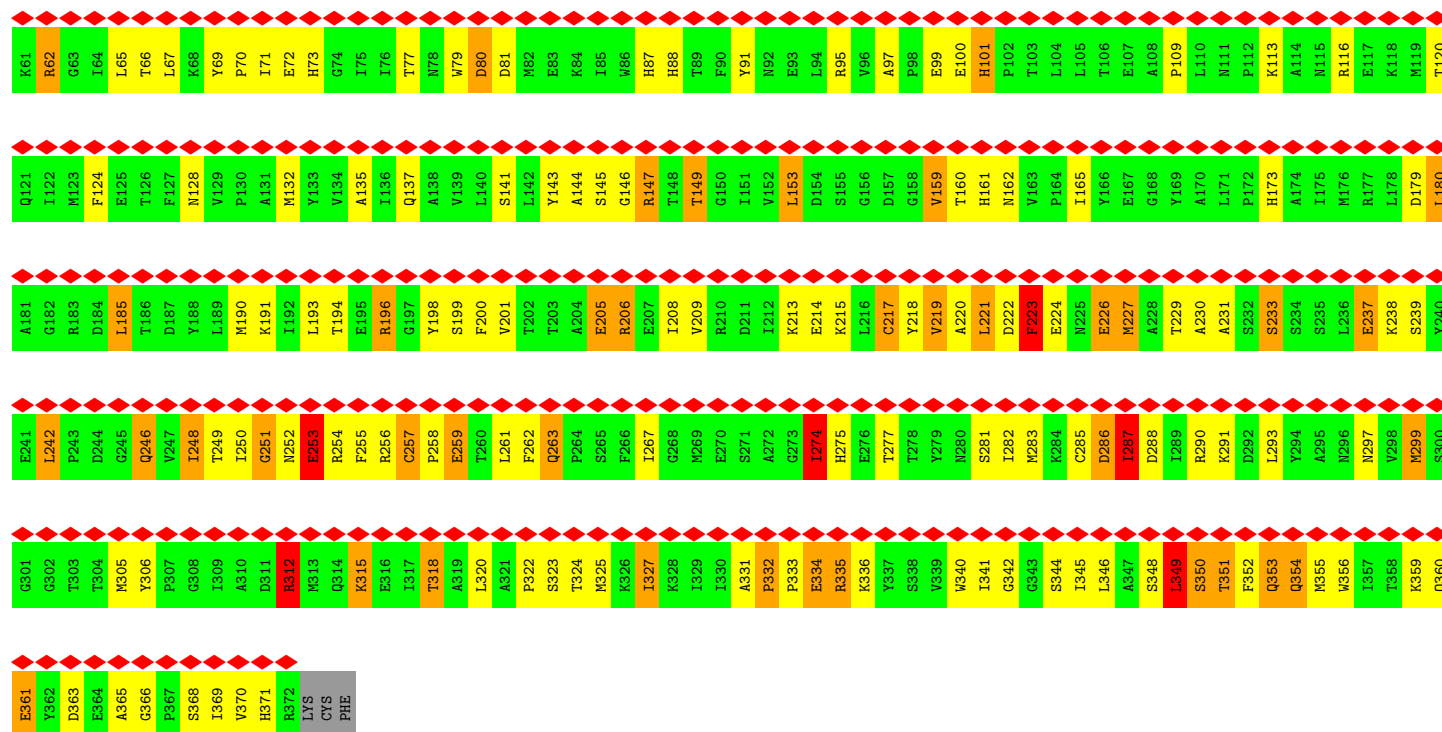


• Molecule 4: SKELETAL MUSCLE ACTIN

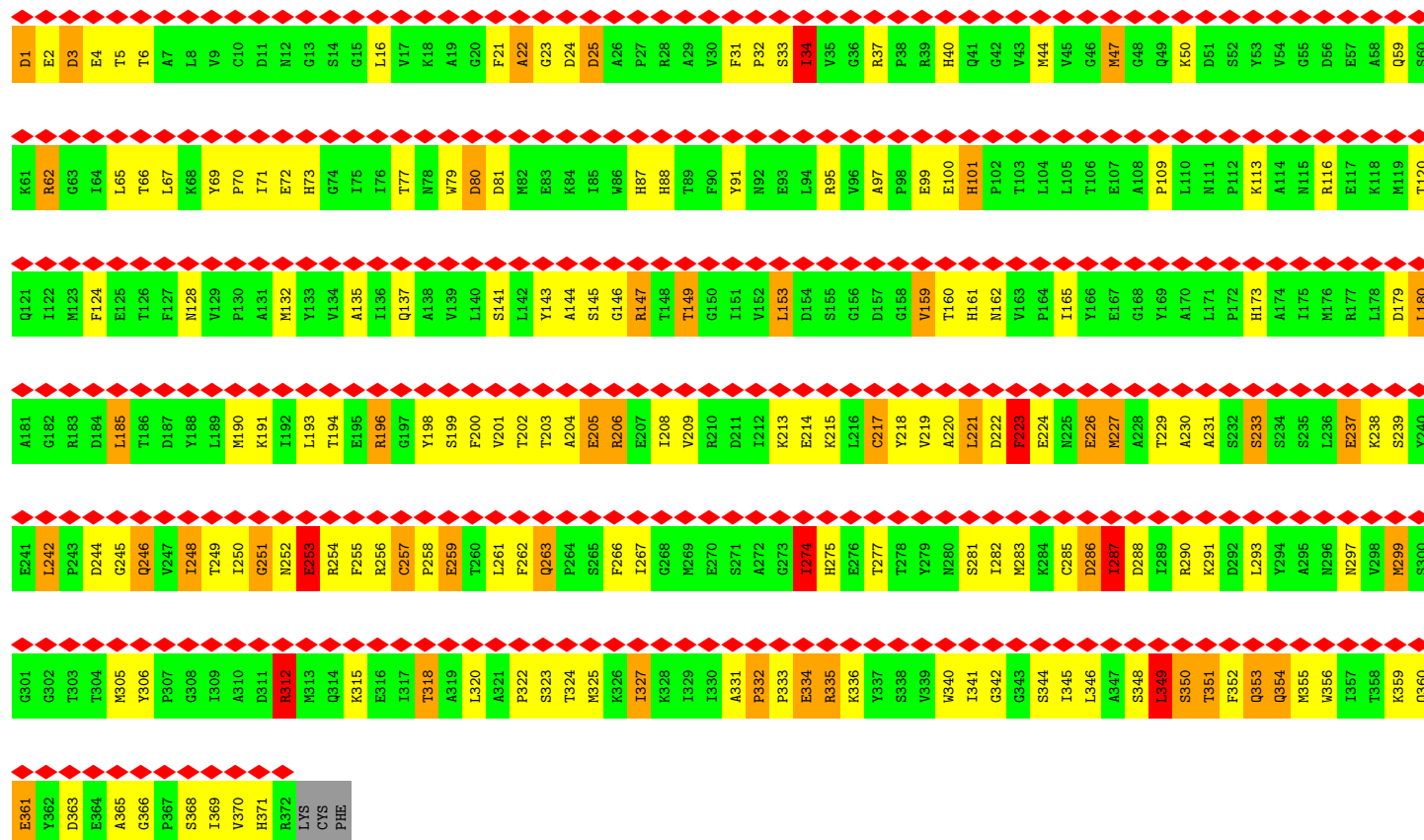


• Molecule 4: SKELETAL MUSCLE ACTIN

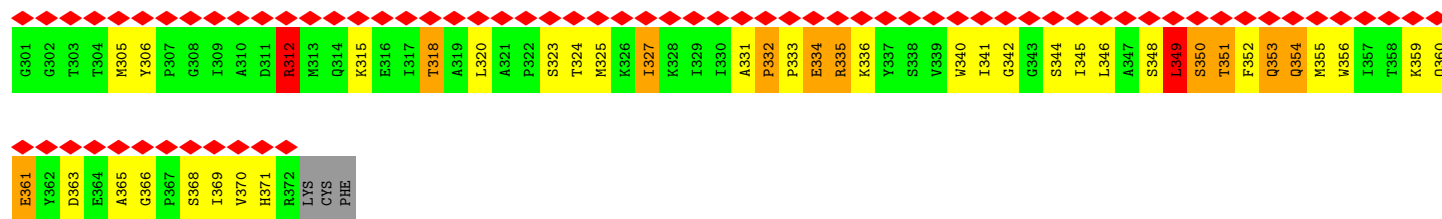




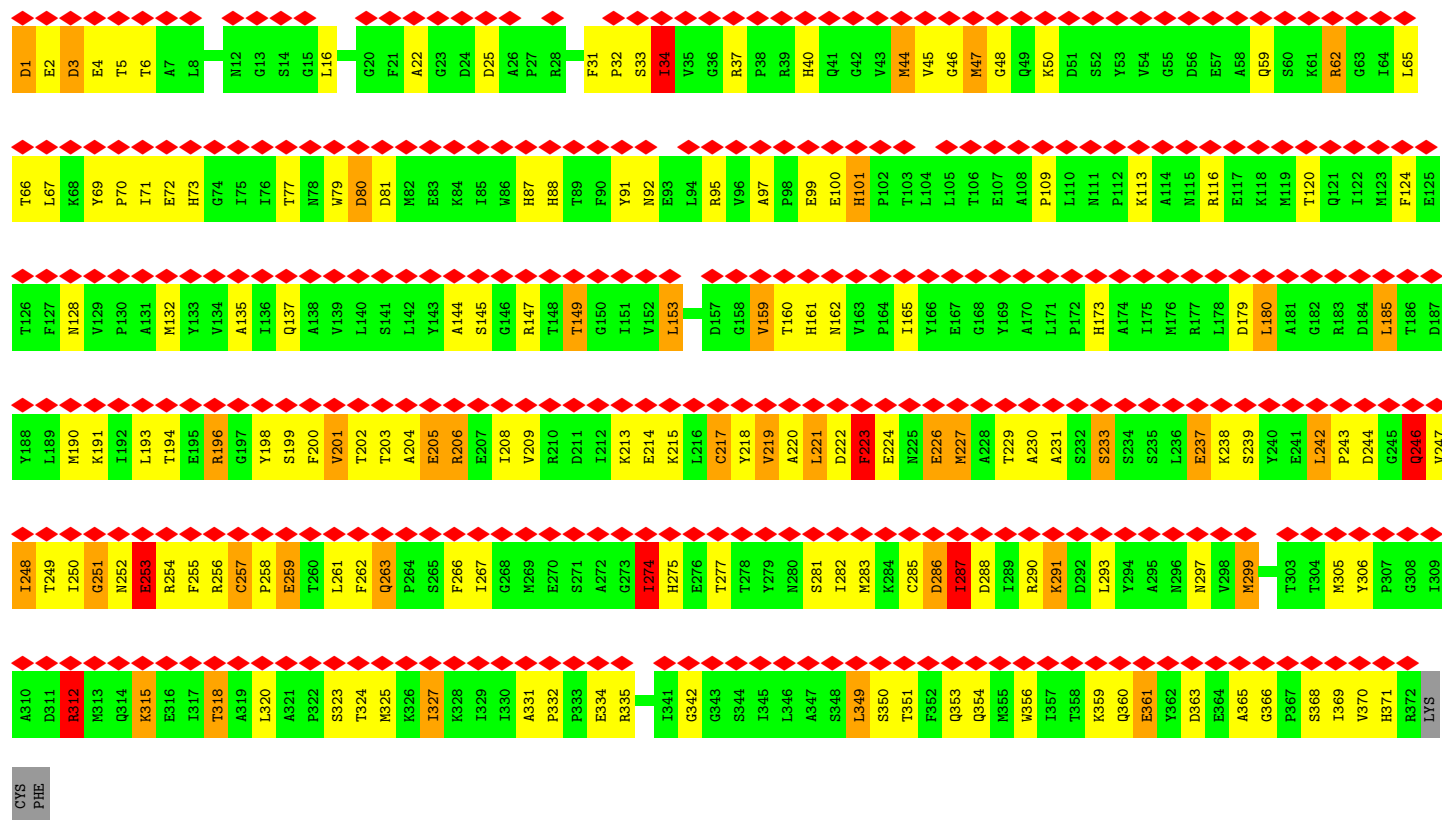
• Molecule 4: SKELETAL MUSCLE ACTIN



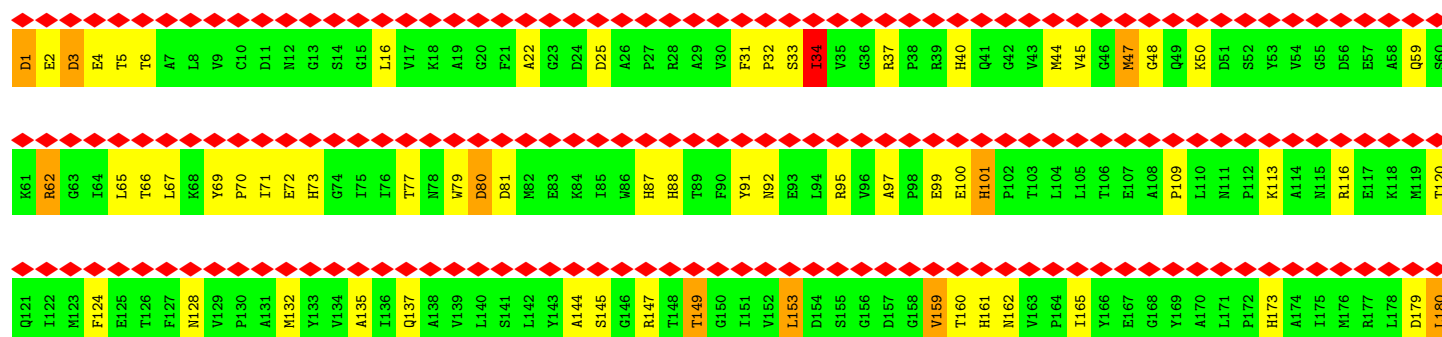




## • Molecule 4: SKELETAL MUSCLE ACTIN



## • Molecule 4: SKELETAL MUSCLE ACTIN





## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | TOMOGRAPHY                | Depositor |
| Imposed symmetry                     | POINT, C1                 | Depositor |
| Number of tilted images used         | Not provided              |           |
| Resolution determination method      | Not provided              |           |
| CTF correction method                | Not provided              |           |
| Microscope                           | FEI/PHILIPS EM400         | Depositor |
| Voltage (kV)                         | 100                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided              |           |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | 17000                     | Depositor |
| Image detector                       | KODAK SO-163 FILM         | Depositor |
| Maximum voxel value                  | 366.680                   | Depositor |
| Minimum voxel value                  | -417.992                  | Depositor |
| Average voxel value                  | 1.860                     | Depositor |
| Voxel value standard deviation       | 47.792                    | Depositor |
| Recommended contour level            | 81.2                      | Depositor |
| Tomogram size ( $\text{\AA}$ )       | 9280, 9280, 464           | wwPDB     |
| Tomogram dimensions                  | 600, 600, 30              | wwPDB     |
| Tomogram angles ( $^\circ$ )         | 90, 90, 90                | wwPDB     |
| Grid spacing ( $\text{\AA}$ )        | 15.4667, 15.4667, 15.4667 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$        |
| 1   | A     | 1.85         | 44/6448 (0.7%)   | 2.12        | 152/8729 (1.7%)    |
| 1   | D     | 1.85         | 39/6448 (0.6%)   | 2.13        | 151/8729 (1.7%)    |
| 1   | G     | 1.86         | 41/6448 (0.6%)   | 2.13        | 156/8729 (1.8%)    |
| 1   | J     | 2.05         | 44/6449 (0.7%)   | 2.16        | 149/8732 (1.7%)    |
| 2   | B     | 1.38         | 16/1148 (1.4%)   | 1.47        | 21/1548 (1.4%)     |
| 2   | E     | 1.37         | 16/1148 (1.4%)   | 1.47        | 21/1548 (1.4%)     |
| 2   | H     | 1.37         | 16/1148 (1.4%)   | 1.47        | 21/1548 (1.4%)     |
| 2   | K     | 1.37         | 15/1148 (1.3%)   | 1.47        | 21/1548 (1.4%)     |
| 3   | C     | 0.88         | 4/1136 (0.4%)    | 1.18        | 6/1525 (0.4%)      |
| 3   | F     | 0.88         | 4/1136 (0.4%)    | 1.18        | 6/1525 (0.4%)      |
| 3   | I     | 0.88         | 4/1136 (0.4%)    | 1.18        | 5/1525 (0.3%)      |
| 3   | L     | 0.87         | 4/1136 (0.4%)    | 1.18        | 5/1525 (0.3%)      |
| 4   | 0     | 1.17         | 12/2968 (0.4%)   | 2.00        | 96/4023 (2.4%)     |
| 4   | 1     | 1.17         | 13/2968 (0.4%)   | 2.00        | 101/4023 (2.5%)    |
| 4   | 2     | 1.17         | 13/2968 (0.4%)   | 2.00        | 98/4023 (2.4%)     |
| 4   | 3     | 1.17         | 13/2968 (0.4%)   | 2.00        | 98/4023 (2.4%)     |
| 4   | 4     | 1.17         | 13/2968 (0.4%)   | 2.00        | 100/4023 (2.5%)    |
| 4   | 5     | 1.17         | 13/2968 (0.4%)   | 2.00        | 98/4023 (2.4%)     |
| 4   | 7     | 1.17         | 13/2968 (0.4%)   | 2.00        | 99/4023 (2.5%)     |
| 4   | 8     | 1.17         | 12/2968 (0.4%)   | 2.00        | 97/4023 (2.4%)     |
| 4   | 9     | 1.17         | 12/2968 (0.4%)   | 2.00        | 98/4023 (2.4%)     |
| 4   | V     | 1.17         | 12/2968 (0.4%)   | 2.00        | 98/4023 (2.4%)     |
| 4   | W     | 1.17         | 13/2968 (0.4%)   | 2.00        | 98/4023 (2.4%)     |
| 4   | X     | 1.17         | 13/2968 (0.4%)   | 2.00        | 98/4023 (2.4%)     |
| 4   | Y     | 1.17         | 13/2968 (0.4%)   | 2.00        | 99/4023 (2.5%)     |
| 4   | Z     | 1.17         | 13/2968 (0.4%)   | 2.00        | 99/4023 (2.5%)     |
| All | All   | 1.46         | 425/76481 (0.6%) | 1.98        | 2091/103533 (2.0%) |

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     | 1                   | 4                   |
| 1   | D     | 1                   | 4                   |
| 1   | G     | 1                   | 4                   |
| 1   | J     | 1                   | 6                   |
| 2   | B     | 0                   | 3                   |
| 2   | E     | 0                   | 3                   |
| 2   | H     | 0                   | 3                   |
| 2   | K     | 0                   | 3                   |
| 3   | C     | 0                   | 2                   |
| 3   | F     | 0                   | 2                   |
| 3   | I     | 0                   | 2                   |
| 3   | L     | 0                   | 2                   |
| 4   | 0     | 0                   | 1                   |
| 4   | 1     | 0                   | 1                   |
| 4   | 2     | 0                   | 1                   |
| 4   | 3     | 0                   | 1                   |
| 4   | 4     | 0                   | 1                   |
| 4   | 5     | 0                   | 1                   |
| 4   | 7     | 0                   | 1                   |
| 4   | 8     | 0                   | 1                   |
| 4   | 9     | 0                   | 1                   |
| 4   | V     | 0                   | 1                   |
| 4   | W     | 0                   | 1                   |
| 4   | X     | 0                   | 1                   |
| 4   | Y     | 0                   | 1                   |
| 4   | Z     | 0                   | 1                   |
| All | All   | 4                   | 52                  |

All (425) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | J     | 709 | LYS  | C-N    | -68.49 | 0.33        | 1.33     |
| 1   | A     | 648 | THR  | CB-OG1 | 42.59  | 2.11        | 1.43     |
| 1   | G     | 648 | THR  | CB-OG1 | 42.57  | 2.11        | 1.43     |
| 1   | J     | 648 | THR  | CB-OG1 | 42.55  | 2.11        | 1.43     |
| 1   | D     | 648 | THR  | CB-OG1 | 42.53  | 2.11        | 1.43     |
| 1   | D     | 623 | PHE  | CB-CG  | 35.89  | 2.33        | 1.50     |
| 1   | J     | 623 | PHE  | CB-CG  | 35.88  | 2.33        | 1.50     |
| 1   | A     | 623 | PHE  | CB-CG  | 35.85  | 2.33        | 1.50     |
| 1   | G     | 623 | PHE  | CB-CG  | 35.80  | 2.33        | 1.50     |
| 1   | G     | 649 | VAL  | CB-CG1 | 33.96  | 2.64        | 1.52     |
| 1   | J     | 649 | VAL  | CB-CG1 | 33.96  | 2.64        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | D     | 649 | VAL  | CB-CG1 | 33.91  | 2.64        | 1.52     |
| 1   | A     | 649 | VAL  | CB-CG1 | 33.91  | 2.64        | 1.52     |
| 1   | J     | 648 | THR  | CB-CG2 | -30.76 | 0.51        | 1.52     |
| 1   | A     | 648 | THR  | CB-CG2 | -30.75 | 0.51        | 1.52     |
| 1   | D     | 648 | THR  | CB-CG2 | -30.72 | 0.51        | 1.52     |
| 1   | G     | 648 | THR  | CB-CG2 | -30.71 | 0.51        | 1.52     |
| 1   | A     | 649 | VAL  | CB-CG2 | 29.51  | 2.50        | 1.52     |
| 1   | G     | 649 | VAL  | CB-CG2 | 29.48  | 2.49        | 1.52     |
| 1   | J     | 649 | VAL  | CB-CG2 | 29.47  | 2.49        | 1.52     |
| 1   | D     | 649 | VAL  | CB-CG2 | 29.43  | 2.49        | 1.52     |
| 1   | A     | 649 | VAL  | C-N    | -21.99 | 1.02        | 1.33     |
| 1   | G     | 649 | VAL  | C-N    | -21.97 | 1.02        | 1.33     |
| 1   | D     | 649 | VAL  | C-N    | -21.87 | 1.03        | 1.33     |
| 1   | J     | 649 | VAL  | C-N    | -21.86 | 1.03        | 1.33     |
| 2   | E     | 140 | PHE  | C-N    | -20.23 | 1.09        | 1.33     |
| 2   | K     | 140 | PHE  | C-N    | -20.12 | 1.09        | 1.33     |
| 2   | B     | 140 | PHE  | C-N    | -20.05 | 1.09        | 1.33     |
| 2   | H     | 140 | PHE  | C-N    | -19.99 | 1.09        | 1.33     |
| 1   | D     | 637 | LYS  | C-N    | -18.83 | 1.06        | 1.33     |
| 1   | J     | 637 | LYS  | C-N    | -18.80 | 1.06        | 1.33     |
| 1   | G     | 637 | LYS  | C-N    | -18.61 | 1.06        | 1.33     |
| 1   | A     | 637 | LYS  | C-N    | -18.58 | 1.06        | 1.33     |
| 1   | J     | 785 | GLU  | C-N    | 15.09  | 1.54        | 1.33     |
| 1   | A     | 622 | LEU  | C-N    | 13.08  | 1.54        | 1.33     |
| 1   | J     | 622 | LEU  | C-N    | 13.03  | 1.53        | 1.33     |
| 1   | D     | 622 | LEU  | C-N    | 13.00  | 1.53        | 1.33     |
| 1   | G     | 622 | LEU  | C-N    | 12.99  | 1.53        | 1.33     |
| 2   | K     | 150 | TYR  | CA-CB  | -11.50 | 1.35        | 1.53     |
| 2   | H     | 150 | TYR  | CA-CB  | -11.43 | 1.35        | 1.53     |
| 2   | B     | 150 | TYR  | CA-CB  | -11.42 | 1.35        | 1.53     |
| 1   | G     | 785 | GLU  | C-N    | 11.32  | 1.49        | 1.33     |
| 2   | E     | 150 | TYR  | CA-CB  | -11.29 | 1.36        | 1.53     |
| 2   | B     | 150 | TYR  | N-CA   | -10.97 | 1.33        | 1.46     |
| 1   | D     | 201 | ALA  | CA-C   | -10.88 | 1.47        | 1.53     |
| 1   | A     | 201 | ALA  | CA-C   | -10.84 | 1.47        | 1.53     |
| 2   | H     | 150 | TYR  | N-CA   | -10.74 | 1.33        | 1.46     |
| 2   | K     | 150 | TYR  | N-CA   | -10.73 | 1.33        | 1.46     |
| 2   | E     | 150 | TYR  | N-CA   | -10.71 | 1.33        | 1.46     |
| 2   | K     | 141 | PRO  | N-CD   | -10.65 | 1.32        | 1.47     |
| 1   | G     | 201 | ALA  | CA-C   | -10.60 | 1.47        | 1.53     |
| 2   | E     | 141 | PRO  | N-CD   | -10.46 | 1.33        | 1.47     |
| 2   | B     | 141 | PRO  | N-CD   | -10.43 | 1.33        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | J     | 201 | ALA  | CA-C    | -10.38 | 1.48        | 1.53     |
| 2   | H     | 141 | PRO  | N-CD    | -10.30 | 1.33        | 1.47     |
| 2   | K     | 150 | TYR  | CB-CG   | -9.13  | 1.31        | 1.51     |
| 2   | H     | 150 | TYR  | CB-CG   | -9.06  | 1.31        | 1.51     |
| 2   | B     | 150 | TYR  | CB-CG   | -9.05  | 1.31        | 1.51     |
| 2   | E     | 150 | TYR  | CB-CG   | -9.00  | 1.31        | 1.51     |
| 1   | D     | 218 | LEU  | C-N     | -8.62  | 1.21        | 1.33     |
| 1   | A     | 218 | LEU  | C-N     | -8.55  | 1.21        | 1.33     |
| 1   | J     | 218 | LEU  | C-N     | -8.53  | 1.21        | 1.33     |
| 2   | K     | 131 | GLU  | N-CA    | 8.52   | 1.57        | 1.46     |
| 1   | G     | 218 | LEU  | C-N     | -8.45  | 1.21        | 1.33     |
| 2   | B     | 131 | GLU  | N-CA    | 8.44   | 1.57        | 1.46     |
| 2   | E     | 131 | GLU  | N-CA    | 8.43   | 1.57        | 1.46     |
| 2   | H     | 131 | GLU  | N-CA    | 8.34   | 1.56        | 1.46     |
| 2   | H     | 149 | ASP  | C-N     | -8.29  | 1.23        | 1.33     |
| 2   | E     | 149 | ASP  | C-N     | -8.22  | 1.23        | 1.33     |
| 2   | B     | 149 | ASP  | C-N     | -8.07  | 1.23        | 1.33     |
| 2   | K     | 149 | ASP  | C-N     | -8.03  | 1.23        | 1.33     |
| 1   | G     | 218 | LEU  | CB-CG   | 7.84   | 1.69        | 1.53     |
| 1   | J     | 218 | LEU  | CB-CG   | 7.76   | 1.69        | 1.53     |
| 1   | A     | 218 | LEU  | CB-CG   | 7.72   | 1.69        | 1.53     |
| 1   | D     | 218 | LEU  | CB-CG   | 7.67   | 1.68        | 1.53     |
| 4   | Y     | 101 | HIS  | CD2-NE2 | -7.52  | 1.29        | 1.37     |
| 4   | W     | 101 | HIS  | CD2-NE2 | -7.52  | 1.29        | 1.37     |
| 2   | B     | 140 | PHE  | CA-C    | -7.51  | 1.43        | 1.52     |
| 4   | 1     | 101 | HIS  | CD2-NE2 | -7.50  | 1.29        | 1.37     |
| 4   | V     | 101 | HIS  | CD2-NE2 | -7.50  | 1.29        | 1.37     |
| 4   | 5     | 101 | HIS  | CD2-NE2 | -7.49  | 1.29        | 1.37     |
| 4   | 7     | 101 | HIS  | CD2-NE2 | -7.46  | 1.29        | 1.37     |
| 4   | Z     | 101 | HIS  | CD2-NE2 | -7.45  | 1.29        | 1.37     |
| 4   | 0     | 101 | HIS  | CD2-NE2 | -7.44  | 1.29        | 1.37     |
| 2   | H     | 140 | PHE  | CA-C    | -7.43  | 1.43        | 1.52     |
| 4   | 2     | 101 | HIS  | CD2-NE2 | -7.43  | 1.29        | 1.37     |
| 4   | 3     | 101 | HIS  | CD2-NE2 | -7.43  | 1.29        | 1.37     |
| 4   | 4     | 101 | HIS  | CD2-NE2 | -7.41  | 1.29        | 1.37     |
| 4   | 9     | 101 | HIS  | CD2-NE2 | -7.40  | 1.29        | 1.37     |
| 4   | 8     | 101 | HIS  | CD2-NE2 | -7.39  | 1.29        | 1.37     |
| 2   | E     | 140 | PHE  | CA-C    | -7.38  | 1.43        | 1.52     |
| 4   | 8     | 88  | HIS  | CD2-NE2 | -7.38  | 1.29        | 1.37     |
| 4   | X     | 101 | HIS  | CD2-NE2 | -7.36  | 1.29        | 1.37     |
| 4   | W     | 87  | HIS  | CD2-NE2 | -7.35  | 1.29        | 1.37     |
| 3   | F     | 63  | ILE  | CA-CB   | 7.35   | 1.66        | 1.55     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | 4     | 87  | HIS  | CD2-NE2 | -7.35 | 1.29        | 1.37     |
| 4   | X     | 87  | HIS  | CD2-NE2 | -7.34 | 1.29        | 1.37     |
| 4   | W     | 88  | HIS  | CD2-NE2 | -7.34 | 1.29        | 1.37     |
| 4   | 2     | 275 | HIS  | CD2-NE2 | -7.33 | 1.29        | 1.37     |
| 4   | 3     | 88  | HIS  | CD2-NE2 | -7.33 | 1.29        | 1.37     |
| 4   | 0     | 88  | HIS  | CD2-NE2 | -7.32 | 1.29        | 1.37     |
| 4   | Y     | 88  | HIS  | CD2-NE2 | -7.32 | 1.29        | 1.37     |
| 4   | 3     | 87  | HIS  | CD2-NE2 | -7.32 | 1.29        | 1.37     |
| 4   | 1     | 88  | HIS  | CD2-NE2 | -7.31 | 1.29        | 1.37     |
| 3   | C     | 63  | ILE  | CA-CB   | 7.31  | 1.66        | 1.55     |
| 4   | 5     | 87  | HIS  | CD2-NE2 | -7.31 | 1.29        | 1.37     |
| 4   | 4     | 275 | HIS  | CD2-NE2 | -7.31 | 1.29        | 1.37     |
| 4   | 4     | 88  | HIS  | CD2-NE2 | -7.31 | 1.29        | 1.37     |
| 4   | 9     | 88  | HIS  | CD2-NE2 | -7.31 | 1.29        | 1.37     |
| 3   | L     | 63  | ILE  | CA-CB   | 7.31  | 1.66        | 1.55     |
| 4   | 5     | 88  | HIS  | CD2-NE2 | -7.30 | 1.29        | 1.37     |
| 4   | 7     | 88  | HIS  | CD2-NE2 | -7.30 | 1.29        | 1.37     |
| 4   | X     | 88  | HIS  | CD2-NE2 | -7.29 | 1.29        | 1.37     |
| 2   | K     | 140 | PHE  | CA-C    | -7.29 | 1.43        | 1.52     |
| 4   | Z     | 88  | HIS  | CD2-NE2 | -7.28 | 1.29        | 1.37     |
| 4   | 0     | 275 | HIS  | CD2-NE2 | -7.27 | 1.29        | 1.37     |
| 3   | I     | 63  | ILE  | CA-CB   | 7.27  | 1.66        | 1.55     |
| 4   | Z     | 87  | HIS  | CD2-NE2 | -7.26 | 1.29        | 1.37     |
| 4   | Z     | 275 | HIS  | CD2-NE2 | -7.26 | 1.29        | 1.37     |
| 1   | J     | 496 | PHE  | C-N     | -7.26 | 1.24        | 1.33     |
| 4   | 2     | 87  | HIS  | CD2-NE2 | -7.26 | 1.29        | 1.37     |
| 4   | V     | 88  | HIS  | CD2-NE2 | -7.25 | 1.29        | 1.37     |
| 4   | 7     | 87  | HIS  | CD2-NE2 | -7.25 | 1.29        | 1.37     |
| 4   | 8     | 87  | HIS  | CD2-NE2 | -7.24 | 1.29        | 1.37     |
| 4   | 5     | 275 | HIS  | CD2-NE2 | -7.24 | 1.29        | 1.37     |
| 4   | 9     | 87  | HIS  | CD2-NE2 | -7.23 | 1.29        | 1.37     |
| 4   | 2     | 88  | HIS  | CD2-NE2 | -7.23 | 1.29        | 1.37     |
| 4   | 3     | 275 | HIS  | CD2-NE2 | -7.23 | 1.29        | 1.37     |
| 4   | V     | 275 | HIS  | CD2-NE2 | -7.22 | 1.29        | 1.37     |
| 4   | 1     | 275 | HIS  | CD2-NE2 | -7.22 | 1.29        | 1.37     |
| 4   | 1     | 87  | HIS  | CD2-NE2 | -7.21 | 1.29        | 1.37     |
| 4   | Y     | 87  | HIS  | CD2-NE2 | -7.20 | 1.29        | 1.37     |
| 1   | D     | 496 | PHE  | C-N     | -7.19 | 1.24        | 1.33     |
| 4   | 8     | 275 | HIS  | CD2-NE2 | -7.19 | 1.29        | 1.37     |
| 4   | 0     | 87  | HIS  | CD2-NE2 | -7.18 | 1.29        | 1.37     |
| 4   | W     | 275 | HIS  | CD2-NE2 | -7.17 | 1.29        | 1.37     |
| 4   | V     | 87  | HIS  | CD2-NE2 | -7.17 | 1.29        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 496 | PHE  | C-N     | -7.15 | 1.25        | 1.33     |
| 2   | B     | 150 | TYR  | CG-CD2  | -7.15 | 1.24        | 1.39     |
| 4   | X     | 40  | HIS  | CD2-NE2 | -7.15 | 1.29        | 1.37     |
| 4   | 7     | 275 | HIS  | CD2-NE2 | -7.14 | 1.29        | 1.37     |
| 4   | 9     | 275 | HIS  | CD2-NE2 | -7.14 | 1.29        | 1.37     |
| 4   | Y     | 275 | HIS  | CD2-NE2 | -7.13 | 1.30        | 1.37     |
| 4   | 8     | 40  | HIS  | CD2-NE2 | -7.12 | 1.30        | 1.37     |
| 2   | H     | 150 | TYR  | CG-CD2  | -7.12 | 1.24        | 1.39     |
| 4   | 0     | 40  | HIS  | CD2-NE2 | -7.11 | 1.30        | 1.37     |
| 4   | 3     | 40  | HIS  | CD2-NE2 | -7.11 | 1.30        | 1.37     |
| 4   | 5     | 40  | HIS  | CD2-NE2 | -7.10 | 1.30        | 1.37     |
| 4   | X     | 275 | HIS  | CD2-NE2 | -7.10 | 1.30        | 1.37     |
| 4   | 1     | 40  | HIS  | CD2-NE2 | -7.10 | 1.30        | 1.37     |
| 4   | V     | 40  | HIS  | CD2-NE2 | -7.07 | 1.30        | 1.37     |
| 1   | G     | 496 | PHE  | C-N     | -7.06 | 1.25        | 1.33     |
| 2   | K     | 141 | PRO  | CA-CB   | -7.06 | 1.44        | 1.54     |
| 2   | K     | 150 | TYR  | CG-CD2  | -7.04 | 1.24        | 1.39     |
| 2   | E     | 150 | TYR  | CG-CD2  | -7.04 | 1.24        | 1.39     |
| 4   | Z     | 40  | HIS  | CD2-NE2 | -7.03 | 1.30        | 1.37     |
| 4   | 2     | 40  | HIS  | CD2-NE2 | -7.03 | 1.30        | 1.37     |
| 4   | W     | 40  | HIS  | CD2-NE2 | -7.02 | 1.30        | 1.37     |
| 4   | Y     | 40  | HIS  | CD2-NE2 | -7.01 | 1.30        | 1.37     |
| 2   | E     | 141 | PRO  | CA-CB   | -7.00 | 1.44        | 1.54     |
| 1   | J     | 288 | PHE  | CA-C    | -6.99 | 1.44        | 1.52     |
| 4   | 4     | 40  | HIS  | CD2-NE2 | -6.99 | 1.30        | 1.37     |
| 4   | 9     | 40  | HIS  | CD2-NE2 | -6.97 | 1.30        | 1.37     |
| 2   | H     | 141 | PRO  | CA-CB   | -6.96 | 1.44        | 1.54     |
| 1   | D     | 177 | ILE  | C-O     | -6.94 | 1.16        | 1.24     |
| 2   | H     | 138 | ALA  | C-N     | -6.93 | 1.23        | 1.33     |
| 2   | B     | 141 | PRO  | CA-CB   | -6.92 | 1.44        | 1.54     |
| 4   | 7     | 40  | HIS  | CD2-NE2 | -6.91 | 1.30        | 1.37     |
| 1   | A     | 288 | PHE  | CA-C    | -6.90 | 1.44        | 1.52     |
| 1   | G     | 288 | PHE  | CA-C    | -6.88 | 1.44        | 1.52     |
| 1   | G     | 177 | ILE  | C-O     | -6.87 | 1.16        | 1.24     |
| 2   | K     | 138 | ALA  | C-N     | -6.87 | 1.23        | 1.33     |
| 1   | D     | 288 | PHE  | CA-C    | -6.87 | 1.44        | 1.52     |
| 2   | B     | 138 | ALA  | C-N     | -6.86 | 1.23        | 1.33     |
| 2   | B     | 140 | PHE  | C-O     | -6.83 | 1.15        | 1.24     |
| 2   | K     | 140 | PHE  | C-O     | -6.82 | 1.15        | 1.24     |
| 2   | E     | 138 | ALA  | C-N     | -6.81 | 1.23        | 1.33     |
| 1   | A     | 177 | ILE  | C-O     | -6.79 | 1.16        | 1.24     |
| 1   | D     | 641 | LYS  | C-N     | -6.79 | 1.25        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 140 | PHE  | C-O     | -6.75 | 1.15        | 1.24     |
| 1   | J     | 177 | ILE  | C-O     | -6.73 | 1.16        | 1.24     |
| 4   | 4     | 371 | HIS  | CD2-NE2 | -6.71 | 1.30        | 1.37     |
| 4   | X     | 371 | HIS  | CD2-NE2 | -6.66 | 1.30        | 1.37     |
| 1   | G     | 496 | PHE  | C-O     | -6.66 | 1.16        | 1.24     |
| 1   | A     | 637 | LYS  | C-O     | 6.65  | 1.32        | 1.24     |
| 1   | J     | 568 | PRO  | CA-C    | -6.65 | 1.44        | 1.52     |
| 4   | 8     | 371 | HIS  | CD2-NE2 | -6.64 | 1.30        | 1.37     |
| 1   | J     | 641 | LYS  | C-N     | -6.61 | 1.25        | 1.34     |
| 1   | G     | 637 | LYS  | C-O     | 6.60  | 1.32        | 1.24     |
| 1   | A     | 496 | PHE  | C-O     | -6.60 | 1.16        | 1.24     |
| 1   | G     | 201 | ALA  | C-N     | -6.59 | 1.24        | 1.33     |
| 2   | E     | 140 | PHE  | C-O     | -6.59 | 1.15        | 1.24     |
| 1   | G     | 641 | LYS  | C-N     | -6.59 | 1.25        | 1.34     |
| 1   | A     | 641 | LYS  | C-N     | -6.58 | 1.25        | 1.34     |
| 4   | 3     | 371 | HIS  | CD2-NE2 | -6.58 | 1.30        | 1.37     |
| 4   | W     | 371 | HIS  | CD2-NE2 | -6.58 | 1.30        | 1.37     |
| 4   | 9     | 371 | HIS  | CD2-NE2 | -6.58 | 1.30        | 1.37     |
| 1   | J     | 637 | LYS  | C-O     | 6.57  | 1.32        | 1.24     |
| 4   | 0     | 371 | HIS  | CD2-NE2 | -6.56 | 1.30        | 1.37     |
| 1   | D     | 568 | PRO  | CA-C    | -6.56 | 1.44        | 1.52     |
| 4   | Z     | 371 | HIS  | CD2-NE2 | -6.55 | 1.30        | 1.37     |
| 4   | 3     | 101 | HIS  | CG-ND1  | -6.54 | 1.31        | 1.38     |
| 4   | 2     | 371 | HIS  | CD2-NE2 | -6.54 | 1.30        | 1.37     |
| 4   | 1     | 371 | HIS  | CD2-NE2 | -6.54 | 1.30        | 1.37     |
| 4   | 4     | 101 | HIS  | CG-ND1  | -6.53 | 1.31        | 1.38     |
| 1   | A     | 523 | ILE  | CA-CB   | -6.53 | 1.46        | 1.54     |
| 4   | V     | 371 | HIS  | CD2-NE2 | -6.52 | 1.30        | 1.37     |
| 4   | 1     | 88  | HIS  | CG-ND1  | -6.50 | 1.31        | 1.38     |
| 4   | Y     | 371 | HIS  | CD2-NE2 | -6.50 | 1.30        | 1.37     |
| 1   | D     | 496 | PHE  | C-O     | -6.50 | 1.16        | 1.24     |
| 4   | 1     | 101 | HIS  | CG-ND1  | -6.50 | 1.31        | 1.38     |
| 4   | 5     | 371 | HIS  | CD2-NE2 | -6.47 | 1.30        | 1.37     |
| 1   | D     | 637 | LYS  | C-O     | 6.47  | 1.32        | 1.24     |
| 1   | J     | 201 | ALA  | C-N     | -6.46 | 1.24        | 1.33     |
| 1   | G     | 568 | PRO  | CA-C    | -6.46 | 1.44        | 1.52     |
| 1   | D     | 523 | ILE  | CA-CB   | -6.46 | 1.46        | 1.54     |
| 4   | V     | 101 | HIS  | CG-ND1  | -6.45 | 1.31        | 1.38     |
| 4   | 4     | 88  | HIS  | CG-ND1  | -6.45 | 1.31        | 1.38     |
| 3   | I     | 62  | ALA  | C-N     | -6.45 | 1.25        | 1.33     |
| 4   | 9     | 101 | HIS  | CG-ND1  | -6.44 | 1.31        | 1.38     |
| 1   | A     | 568 | PRO  | CA-C    | -6.44 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | Z     | 101 | HIS  | CG-ND1  | -6.43 | 1.31        | 1.38     |
| 4   | 3     | 88  | HIS  | CG-ND1  | -6.42 | 1.31        | 1.38     |
| 4   | W     | 101 | HIS  | CG-ND1  | -6.42 | 1.31        | 1.38     |
| 4   | 7     | 371 | HIS  | CD2-NE2 | -6.42 | 1.30        | 1.37     |
| 4   | 9     | 88  | HIS  | CG-ND1  | -6.42 | 1.31        | 1.38     |
| 1   | G     | 523 | ILE  | CA-CB   | -6.41 | 1.46        | 1.54     |
| 4   | 7     | 88  | HIS  | CG-ND1  | -6.41 | 1.31        | 1.38     |
| 1   | J     | 496 | PHE  | C-O     | -6.41 | 1.16        | 1.24     |
| 4   | 5     | 88  | HIS  | CG-ND1  | -6.41 | 1.31        | 1.38     |
| 4   | 7     | 101 | HIS  | CG-ND1  | -6.41 | 1.31        | 1.38     |
| 4   | 0     | 101 | HIS  | CG-ND1  | -6.41 | 1.31        | 1.38     |
| 4   | X     | 88  | HIS  | CG-ND1  | -6.41 | 1.31        | 1.38     |
| 4   | 5     | 101 | HIS  | CG-ND1  | -6.40 | 1.31        | 1.38     |
| 4   | X     | 101 | HIS  | CG-ND1  | -6.40 | 1.31        | 1.38     |
| 4   | 0     | 88  | HIS  | CG-ND1  | -6.39 | 1.31        | 1.38     |
| 4   | 2     | 88  | HIS  | CG-ND1  | -6.39 | 1.31        | 1.38     |
| 4   | 8     | 88  | HIS  | CG-ND1  | -6.39 | 1.31        | 1.38     |
| 4   | W     | 88  | HIS  | CG-ND1  | -6.39 | 1.31        | 1.38     |
| 4   | V     | 88  | HIS  | CG-ND1  | -6.39 | 1.31        | 1.38     |
| 4   | Y     | 88  | HIS  | CG-ND1  | -6.39 | 1.31        | 1.38     |
| 1   | D     | 201 | ALA  | C-N     | -6.38 | 1.24        | 1.33     |
| 4   | Z     | 88  | HIS  | CG-ND1  | -6.38 | 1.31        | 1.38     |
| 2   | B     | 123 | THR  | C-N     | -6.38 | 1.24        | 1.33     |
| 4   | Y     | 101 | HIS  | CG-ND1  | -6.37 | 1.31        | 1.38     |
| 1   | J     | 523 | ILE  | CA-CB   | -6.37 | 1.47        | 1.54     |
| 4   | 2     | 101 | HIS  | CG-ND1  | -6.35 | 1.31        | 1.38     |
| 4   | 8     | 101 | HIS  | CG-ND1  | -6.34 | 1.31        | 1.38     |
| 3   | C     | 62  | ALA  | C-N     | -6.32 | 1.26        | 1.33     |
| 2   | K     | 123 | THR  | C-N     | -6.32 | 1.24        | 1.33     |
| 2   | E     | 123 | THR  | C-N     | -6.31 | 1.24        | 1.33     |
| 1   | A     | 201 | ALA  | C-N     | -6.29 | 1.24        | 1.33     |
| 2   | H     | 123 | THR  | C-N     | -6.21 | 1.24        | 1.33     |
| 3   | L     | 62  | ALA  | C-N     | -6.18 | 1.26        | 1.33     |
| 3   | F     | 62  | ALA  | C-N     | -6.15 | 1.26        | 1.33     |
| 3   | L     | 64  | THR  | N-CA    | -6.14 | 1.38        | 1.45     |
| 3   | F     | 64  | THR  | N-CA    | -6.08 | 1.38        | 1.46     |
| 4   | 1     | 161 | HIS  | CD2-NE2 | -6.04 | 1.31        | 1.37     |
| 4   | W     | 173 | HIS  | CD2-NE2 | -6.03 | 1.31        | 1.37     |
| 4   | 2     | 161 | HIS  | CD2-NE2 | -6.03 | 1.31        | 1.37     |
| 3   | I     | 64  | THR  | N-CA    | -6.02 | 1.38        | 1.46     |
| 3   | F     | 63  | ILE  | CB-CG1  | 6.02  | 1.65        | 1.53     |
| 3   | C     | 63  | ILE  | CB-CG1  | 6.02  | 1.65        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | V     | 173 | HIS  | CD2-NE2 | -6.00 | 1.31        | 1.37     |
| 4   | 8     | 161 | HIS  | CD2-NE2 | -6.00 | 1.31        | 1.37     |
| 4   | V     | 161 | HIS  | CD2-NE2 | -5.98 | 1.31        | 1.37     |
| 4   | 3     | 161 | HIS  | CD2-NE2 | -5.98 | 1.31        | 1.37     |
| 4   | X     | 161 | HIS  | CD2-NE2 | -5.97 | 1.31        | 1.37     |
| 3   | L     | 63  | ILE  | CB-CG1  | 5.96  | 1.65        | 1.53     |
| 4   | X     | 173 | HIS  | CD2-NE2 | -5.96 | 1.31        | 1.37     |
| 3   | C     | 64  | THR  | N-CA    | -5.95 | 1.38        | 1.45     |
| 1   | J     | 358 | VAL  | C-O     | -5.95 | 1.17        | 1.24     |
| 4   | Y     | 161 | HIS  | CD2-NE2 | -5.94 | 1.31        | 1.37     |
| 4   | 1     | 173 | HIS  | CD2-NE2 | -5.94 | 1.31        | 1.37     |
| 1   | A     | 514 | ASP  | C-O     | -5.93 | 1.16        | 1.23     |
| 4   | Z     | 161 | HIS  | CD2-NE2 | -5.92 | 1.31        | 1.37     |
| 4   | W     | 161 | HIS  | CD2-NE2 | -5.92 | 1.31        | 1.37     |
| 4   | 9     | 161 | HIS  | CD2-NE2 | -5.92 | 1.31        | 1.37     |
| 4   | 4     | 161 | HIS  | CD2-NE2 | -5.91 | 1.31        | 1.37     |
| 4   | 5     | 161 | HIS  | CD2-NE2 | -5.91 | 1.31        | 1.37     |
| 4   | 5     | 173 | HIS  | CD2-NE2 | -5.91 | 1.31        | 1.37     |
| 4   | 2     | 173 | HIS  | CD2-NE2 | -5.90 | 1.31        | 1.37     |
| 3   | I     | 63  | ILE  | CB-CG1  | 5.89  | 1.65        | 1.53     |
| 4   | 0     | 161 | HIS  | CD2-NE2 | -5.89 | 1.31        | 1.37     |
| 4   | 4     | 173 | HIS  | CD2-NE2 | -5.89 | 1.31        | 1.37     |
| 4   | 0     | 173 | HIS  | CD2-NE2 | -5.88 | 1.31        | 1.37     |
| 4   | Z     | 173 | HIS  | CD2-NE2 | -5.87 | 1.31        | 1.37     |
| 4   | 3     | 173 | HIS  | CD2-NE2 | -5.85 | 1.31        | 1.37     |
| 4   | 8     | 173 | HIS  | CD2-NE2 | -5.84 | 1.31        | 1.37     |
| 4   | 9     | 173 | HIS  | CD2-NE2 | -5.84 | 1.31        | 1.37     |
| 4   | 7     | 161 | HIS  | CD2-NE2 | -5.83 | 1.31        | 1.37     |
| 4   | 7     | 173 | HIS  | CD2-NE2 | -5.83 | 1.31        | 1.37     |
| 1   | G     | 358 | VAL  | C-O     | -5.82 | 1.17        | 1.24     |
| 4   | Y     | 173 | HIS  | CD2-NE2 | -5.81 | 1.31        | 1.37     |
| 1   | D     | 358 | VAL  | C-O     | -5.79 | 1.17        | 1.24     |
| 1   | A     | 358 | VAL  | C-O     | -5.78 | 1.17        | 1.24     |
| 1   | J     | 434 | TYR  | CA-CB   | -5.77 | 1.44        | 1.53     |
| 1   | J     | 514 | ASP  | C-O     | -5.77 | 1.17        | 1.23     |
| 1   | A     | 434 | TYR  | CA-CB   | -5.76 | 1.44        | 1.53     |
| 1   | A     | 217 | THR  | N-CA    | 5.75  | 1.53        | 1.45     |
| 1   | D     | 514 | ASP  | C-O     | -5.75 | 1.17        | 1.23     |
| 1   | G     | 514 | ASP  | C-O     | -5.74 | 1.17        | 1.23     |
| 1   | G     | 233 | GLY  | C-O     | -5.70 | 1.20        | 1.24     |
| 1   | A     | 625 | THR  | CB-CG2  | 5.67  | 1.71        | 1.52     |
| 1   | D     | 434 | TYR  | CA-CB   | -5.63 | 1.44        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 434 | TYR  | CA-CB   | -5.63 | 1.44        | 1.53     |
| 1   | D     | 625 | THR  | CB-CG2  | 5.60  | 1.71        | 1.52     |
| 1   | G     | 625 | THR  | CB-CG2  | 5.60  | 1.71        | 1.52     |
| 1   | D     | 217 | THR  | N-CA    | 5.60  | 1.52        | 1.45     |
| 1   | J     | 578 | HIS  | N-CA    | 5.59  | 1.53        | 1.46     |
| 1   | J     | 625 | THR  | CB-CG2  | 5.59  | 1.71        | 1.52     |
| 1   | J     | 217 | THR  | N-CA    | 5.58  | 1.52        | 1.45     |
| 4   | 2     | 275 | HIS  | CG-ND1  | -5.57 | 1.32        | 1.38     |
| 4   | 4     | 275 | HIS  | CG-ND1  | -5.54 | 1.32        | 1.38     |
| 4   | Y     | 275 | HIS  | CG-ND1  | -5.54 | 1.32        | 1.38     |
| 4   | W     | 275 | HIS  | CG-ND1  | -5.54 | 1.32        | 1.38     |
| 4   | 1     | 275 | HIS  | CG-ND1  | -5.53 | 1.32        | 1.38     |
| 1   | G     | 217 | THR  | N-CA    | 5.53  | 1.52        | 1.45     |
| 4   | X     | 275 | HIS  | CG-ND1  | -5.53 | 1.32        | 1.38     |
| 1   | D     | 233 | GLY  | C-O     | -5.51 | 1.20        | 1.24     |
| 4   | 8     | 275 | HIS  | CG-ND1  | -5.51 | 1.32        | 1.38     |
| 4   | 7     | 275 | HIS  | CG-ND1  | -5.51 | 1.32        | 1.38     |
| 4   | V     | 275 | HIS  | CG-ND1  | -5.50 | 1.32        | 1.38     |
| 1   | J     | 641 | LYS  | C-O     | 5.50  | 1.31        | 1.24     |
| 4   | Z     | 275 | HIS  | CG-ND1  | -5.50 | 1.32        | 1.38     |
| 4   | 3     | 275 | HIS  | CG-ND1  | -5.49 | 1.32        | 1.38     |
| 4   | 9     | 275 | HIS  | CG-ND1  | -5.49 | 1.32        | 1.38     |
| 4   | 0     | 275 | HIS  | CG-ND1  | -5.49 | 1.32        | 1.38     |
| 1   | A     | 578 | HIS  | N-CA    | 5.47  | 1.53        | 1.46     |
| 1   | A     | 233 | GLY  | C-O     | -5.45 | 1.20        | 1.24     |
| 4   | 5     | 275 | HIS  | CG-ND1  | -5.44 | 1.32        | 1.38     |
| 1   | D     | 578 | HIS  | N-CA    | 5.43  | 1.53        | 1.46     |
| 1   | D     | 641 | LYS  | C-O     | 5.43  | 1.31        | 1.24     |
| 1   | D     | 340 | ILE  | CA-C    | -5.42 | 1.45        | 1.52     |
| 1   | J     | 482 | PHE  | C-O     | -5.41 | 1.17        | 1.24     |
| 1   | G     | 340 | ILE  | CA-C    | -5.39 | 1.45        | 1.52     |
| 1   | D     | 104 | TYR  | C-O     | -5.37 | 1.17        | 1.24     |
| 1   | A     | 641 | LYS  | C-O     | 5.37  | 1.30        | 1.24     |
| 1   | G     | 641 | LYS  | C-O     | 5.36  | 1.30        | 1.24     |
| 2   | E     | 129 | THR  | N-CA    | 5.36  | 1.53        | 1.46     |
| 1   | A     | 340 | ILE  | CA-C    | -5.34 | 1.45        | 1.52     |
| 1   | G     | 578 | HIS  | N-CA    | 5.33  | 1.53        | 1.46     |
| 1   | A     | 482 | PHE  | C-O     | -5.32 | 1.17        | 1.24     |
| 1   | J     | 340 | ILE  | CA-C    | -5.31 | 1.45        | 1.52     |
| 1   | J     | 476 | GLU  | CD-OE1  | 5.30  | 1.35        | 1.25     |
| 2   | B     | 137 | TRP  | NE1-CE2 | -5.29 | 1.31        | 1.37     |
| 1   | J     | 252 | ILE  | CA-C    | -5.29 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 252 | ILE  | CA-C   | -5.28 | 1.46        | 1.52     |
| 1   | G     | 309 | PRO  | CA-CB  | -5.27 | 1.46        | 1.53     |
| 1   | G     | 671 | PHE  | C-O    | -5.27 | 1.17        | 1.23     |
| 2   | B     | 129 | THR  | N-CA   | 5.26  | 1.53        | 1.46     |
| 1   | A     | 671 | PHE  | C-O    | -5.26 | 1.17        | 1.23     |
| 1   | D     | 309 | PRO  | CA-CB  | -5.25 | 1.46        | 1.53     |
| 1   | G     | 482 | PHE  | C-O    | -5.25 | 1.18        | 1.24     |
| 2   | K     | 129 | THR  | N-CA   | 5.24  | 1.53        | 1.46     |
| 1   | D     | 671 | PHE  | C-O    | -5.23 | 1.17        | 1.23     |
| 1   | D     | 476 | GLU  | CD-OE1 | 5.22  | 1.35        | 1.25     |
| 4   | 0     | 259 | GLU  | CA-CB  | 5.22  | 1.62        | 1.53     |
| 1   | J     | 233 | GLY  | C-O    | -5.21 | 1.20        | 1.24     |
| 1   | D     | 482 | PHE  | C-O    | -5.21 | 1.18        | 1.24     |
| 1   | G     | 104 | TYR  | C-O    | -5.21 | 1.17        | 1.24     |
| 1   | G     | 177 | ILE  | CA-CB  | -5.21 | 1.48        | 1.54     |
| 1   | G     | 252 | ILE  | CA-C   | -5.21 | 1.46        | 1.52     |
| 1   | A     | 476 | GLU  | CD-OE1 | 5.20  | 1.35        | 1.25     |
| 1   | J     | 104 | TYR  | C-O    | -5.20 | 1.17        | 1.24     |
| 4   | 7     | 259 | GLU  | CA-CB  | 5.19  | 1.62        | 1.53     |
| 1   | D     | 619 | LEU  | CA-C   | -5.19 | 1.46        | 1.52     |
| 1   | G     | 476 | GLU  | CD-OE1 | 5.19  | 1.35        | 1.25     |
| 1   | J     | 157 | SER  | CA-C   | -5.19 | 1.46        | 1.52     |
| 2   | K     | 149 | ASP  | CA-C   | -5.18 | 1.46        | 1.53     |
| 1   | J     | 671 | PHE  | C-O    | -5.17 | 1.17        | 1.23     |
| 1   | A     | 309 | PRO  | CA-CB  | -5.17 | 1.46        | 1.53     |
| 1   | G     | 619 | LEU  | CA-C   | -5.17 | 1.46        | 1.52     |
| 4   | 3     | 259 | GLU  | CA-CB  | 5.17  | 1.62        | 1.53     |
| 1   | A     | 252 | ILE  | CA-C   | -5.16 | 1.47        | 1.52     |
| 4   | V     | 259 | GLU  | CA-CB  | 5.15  | 1.62        | 1.53     |
| 4   | W     | 259 | GLU  | CA-CB  | 5.15  | 1.62        | 1.53     |
| 1   | A     | 41  | VAL  | CA-CB  | -5.14 | 1.49        | 1.54     |
| 1   | A     | 619 | LEU  | CA-C   | -5.14 | 1.46        | 1.52     |
| 4   | X     | 259 | GLU  | CA-CB  | 5.14  | 1.62        | 1.53     |
| 2   | E     | 149 | ASP  | CA-C   | -5.13 | 1.46        | 1.53     |
| 4   | Y     | 259 | GLU  | CA-CB  | 5.13  | 1.62        | 1.53     |
| 4   | Z     | 259 | GLU  | CA-CB  | 5.13  | 1.62        | 1.53     |
| 1   | A     | 177 | ILE  | CA-CB  | -5.12 | 1.48        | 1.54     |
| 1   | J     | 309 | PRO  | CA-CB  | -5.12 | 1.46        | 1.53     |
| 4   | 1     | 259 | GLU  | CA-CB  | 5.12  | 1.62        | 1.53     |
| 4   | 9     | 259 | GLU  | CA-CB  | 5.12  | 1.62        | 1.53     |
| 1   | A     | 334 | THR  | CA-C   | -5.12 | 1.46        | 1.52     |
| 1   | J     | 202 | SER  | CB-OG  | 5.12  | 1.52        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 129 | THR  | N-CA    | 5.11  | 1.53        | 1.46     |
| 4   | 4     | 259 | GLU  | CA-CB   | 5.11  | 1.62        | 1.53     |
| 2   | E     | 137 | TRP  | NE1-CE2 | -5.11 | 1.31        | 1.37     |
| 4   | 5     | 259 | GLU  | CA-CB   | 5.10  | 1.62        | 1.53     |
| 4   | 4     | 214 | GLU  | CA-CB   | 5.10  | 1.61        | 1.53     |
| 1   | D     | 766 | PHE  | N-CA    | -5.10 | 1.39        | 1.46     |
| 4   | 8     | 259 | GLU  | CA-CB   | 5.10  | 1.62        | 1.53     |
| 4   | 2     | 259 | GLU  | CA-CB   | 5.09  | 1.62        | 1.53     |
| 4   | 5     | 214 | GLU  | CA-CB   | 5.09  | 1.61        | 1.53     |
| 1   | J     | 277 | PHE  | CA-C    | -5.09 | 1.46        | 1.52     |
| 4   | Y     | 214 | GLU  | CA-CB   | 5.08  | 1.61        | 1.53     |
| 1   | A     | 104 | TYR  | C-O     | -5.08 | 1.17        | 1.24     |
| 1   | A     | 157 | SER  | CA-C    | -5.07 | 1.46        | 1.52     |
| 4   | 2     | 214 | GLU  | CA-CB   | 5.07  | 1.61        | 1.53     |
| 4   | 3     | 214 | GLU  | CA-CB   | 5.07  | 1.61        | 1.53     |
| 4   | W     | 214 | GLU  | CA-CB   | 5.07  | 1.61        | 1.53     |
| 1   | J     | 41  | VAL  | CA-CB   | -5.06 | 1.49        | 1.54     |
| 1   | J     | 177 | ILE  | CA-CB   | -5.06 | 1.48        | 1.54     |
| 1   | A     | 766 | PHE  | N-CA    | -5.05 | 1.39        | 1.46     |
| 2   | B     | 149 | ASP  | CA-C    | -5.05 | 1.46        | 1.53     |
| 2   | H     | 130 | PRO  | C-N     | 5.05  | 1.40        | 1.33     |
| 1   | A     | 202 | SER  | CB-OG   | 5.04  | 1.52        | 1.42     |
| 2   | H     | 149 | ASP  | CA-C    | -5.04 | 1.46        | 1.53     |
| 1   | D     | 177 | ILE  | CA-CB   | -5.04 | 1.48        | 1.54     |
| 1   | J     | 619 | LEU  | CA-C    | -5.04 | 1.46        | 1.52     |
| 4   | X     | 214 | GLU  | CA-CB   | 5.04  | 1.61        | 1.53     |
| 1   | G     | 644 | SER  | C-O     | 5.03  | 1.30        | 1.24     |
| 1   | D     | 202 | SER  | CB-OG   | 5.03  | 1.52        | 1.42     |
| 4   | 1     | 214 | GLU  | CA-CB   | 5.02  | 1.61        | 1.53     |
| 1   | A     | 672 | VAL  | C-O     | -5.02 | 1.18        | 1.24     |
| 1   | G     | 202 | SER  | CB-OG   | 5.02  | 1.52        | 1.42     |
| 4   | 7     | 214 | GLU  | CA-CB   | 5.02  | 1.61        | 1.53     |
| 4   | Z     | 214 | GLU  | CA-CB   | 5.02  | 1.61        | 1.53     |
| 1   | A     | 277 | PHE  | CA-C    | -5.01 | 1.46        | 1.52     |
| 1   | G     | 411 | GLU  | CD-OE1  | 5.01  | 1.34        | 1.25     |
| 1   | J     | 766 | PHE  | N-CA    | -5.00 | 1.40        | 1.46     |

All (2091) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | G     | 637 | LYS  | O-C-N | -74.34 | 23.72       | 122.59   |
| 1   | D     | 637 | LYS  | O-C-N | -74.28 | 23.80       | 122.59   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | J     | 637 | LYS  | O-C-N      | -74.27 | 23.81       | 122.59   |
| 1   | A     | 637 | LYS  | O-C-N      | -74.23 | 23.87       | 122.59   |
| 1   | J     | 648 | THR  | CA-CB-OG1  | -44.78 | 42.43       | 109.60   |
| 1   | D     | 648 | THR  | CA-CB-OG1  | -44.77 | 42.44       | 109.60   |
| 1   | A     | 648 | THR  | CA-CB-OG1  | -44.77 | 42.45       | 109.60   |
| 1   | G     | 648 | THR  | CA-CB-OG1  | -44.74 | 42.49       | 109.60   |
| 1   | J     | 709 | LYS  | O-C-N      | -30.22 | 85.18       | 122.35   |
| 1   | A     | 623 | PHE  | CA-CB-CG   | -29.33 | 84.47       | 113.80   |
| 1   | J     | 623 | PHE  | CA-CB-CG   | -29.33 | 84.47       | 113.80   |
| 1   | D     | 623 | PHE  | CA-CB-CG   | -29.30 | 84.50       | 113.80   |
| 1   | G     | 623 | PHE  | CA-CB-CG   | -29.15 | 84.65       | 113.80   |
| 1   | G     | 649 | VAL  | CA-CB-CG1  | -24.88 | 68.10       | 110.40   |
| 1   | D     | 649 | VAL  | CA-CB-CG1  | -24.84 | 68.17       | 110.40   |
| 1   | J     | 649 | VAL  | CA-CB-CG1  | -24.83 | 68.20       | 110.40   |
| 1   | A     | 649 | VAL  | CA-CB-CG1  | -24.82 | 68.20       | 110.40   |
| 1   | J     | 649 | VAL  | CG1-CB-CG2 | -24.69 | 56.48       | 110.80   |
| 1   | D     | 649 | VAL  | CG1-CB-CG2 | -24.68 | 56.50       | 110.80   |
| 1   | G     | 649 | VAL  | CG1-CB-CG2 | -24.68 | 56.50       | 110.80   |
| 1   | A     | 649 | VAL  | CG1-CB-CG2 | -24.67 | 56.52       | 110.80   |
| 1   | G     | 649 | VAL  | CA-CB-CG2  | -24.59 | 68.59       | 110.40   |
| 1   | A     | 649 | VAL  | CA-CB-CG2  | -24.58 | 68.62       | 110.40   |
| 1   | D     | 649 | VAL  | CA-CB-CG2  | -24.56 | 68.64       | 110.40   |
| 1   | J     | 649 | VAL  | CA-CB-CG2  | -24.55 | 68.66       | 110.40   |
| 1   | D     | 648 | THR  | CA-CB-CG2  | -19.91 | 76.65       | 110.50   |
| 1   | J     | 648 | THR  | CA-CB-CG2  | -19.88 | 76.71       | 110.50   |
| 1   | A     | 648 | THR  | CA-CB-CG2  | -19.84 | 76.76       | 110.50   |
| 1   | G     | 648 | THR  | CA-CB-CG2  | -19.84 | 76.78       | 110.50   |
| 1   | D     | 728 | ASN  | O-C-N      | 16.30  | 138.32      | 122.18   |
| 1   | A     | 728 | ASN  | O-C-N      | 16.10  | 138.12      | 122.18   |
| 1   | J     | 728 | ASN  | O-C-N      | 16.09  | 138.11      | 122.18   |
| 1   | G     | 728 | ASN  | O-C-N      | 15.89  | 137.91      | 122.18   |
| 3   | C     | 63  | ILE  | O-C-N      | 14.31  | 138.42      | 122.82   |
| 3   | I     | 63  | ILE  | O-C-N      | 14.26  | 138.36      | 122.82   |
| 2   | E     | 150 | TYR  | CD1-CG-CD2 | 14.20  | 139.40      | 118.10   |
| 2   | H     | 150 | TYR  | CD1-CG-CD2 | 14.19  | 139.38      | 118.10   |
| 2   | B     | 150 | TYR  | CD1-CG-CD2 | 14.14  | 139.30      | 118.10   |
| 2   | K     | 150 | TYR  | CD1-CG-CD2 | 14.12  | 139.28      | 118.10   |
| 3   | L     | 63  | ILE  | O-C-N      | 14.10  | 138.19      | 122.82   |
| 3   | F     | 63  | ILE  | O-C-N      | 14.08  | 138.16      | 122.82   |
| 1   | A     | 568 | PRO  | O-C-N      | 13.53  | 139.78      | 123.01   |
| 1   | G     | 568 | PRO  | O-C-N      | 13.52  | 139.77      | 123.01   |
| 1   | D     | 568 | PRO  | O-C-N      | 13.49  | 139.74      | 123.01   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | J     | 568 | PRO  | O-C-N      | 13.44  | 139.67      | 123.01   |
| 1   | D     | 98  | HIS  | CB-CA-C    | -11.85 | 87.28       | 111.22   |
| 1   | J     | 98  | HIS  | CB-CA-C    | -11.85 | 87.28       | 111.22   |
| 1   | A     | 98  | HIS  | CB-CA-C    | -11.84 | 87.30       | 111.22   |
| 1   | G     | 98  | HIS  | CB-CA-C    | -11.84 | 87.31       | 111.22   |
| 1   | J     | 709 | LYS  | CA-C-N     | 11.81  | 144.56      | 121.41   |
| 1   | J     | 709 | LYS  | C-N-CA     | 11.81  | 144.56      | 121.41   |
| 2   | E     | 150 | TYR  | CB-CG-CD2  | -11.35 | 103.77      | 120.80   |
| 2   | B     | 150 | TYR  | CB-CG-CD2  | -11.32 | 103.81      | 120.80   |
| 2   | H     | 150 | TYR  | CB-CG-CD2  | -11.32 | 103.82      | 120.80   |
| 2   | K     | 150 | TYR  | CB-CG-CD2  | -11.29 | 103.87      | 120.80   |
| 1   | A     | 201 | ALA  | CA-C-O     | 11.11  | 125.33      | 118.33   |
| 2   | H     | 150 | TYR  | CG-CD2-CE2 | -11.08 | 104.59      | 121.20   |
| 1   | J     | 201 | ALA  | CA-C-O     | 11.06  | 125.30      | 118.33   |
| 1   | D     | 201 | ALA  | CA-C-O     | 10.97  | 125.24      | 118.33   |
| 2   | E     | 150 | TYR  | CG-CD2-CE2 | -10.93 | 104.81      | 121.20   |
| 1   | G     | 201 | ALA  | CA-C-O     | 10.92  | 125.21      | 118.33   |
| 2   | K     | 150 | TYR  | CG-CD2-CE2 | -10.88 | 104.88      | 121.20   |
| 2   | B     | 150 | TYR  | CG-CD2-CE2 | -10.86 | 104.91      | 121.20   |
| 1   | G     | 320 | ILE  | CB-CA-C    | -10.63 | 100.50      | 110.91   |
| 1   | J     | 320 | ILE  | CB-CA-C    | -10.49 | 100.63      | 110.91   |
| 1   | D     | 320 | ILE  | CB-CA-C    | -10.45 | 100.67      | 110.91   |
| 1   | A     | 320 | ILE  | CB-CA-C    | -10.45 | 100.67      | 110.91   |
| 2   | E     | 150 | TYR  | N-CA-CB    | -10.30 | 93.67       | 110.77   |
| 2   | H     | 150 | TYR  | N-CA-CB    | -10.27 | 93.72       | 110.77   |
| 1   | A     | 739 | ASP  | CA-CB-CG   | -10.27 | 102.33      | 112.60   |
| 2   | K     | 150 | TYR  | N-CA-CB    | -10.26 | 93.73       | 110.77   |
| 2   | B     | 150 | TYR  | N-CA-CB    | -10.20 | 93.83       | 110.77   |
| 1   | G     | 653 | PHE  | CA-CB-CG   | -10.20 | 103.60      | 113.80   |
| 1   | A     | 653 | PHE  | CA-CB-CG   | -10.19 | 103.61      | 113.80   |
| 1   | G     | 739 | ASP  | CA-CB-CG   | -10.18 | 102.42      | 112.60   |
| 1   | J     | 653 | PHE  | CA-CB-CG   | -10.18 | 103.62      | 113.80   |
| 1   | J     | 739 | ASP  | CA-CB-CG   | -10.18 | 102.42      | 112.60   |
| 1   | D     | 653 | PHE  | CA-CB-CG   | -10.09 | 103.71      | 113.80   |
| 2   | E     | 141 | PRO  | CA-N-CD    | 10.05  | 126.07      | 112.00   |
| 2   | H     | 141 | PRO  | CA-N-CD    | 10.04  | 126.06      | 112.00   |
| 1   | D     | 739 | ASP  | CA-CB-CG   | -10.04 | 102.56      | 112.60   |
| 2   | K     | 141 | PRO  | CA-N-CD    | 10.00  | 125.99      | 112.00   |
| 2   | B     | 141 | PRO  | CA-N-CD    | 9.98   | 125.97      | 112.00   |
| 2   | E     | 150 | TYR  | CG-CD1-CE1 | -9.83  | 106.45      | 121.20   |
| 1   | G     | 693 | HIS  | CA-CB-CG   | -9.83  | 103.97      | 113.80   |
| 2   | H     | 150 | TYR  | CG-CD1-CE1 | -9.80  | 106.50      | 121.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | K     | 150 | TYR  | CG-CD1-CE1 | -9.79 | 106.52      | 121.20   |
| 1   | J     | 693 | HIS  | CA-CB-CG   | -9.77 | 104.03      | 113.80   |
| 1   | D     | 693 | HIS  | CA-CB-CG   | -9.76 | 104.04      | 113.80   |
| 2   | B     | 150 | TYR  | CG-CD1-CE1 | -9.74 | 106.58      | 121.20   |
| 1   | A     | 693 | HIS  | CA-CB-CG   | -9.61 | 104.19      | 113.80   |
| 2   | K     | 138 | ALA  | O-C-N      | -9.44 | 108.65      | 122.43   |
| 4   | 3     | 147 | ARG  | N-CA-C     | 9.41  | 123.33      | 110.35   |
| 4   | Z     | 147 | ARG  | N-CA-C     | 9.40  | 123.32      | 110.35   |
| 4   | 4     | 147 | ARG  | N-CA-C     | 9.40  | 123.32      | 110.35   |
| 4   | 8     | 147 | ARG  | N-CA-C     | 9.40  | 123.32      | 110.35   |
| 4   | X     | 147 | ARG  | N-CA-C     | 9.39  | 123.31      | 110.35   |
| 4   | 0     | 147 | ARG  | N-CA-C     | 9.38  | 123.29      | 110.35   |
| 4   | 9     | 147 | ARG  | N-CA-C     | 9.38  | 123.29      | 110.35   |
| 4   | W     | 147 | ARG  | N-CA-C     | 9.38  | 123.29      | 110.35   |
| 4   | 2     | 147 | ARG  | N-CA-C     | 9.37  | 123.28      | 110.35   |
| 4   | 1     | 147 | ARG  | N-CA-C     | 9.36  | 123.27      | 110.35   |
| 1   | J     | 604 | ASN  | CA-CB-CG   | 9.36  | 121.96      | 112.60   |
| 4   | V     | 147 | ARG  | N-CA-C     | 9.36  | 123.26      | 110.35   |
| 1   | G     | 604 | ASN  | CA-CB-CG   | 9.35  | 121.95      | 112.60   |
| 4   | 7     | 147 | ARG  | N-CA-C     | 9.35  | 123.26      | 110.35   |
| 4   | Y     | 147 | ARG  | N-CA-C     | 9.34  | 123.25      | 110.35   |
| 1   | A     | 604 | ASN  | CA-CB-CG   | 9.34  | 121.94      | 112.60   |
| 4   | 5     | 147 | ARG  | N-CA-C     | 9.33  | 123.23      | 110.35   |
| 2   | B     | 138 | ALA  | O-C-N      | -9.31 | 108.83      | 122.43   |
| 2   | E     | 138 | ALA  | O-C-N      | -9.31 | 108.83      | 122.43   |
| 1   | D     | 604 | ASN  | CA-CB-CG   | 9.30  | 121.91      | 112.60   |
| 4   | 1     | 3   | ASP  | CA-CB-CG   | 9.30  | 121.90      | 112.60   |
| 2   | H     | 138 | ALA  | O-C-N      | -9.30 | 108.85      | 122.43   |
| 4   | 3     | 3   | ASP  | CA-CB-CG   | 9.30  | 121.90      | 112.60   |
| 4   | 7     | 3   | ASP  | CA-CB-CG   | 9.28  | 121.88      | 112.60   |
| 4   | 0     | 3   | ASP  | CA-CB-CG   | 9.27  | 121.87      | 112.60   |
| 4   | Y     | 3   | ASP  | CA-CB-CG   | 9.24  | 121.84      | 112.60   |
| 4   | Z     | 3   | ASP  | CA-CB-CG   | 9.23  | 121.83      | 112.60   |
| 4   | 4     | 3   | ASP  | CA-CB-CG   | 9.23  | 121.83      | 112.60   |
| 4   | 5     | 3   | ASP  | CA-CB-CG   | 9.22  | 121.82      | 112.60   |
| 4   | X     | 3   | ASP  | CA-CB-CG   | 9.22  | 121.82      | 112.60   |
| 4   | 8     | 3   | ASP  | CA-CB-CG   | 9.21  | 121.81      | 112.60   |
| 4   | W     | 3   | ASP  | CA-CB-CG   | 9.20  | 121.80      | 112.60   |
| 4   | V     | 3   | ASP  | CA-CB-CG   | 9.20  | 121.80      | 112.60   |
| 4   | 2     | 3   | ASP  | CA-CB-CG   | 9.18  | 121.78      | 112.60   |
| 4   | 9     | 3   | ASP  | CA-CB-CG   | 9.17  | 121.77      | 112.60   |
| 4   | 8     | 179 | ASP  | CA-CB-CG   | 8.83  | 121.43      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | 0     | 179 | ASP  | CA-CB-CG | 8.83  | 121.43      | 112.60   |
| 1   | A     | 264 | ASP  | CB-CA-C  | -8.82 | 100.49      | 111.43   |
| 4   | V     | 179 | ASP  | CA-CB-CG | 8.82  | 121.42      | 112.60   |
| 4   | 3     | 179 | ASP  | CA-CB-CG | 8.82  | 121.42      | 112.60   |
| 4   | 7     | 179 | ASP  | CA-CB-CG | 8.81  | 121.42      | 112.60   |
| 4   | 4     | 179 | ASP  | CA-CB-CG | 8.81  | 121.41      | 112.60   |
| 1   | J     | 264 | ASP  | CB-CA-C  | -8.80 | 100.52      | 111.43   |
| 4   | 5     | 179 | ASP  | CA-CB-CG | 8.78  | 121.38      | 112.60   |
| 1   | D     | 264 | ASP  | CB-CA-C  | -8.78 | 100.55      | 111.43   |
| 4   | 2     | 179 | ASP  | CA-CB-CG | 8.78  | 121.38      | 112.60   |
| 4   | 9     | 179 | ASP  | CA-CB-CG | 8.77  | 121.37      | 112.60   |
| 4   | W     | 179 | ASP  | CA-CB-CG | 8.77  | 121.37      | 112.60   |
| 4   | 1     | 179 | ASP  | CA-CB-CG | 8.76  | 121.36      | 112.60   |
| 1   | G     | 264 | ASP  | CB-CA-C  | -8.76 | 100.57      | 111.43   |
| 4   | Y     | 179 | ASP  | CA-CB-CG | 8.74  | 121.34      | 112.60   |
| 4   | Z     | 179 | ASP  | CA-CB-CG | 8.72  | 121.32      | 112.60   |
| 4   | X     | 179 | ASP  | CA-CB-CG | 8.71  | 121.31      | 112.60   |
| 1   | J     | 752 | ASP  | CA-CB-CG | 8.68  | 121.28      | 112.60   |
| 1   | G     | 752 | ASP  | CA-CB-CG | 8.61  | 121.21      | 112.60   |
| 1   | D     | 784 | ALA  | N-CA-C   | -8.60 | 101.86      | 111.07   |
| 1   | A     | 784 | ALA  | N-CA-C   | -8.60 | 101.87      | 111.07   |
| 1   | D     | 752 | ASP  | CA-CB-CG | 8.60  | 121.20      | 112.60   |
| 1   | A     | 752 | ASP  | CA-CB-CG | 8.58  | 121.18      | 112.60   |
| 1   | J     | 264 | ASP  | N-CA-CB  | -8.40 | 97.92       | 110.86   |
| 1   | A     | 264 | ASP  | N-CA-CB  | -8.37 | 97.97       | 110.86   |
| 1   | J     | 219 | GLU  | N-CA-C   | -8.35 | 93.01       | 110.80   |
| 1   | G     | 219 | GLU  | N-CA-C   | -8.34 | 93.03       | 110.80   |
| 1   | G     | 756 | THR  | N-CA-CB  | -8.33 | 97.56       | 110.39   |
| 1   | D     | 264 | ASP  | N-CA-CB  | -8.32 | 98.04       | 110.86   |
| 1   | D     | 752 | ASP  | CB-CA-C  | 8.32  | 121.46      | 111.22   |
| 1   | G     | 264 | ASP  | N-CA-CB  | -8.32 | 98.04       | 110.86   |
| 1   | G     | 141 | LEU  | CB-CA-C  | -8.30 | 97.79       | 110.90   |
| 1   | J     | 752 | ASP  | CB-CA-C  | 8.29  | 121.42      | 111.22   |
| 1   | J     | 141 | LEU  | CB-CA-C  | -8.29 | 97.81       | 110.90   |
| 1   | A     | 219 | GLU  | N-CA-C   | -8.28 | 93.17       | 110.80   |
| 1   | A     | 752 | ASP  | CB-CA-C  | 8.28  | 121.40      | 111.22   |
| 1   | G     | 752 | ASP  | CB-CA-C  | 8.27  | 121.39      | 111.22   |
| 1   | J     | 756 | THR  | N-CA-CB  | -8.27 | 97.66       | 110.39   |
| 1   | D     | 756 | THR  | N-CA-CB  | -8.26 | 97.67       | 110.39   |
| 1   | A     | 315 | VAL  | N-CA-C   | 8.25  | 120.01      | 112.17   |
| 1   | J     | 75  | ASP  | N-CA-CB  | 8.25  | 123.00      | 110.79   |
| 1   | D     | 141 | LEU  | CB-CA-C  | -8.24 | 97.89       | 110.90   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 756 | THR  | N-CA-CB   | -8.23 | 97.71       | 110.39   |
| 1   | D     | 219 | GLU  | N-CA-C    | -8.21 | 93.32       | 110.80   |
| 1   | A     | 141 | LEU  | CB-CA-C   | -8.20 | 97.94       | 110.90   |
| 1   | D     | 315 | VAL  | N-CA-C    | 8.19  | 119.95      | 112.17   |
| 1   | A     | 75  | ASP  | N-CA-CB   | 8.19  | 122.91      | 110.79   |
| 1   | G     | 315 | VAL  | N-CA-C    | 8.15  | 119.92      | 112.17   |
| 1   | J     | 800 | ARG  | NE-CZ-NH2 | -8.11 | 111.91      | 119.20   |
| 1   | G     | 625 | THR  | CA-CB-OG1 | 8.08  | 121.72      | 109.60   |
| 1   | J     | 315 | VAL  | N-CA-C    | 8.07  | 119.84      | 112.17   |
| 1   | D     | 75  | ASP  | N-CA-CB   | 8.06  | 122.72      | 110.79   |
| 1   | D     | 625 | THR  | CA-CB-OG1 | 8.06  | 121.69      | 109.60   |
| 4   | 1     | 363 | ASP  | CA-CB-CG  | 8.03  | 120.62      | 112.60   |
| 4   | 3     | 363 | ASP  | CA-CB-CG  | 8.03  | 120.63      | 112.60   |
| 4   | Z     | 363 | ASP  | CA-CB-CG  | 8.02  | 120.62      | 112.60   |
| 1   | J     | 625 | THR  | CA-CB-OG1 | 8.02  | 121.62      | 109.60   |
| 4   | X     | 363 | ASP  | CA-CB-CG  | 8.02  | 120.62      | 112.60   |
| 4   | W     | 363 | ASP  | CA-CB-CG  | 8.01  | 120.61      | 112.60   |
| 1   | A     | 625 | THR  | CA-CB-OG1 | 8.00  | 121.61      | 109.60   |
| 4   | 2     | 363 | ASP  | CA-CB-CG  | 8.00  | 120.60      | 112.60   |
| 4   | Y     | 363 | ASP  | CA-CB-CG  | 7.99  | 120.59      | 112.60   |
| 4   | 7     | 363 | ASP  | CA-CB-CG  | 7.98  | 120.58      | 112.60   |
| 4   | 9     | 363 | ASP  | CA-CB-CG  | 7.97  | 120.58      | 112.60   |
| 4   | 8     | 363 | ASP  | CA-CB-CG  | 7.97  | 120.57      | 112.60   |
| 4   | 5     | 363 | ASP  | CA-CB-CG  | 7.97  | 120.57      | 112.60   |
| 4   | 4     | 363 | ASP  | CA-CB-CG  | 7.96  | 120.56      | 112.60   |
| 1   | G     | 473 | ASN  | CA-CB-CG  | -7.96 | 104.64      | 112.60   |
| 1   | D     | 641 | LYS  | CA-C-N    | 7.95  | 131.98      | 120.38   |
| 1   | D     | 641 | LYS  | C-N-CA    | 7.95  | 131.98      | 120.38   |
| 4   | 0     | 363 | ASP  | CA-CB-CG  | 7.94  | 120.54      | 112.60   |
| 1   | A     | 473 | ASN  | CA-CB-CG  | -7.93 | 104.67      | 112.60   |
| 4   | V     | 363 | ASP  | CA-CB-CG  | 7.92  | 120.52      | 112.60   |
| 4   | 1     | 286 | ASP  | CA-CB-CG  | 7.89  | 120.50      | 112.60   |
| 4   | 7     | 286 | ASP  | CA-CB-CG  | 7.89  | 120.49      | 112.60   |
| 4   | 0     | 286 | ASP  | CA-CB-CG  | 7.89  | 120.49      | 112.60   |
| 1   | D     | 800 | ARG  | NE-CZ-NH2 | -7.89 | 112.10      | 119.20   |
| 4   | V     | 128 | ASN  | CA-CB-CG  | 7.89  | 120.49      | 112.60   |
| 4   | 4     | 286 | ASP  | CA-CB-CG  | 7.88  | 120.48      | 112.60   |
| 4   | 8     | 286 | ASP  | CA-CB-CG  | 7.88  | 120.48      | 112.60   |
| 4   | W     | 286 | ASP  | CA-CB-CG  | 7.88  | 120.48      | 112.60   |
| 4   | Z     | 128 | ASN  | CA-CB-CG  | 7.88  | 120.48      | 112.60   |
| 4   | W     | 128 | ASN  | CA-CB-CG  | 7.87  | 120.47      | 112.60   |
| 4   | Z     | 286 | ASP  | CA-CB-CG  | 7.87  | 120.47      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 5     | 128 | ASN  | CA-CB-CG  | 7.87  | 120.47      | 112.60   |
| 1   | D     | 473 | ASN  | CA-CB-CG  | -7.87 | 104.73      | 112.60   |
| 4   | 0     | 128 | ASN  | CA-CB-CG  | 7.87  | 120.47      | 112.60   |
| 4   | 8     | 128 | ASN  | CA-CB-CG  | 7.86  | 120.46      | 112.60   |
| 4   | 9     | 286 | ASP  | CA-CB-CG  | 7.86  | 120.46      | 112.60   |
| 4   | 2     | 286 | ASP  | CA-CB-CG  | 7.86  | 120.46      | 112.60   |
| 4   | X     | 286 | ASP  | CA-CB-CG  | 7.86  | 120.46      | 112.60   |
| 4   | 7     | 128 | ASN  | CA-CB-CG  | 7.86  | 120.46      | 112.60   |
| 4   | Y     | 286 | ASP  | CA-CB-CG  | 7.86  | 120.46      | 112.60   |
| 4   | 5     | 286 | ASP  | CA-CB-CG  | 7.85  | 120.45      | 112.60   |
| 1   | J     | 473 | ASN  | CA-CB-CG  | -7.85 | 104.75      | 112.60   |
| 1   | J     | 547 | ASP  | N-CA-C    | -7.85 | 102.67      | 111.07   |
| 1   | A     | 800 | ARG  | NE-CZ-NH2 | -7.84 | 112.15      | 119.20   |
| 2   | K     | 129 | THR  | CB-CA-C   | -7.84 | 94.73       | 110.17   |
| 1   | A     | 641 | LYS  | CA-C-N    | 7.84  | 131.82      | 120.38   |
| 1   | A     | 641 | LYS  | C-N-CA    | 7.84  | 131.82      | 120.38   |
| 4   | V     | 286 | ASP  | CA-CB-CG  | 7.83  | 120.44      | 112.60   |
| 4   | 9     | 128 | ASN  | CA-CB-CG  | 7.83  | 120.43      | 112.60   |
| 4   | 4     | 128 | ASN  | CA-CB-CG  | 7.83  | 120.43      | 112.60   |
| 1   | G     | 547 | ASP  | N-CA-C    | -7.82 | 102.76      | 111.28   |
| 1   | D     | 547 | ASP  | N-CA-C    | -7.82 | 102.71      | 111.07   |
| 1   | G     | 800 | ARG  | NE-CZ-NH2 | -7.82 | 112.17      | 119.20   |
| 4   | 3     | 128 | ASN  | CA-CB-CG  | 7.82  | 120.42      | 112.60   |
| 4   | Y     | 128 | ASN  | CA-CB-CG  | 7.81  | 120.41      | 112.60   |
| 4   | 1     | 128 | ASN  | CA-CB-CG  | 7.81  | 120.41      | 112.60   |
| 4   | 2     | 128 | ASN  | CA-CB-CG  | 7.81  | 120.41      | 112.60   |
| 4   | X     | 128 | ASN  | CA-CB-CG  | 7.81  | 120.41      | 112.60   |
| 4   | 3     | 286 | ASP  | CA-CB-CG  | 7.81  | 120.41      | 112.60   |
| 1   | J     | 641 | LYS  | CA-C-N    | 7.80  | 131.77      | 120.38   |
| 1   | J     | 641 | LYS  | C-N-CA    | 7.80  | 131.77      | 120.38   |
| 1   | G     | 641 | LYS  | CA-C-N    | 7.80  | 131.76      | 120.38   |
| 1   | G     | 641 | LYS  | C-N-CA    | 7.80  | 131.76      | 120.38   |
| 1   | A     | 547 | ASP  | N-CA-C    | -7.79 | 102.74      | 111.07   |
| 2   | H     | 129 | THR  | CB-CA-C   | -7.76 | 94.89       | 110.17   |
| 2   | E     | 129 | THR  | CB-CA-C   | -7.75 | 94.90       | 110.17   |
| 2   | B     | 129 | THR  | CB-CA-C   | -7.74 | 94.92       | 110.17   |
| 1   | J     | 784 | ALA  | N-CA-C    | -7.73 | 101.83      | 111.11   |
| 4   | 9     | 25  | ASP  | CA-CB-CG  | 7.72  | 120.32      | 112.60   |
| 1   | J     | 447 | GLN  | N-CA-CB   | 7.71  | 121.46      | 110.12   |
| 1   | A     | 447 | GLN  | N-CA-CB   | 7.69  | 121.42      | 110.12   |
| 4   | 3     | 25  | ASP  | CA-CB-CG  | 7.68  | 120.28      | 112.60   |
| 4   | 4     | 25  | ASP  | CA-CB-CG  | 7.67  | 120.27      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | 5     | 25  | ASP  | CA-CB-CG | 7.67  | 120.27      | 112.60   |
| 1   | G     | 75  | ASP  | N-CA-CB  | 7.66  | 123.02      | 110.91   |
| 4   | 8     | 25  | ASP  | CA-CB-CG | 7.66  | 120.26      | 112.60   |
| 4   | Y     | 25  | ASP  | CA-CB-CG | 7.66  | 120.26      | 112.60   |
| 4   | 1     | 25  | ASP  | CA-CB-CG | 7.65  | 120.25      | 112.60   |
| 4   | 0     | 25  | ASP  | CA-CB-CG | 7.65  | 120.25      | 112.60   |
| 4   | 2     | 223 | PHE  | CA-CB-CG | 7.64  | 121.44      | 113.80   |
| 4   | 4     | 223 | PHE  | CA-CB-CG | 7.64  | 121.44      | 113.80   |
| 4   | V     | 25  | ASP  | CA-CB-CG | 7.64  | 120.24      | 112.60   |
| 2   | B     | 149 | ASP  | N-CA-CB  | 7.63  | 120.91      | 110.38   |
| 4   | 7     | 360 | GLN  | N-CA-C   | -7.63 | 102.66      | 110.97   |
| 3   | F     | 62  | ALA  | CA-C-N   | -7.63 | 112.52      | 122.51   |
| 3   | F     | 62  | ALA  | C-N-CA   | -7.63 | 112.52      | 122.51   |
| 1   | G     | 447 | GLN  | N-CA-CB  | 7.62  | 121.33      | 110.12   |
| 1   | D     | 447 | GLN  | N-CA-CB  | 7.62  | 121.33      | 110.12   |
| 2   | H     | 149 | ASP  | N-CA-CB  | 7.62  | 120.90      | 110.38   |
| 4   | 7     | 25  | ASP  | CA-CB-CG | 7.62  | 120.22      | 112.60   |
| 4   | Z     | 25  | ASP  | CA-CB-CG | 7.62  | 120.22      | 112.60   |
| 4   | X     | 360 | GLN  | N-CA-C   | -7.62 | 102.67      | 110.97   |
| 4   | 8     | 360 | GLN  | N-CA-C   | -7.61 | 102.67      | 110.97   |
| 4   | W     | 25  | ASP  | CA-CB-CG | 7.61  | 120.21      | 112.60   |
| 1   | A     | 698 | ASN  | CB-CA-C  | -7.61 | 98.01       | 110.79   |
| 4   | X     | 25  | ASP  | CA-CB-CG | 7.61  | 120.21      | 112.60   |
| 4   | X     | 223 | PHE  | CA-CB-CG | 7.60  | 121.40      | 113.80   |
| 2   | K     | 149 | ASP  | N-CA-CB  | 7.60  | 120.86      | 110.38   |
| 4   | 4     | 360 | GLN  | N-CA-C   | -7.60 | 102.69      | 110.97   |
| 4   | 7     | 223 | PHE  | CA-CB-CG | 7.60  | 121.40      | 113.80   |
| 4   | 2     | 25  | ASP  | CA-CB-CG | 7.59  | 120.19      | 112.60   |
| 4   | 2     | 360 | GLN  | N-CA-C   | -7.59 | 102.69      | 110.97   |
| 3   | I     | 62  | ALA  | CA-C-N   | -7.59 | 112.57      | 122.51   |
| 3   | I     | 62  | ALA  | C-N-CA   | -7.59 | 112.57      | 122.51   |
| 4   | 9     | 223 | PHE  | CA-CB-CG | 7.58  | 121.39      | 113.80   |
| 4   | 0     | 223 | PHE  | CA-CB-CG | 7.58  | 121.38      | 113.80   |
| 1   | A     | 202 | SER  | CB-CA-C  | -7.58 | 95.34       | 110.42   |
| 1   | D     | 202 | SER  | CB-CA-C  | -7.57 | 95.35       | 110.42   |
| 1   | G     | 784 | ALA  | N-CA-C   | -7.57 | 102.02      | 111.11   |
| 4   | 8     | 223 | PHE  | CA-CB-CG | 7.57  | 121.37      | 113.80   |
| 4   | Y     | 223 | PHE  | CA-CB-CG | 7.57  | 121.37      | 113.80   |
| 4   | 1     | 223 | PHE  | CA-CB-CG | 7.57  | 121.37      | 113.80   |
| 4   | W     | 223 | PHE  | CA-CB-CG | 7.57  | 121.37      | 113.80   |
| 1   | G     | 202 | SER  | CB-CA-C  | -7.57 | 95.36       | 110.42   |
| 4   | 3     | 223 | PHE  | CA-CB-CG | 7.57  | 121.37      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 1     | 252 | ASN  | OD1-CG-ND2 | -7.56 | 115.04      | 122.60   |
| 4   | 3     | 360 | GLN  | N-CA-C     | -7.56 | 102.73      | 110.97   |
| 4   | V     | 223 | PHE  | CA-CB-CG   | 7.56  | 121.36      | 113.80   |
| 1   | J     | 202 | SER  | CB-CA-C    | -7.56 | 95.38       | 110.42   |
| 4   | V     | 360 | GLN  | N-CA-C     | -7.55 | 102.74      | 110.97   |
| 4   | 5     | 223 | PHE  | CA-CB-CG   | 7.55  | 121.35      | 113.80   |
| 4   | 8     | 215 | LYS  | N-CA-C     | 7.54  | 119.29      | 111.14   |
| 4   | Z     | 223 | PHE  | CA-CB-CG   | 7.54  | 121.34      | 113.80   |
| 4   | 7     | 252 | ASN  | OD1-CG-ND2 | -7.54 | 115.06      | 122.60   |
| 4   | 9     | 252 | ASN  | OD1-CG-ND2 | -7.54 | 115.06      | 122.60   |
| 4   | Y     | 360 | GLN  | N-CA-C     | -7.54 | 102.76      | 110.97   |
| 1   | J     | 698 | ASN  | CB-CA-C    | -7.53 | 98.13       | 110.79   |
| 4   | V     | 215 | LYS  | N-CA-C     | 7.53  | 119.28      | 111.14   |
| 4   | 5     | 360 | GLN  | N-CA-C     | -7.53 | 102.76      | 110.97   |
| 2   | K     | 141 | PRO  | N-CA-CB    | -7.53 | 95.78       | 103.08   |
| 4   | Z     | 173 | HIS  | CA-CB-CG   | -7.53 | 106.27      | 113.80   |
| 4   | Z     | 360 | GLN  | N-CA-C     | -7.53 | 102.76      | 110.97   |
| 4   | 0     | 252 | ASN  | OD1-CG-ND2 | -7.52 | 115.08      | 122.60   |
| 4   | 9     | 360 | GLN  | N-CA-C     | -7.52 | 102.77      | 110.97   |
| 1   | G     | 698 | ASN  | CB-CA-C    | -7.52 | 98.15       | 110.79   |
| 4   | W     | 360 | GLN  | N-CA-C     | -7.52 | 102.77      | 110.97   |
| 4   | W     | 252 | ASN  | OD1-CG-ND2 | -7.52 | 115.08      | 122.60   |
| 4   | 0     | 360 | GLN  | N-CA-C     | -7.52 | 102.78      | 110.97   |
| 4   | X     | 173 | HIS  | CA-CB-CG   | -7.51 | 106.29      | 113.80   |
| 4   | Y     | 215 | LYS  | N-CA-C     | 7.51  | 119.25      | 111.14   |
| 4   | 0     | 62  | ARG  | N-CA-C     | 7.51  | 120.34      | 111.71   |
| 3   | L     | 62  | ALA  | CA-C-N     | -7.50 | 112.68      | 122.51   |
| 3   | L     | 62  | ALA  | C-N-CA     | -7.50 | 112.68      | 122.51   |
| 4   | 8     | 252 | ASN  | OD1-CG-ND2 | -7.50 | 115.09      | 122.60   |
| 4   | 5     | 252 | ASN  | OD1-CG-ND2 | -7.50 | 115.10      | 122.60   |
| 4   | Z     | 215 | LYS  | N-CA-C     | 7.50  | 119.24      | 111.14   |
| 4   | 2     | 252 | ASN  | OD1-CG-ND2 | -7.50 | 115.10      | 122.60   |
| 4   | 3     | 173 | HIS  | CA-CB-CG   | -7.50 | 106.31      | 113.80   |
| 4   | 7     | 173 | HIS  | CA-CB-CG   | -7.49 | 106.31      | 113.80   |
| 4   | 9     | 62  | ARG  | N-CA-C     | 7.49  | 120.33      | 111.71   |
| 2   | E     | 149 | ASP  | N-CA-CB    | 7.49  | 120.72      | 110.38   |
| 4   | Y     | 252 | ASN  | OD1-CG-ND2 | -7.49 | 115.11      | 122.60   |
| 4   | 3     | 215 | LYS  | N-CA-C     | 7.48  | 119.22      | 111.14   |
| 1   | D     | 698 | ASN  | CB-CA-C    | -7.48 | 98.22       | 110.79   |
| 4   | 4     | 252 | ASN  | OD1-CG-ND2 | -7.48 | 115.12      | 122.60   |
| 2   | B     | 140 | PHE  | O-C-N      | -7.48 | 112.72      | 121.32   |
| 4   | 9     | 215 | LYS  | N-CA-C     | 7.47  | 119.21      | 111.14   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | C     | 62  | ALA  | CA-C-N     | -7.47 | 112.72      | 122.51   |
| 3   | C     | 62  | ALA  | C-N-CA     | -7.47 | 112.72      | 122.51   |
| 4   | 1     | 215 | LYS  | N-CA-C     | 7.47  | 119.21      | 111.14   |
| 4   | 2     | 62  | ARG  | N-CA-C     | 7.47  | 120.30      | 111.71   |
| 4   | 9     | 173 | HIS  | CA-CB-CG   | -7.47 | 106.33      | 113.80   |
| 4   | Z     | 62  | ARG  | N-CA-C     | 7.47  | 120.30      | 111.71   |
| 4   | W     | 62  | ARG  | N-CA-C     | 7.47  | 120.30      | 111.71   |
| 4   | 2     | 215 | LYS  | N-CA-C     | 7.47  | 119.21      | 111.14   |
| 4   | 5     | 62  | ARG  | N-CA-C     | 7.47  | 120.30      | 111.71   |
| 4   | W     | 173 | HIS  | CA-CB-CG   | -7.47 | 106.33      | 113.80   |
| 4   | Z     | 252 | ASN  | OD1-CG-ND2 | -7.47 | 115.13      | 122.60   |
| 4   | V     | 252 | ASN  | OD1-CG-ND2 | -7.47 | 115.13      | 122.60   |
| 4   | 1     | 360 | GLN  | N-CA-C     | -7.47 | 102.83      | 110.97   |
| 2   | E     | 140 | PHE  | O-C-N      | -7.46 | 112.74      | 121.32   |
| 4   | 0     | 215 | LYS  | N-CA-C     | 7.46  | 119.20      | 111.14   |
| 4   | 3     | 62  | ARG  | N-CA-C     | 7.46  | 120.29      | 111.71   |
| 4   | 1     | 62  | ARG  | N-CA-C     | 7.46  | 120.29      | 111.71   |
| 4   | 3     | 252 | ASN  | OD1-CG-ND2 | -7.46 | 115.14      | 122.60   |
| 4   | 2     | 173 | HIS  | CA-CB-CG   | -7.46 | 106.34      | 113.80   |
| 4   | 8     | 173 | HIS  | CA-CB-CG   | -7.46 | 106.34      | 113.80   |
| 4   | 5     | 215 | LYS  | N-CA-C     | 7.45  | 119.19      | 111.14   |
| 4   | 7     | 62  | ARG  | N-CA-C     | 7.45  | 120.28      | 111.71   |
| 4   | V     | 62  | ARG  | N-CA-C     | 7.45  | 120.27      | 111.71   |
| 4   | Y     | 62  | ARG  | N-CA-C     | 7.45  | 120.27      | 111.71   |
| 4   | 4     | 62  | ARG  | N-CA-C     | 7.44  | 120.27      | 111.71   |
| 4   | V     | 173 | HIS  | CA-CB-CG   | -7.44 | 106.36      | 113.80   |
| 4   | 8     | 62  | ARG  | N-CA-C     | 7.44  | 120.27      | 111.71   |
| 4   | 4     | 173 | HIS  | CA-CB-CG   | -7.44 | 106.36      | 113.80   |
| 4   | X     | 62  | ARG  | N-CA-C     | 7.44  | 120.27      | 111.71   |
| 4   | 4     | 215 | LYS  | N-CA-C     | 7.44  | 119.17      | 111.14   |
| 4   | 7     | 215 | LYS  | N-CA-C     | 7.43  | 119.17      | 111.14   |
| 4   | Y     | 173 | HIS  | CA-CB-CG   | -7.43 | 106.37      | 113.80   |
| 2   | E     | 141 | PRO  | N-CA-CB    | -7.42 | 95.88       | 103.08   |
| 4   | 1     | 173 | HIS  | CA-CB-CG   | -7.42 | 106.38      | 113.80   |
| 4   | X     | 215 | LYS  | N-CA-C     | 7.42  | 119.15      | 111.14   |
| 4   | W     | 215 | LYS  | N-CA-C     | 7.41  | 119.15      | 111.14   |
| 2   | H     | 141 | PRO  | N-CA-CB    | -7.41 | 95.89       | 103.08   |
| 4   | 5     | 173 | HIS  | CA-CB-CG   | -7.41 | 106.39      | 113.80   |
| 4   | X     | 252 | ASN  | OD1-CG-ND2 | -7.41 | 115.19      | 122.60   |
| 2   | B     | 141 | PRO  | N-CA-CB    | -7.39 | 95.91       | 103.08   |
| 4   | 0     | 173 | HIS  | CA-CB-CG   | -7.39 | 106.41      | 113.80   |
| 2   | H     | 140 | PHE  | O-C-N      | -7.37 | 112.84      | 121.32   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 506 | GLU  | CA-C-N    | -7.37 | 112.46      | 122.63   |
| 1   | D     | 506 | GLU  | C-N-CA    | -7.37 | 112.46      | 122.63   |
| 4   | 8     | 34  | ILE  | CA-CB-CG2 | -7.34 | 98.03       | 110.50   |
| 4   | 5     | 34  | ILE  | CA-CB-CG2 | -7.33 | 98.03       | 110.50   |
| 4   | 4     | 34  | ILE  | CA-CB-CG2 | -7.32 | 98.06       | 110.50   |
| 4   | V     | 34  | ILE  | CA-CB-CG2 | -7.31 | 98.07       | 110.50   |
| 4   | Y     | 34  | ILE  | CA-CB-CG2 | -7.31 | 98.08       | 110.50   |
| 4   | 3     | 34  | ILE  | CA-CB-CG2 | -7.31 | 98.08       | 110.50   |
| 4   | Z     | 34  | ILE  | CA-CB-CG2 | -7.30 | 98.08       | 110.50   |
| 2   | K     | 140 | PHE  | O-C-N     | -7.30 | 112.93      | 121.32   |
| 4   | 1     | 34  | ILE  | CA-CB-CG2 | -7.30 | 98.09       | 110.50   |
| 4   | 0     | 34  | ILE  | CA-CB-CG2 | -7.29 | 98.10       | 110.50   |
| 4   | 7     | 34  | ILE  | CA-CB-CG2 | -7.29 | 98.11       | 110.50   |
| 4   | X     | 34  | ILE  | CA-CB-CG2 | -7.28 | 98.12       | 110.50   |
| 4   | 7     | 159 | VAL  | CB-CA-C   | -7.28 | 99.05       | 110.69   |
| 4   | X     | 159 | VAL  | CB-CA-C   | -7.28 | 99.05       | 110.69   |
| 4   | Y     | 159 | VAL  | CB-CA-C   | -7.28 | 99.05       | 110.69   |
| 4   | W     | 34  | ILE  | CA-CB-CG2 | -7.28 | 98.13       | 110.50   |
| 4   | 9     | 34  | ILE  | CA-CB-CG2 | -7.27 | 98.14       | 110.50   |
| 4   | 2     | 34  | ILE  | CA-CB-CG2 | -7.27 | 98.14       | 110.50   |
| 1   | G     | 76  | GLN  | N-CA-C    | -7.26 | 102.72      | 113.61   |
| 1   | D     | 76  | GLN  | N-CA-C    | -7.26 | 102.72      | 113.61   |
| 4   | 0     | 159 | VAL  | CB-CA-C   | -7.26 | 99.07       | 110.69   |
| 4   | W     | 159 | VAL  | CB-CA-C   | -7.26 | 99.07       | 110.69   |
| 4   | 2     | 159 | VAL  | CB-CA-C   | -7.26 | 99.08       | 110.69   |
| 4   | 1     | 159 | VAL  | CB-CA-C   | -7.25 | 99.09       | 110.69   |
| 4   | 3     | 159 | VAL  | CB-CA-C   | -7.25 | 99.08       | 110.69   |
| 4   | 8     | 159 | VAL  | CB-CA-C   | -7.25 | 99.08       | 110.69   |
| 4   | 5     | 159 | VAL  | CB-CA-C   | -7.25 | 99.09       | 110.69   |
| 4   | 4     | 159 | VAL  | CB-CA-C   | -7.25 | 99.10       | 110.69   |
| 4   | Z     | 159 | VAL  | CB-CA-C   | -7.24 | 99.10       | 110.69   |
| 1   | A     | 76  | GLN  | N-CA-C    | -7.24 | 102.75      | 113.61   |
| 4   | V     | 159 | VAL  | CB-CA-C   | -7.24 | 99.11       | 110.69   |
| 4   | X     | 323 | SER  | N-CA-C    | 7.23  | 121.73      | 112.34   |
| 1   | G     | 506 | GLU  | CA-C-N    | -7.22 | 112.66      | 122.63   |
| 1   | G     | 506 | GLU  | C-N-CA    | -7.22 | 112.66      | 122.63   |
| 1   | A     | 506 | GLU  | CA-C-N    | -7.22 | 112.66      | 122.63   |
| 1   | A     | 506 | GLU  | C-N-CA    | -7.22 | 112.66      | 122.63   |
| 4   | 9     | 159 | VAL  | CB-CA-C   | -7.22 | 99.14       | 110.69   |
| 1   | J     | 506 | GLU  | CA-C-N    | -7.21 | 112.68      | 122.63   |
| 1   | J     | 506 | GLU  | C-N-CA    | -7.21 | 112.68      | 122.63   |
| 4   | V     | 323 | SER  | N-CA-C    | 7.21  | 121.71      | 112.34   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | W     | 323 | SER  | N-CA-C    | 7.21  | 121.71      | 112.34   |
| 1   | J     | 76  | GLN  | N-CA-C    | -7.18 | 102.84      | 113.61   |
| 1   | G     | 625 | THR  | CA-CB-CG2 | -7.17 | 98.30       | 110.50   |
| 4   | 7     | 323 | SER  | N-CA-C    | 7.17  | 121.67      | 112.34   |
| 1   | A     | 625 | THR  | CA-CB-CG2 | -7.17 | 98.31       | 110.50   |
| 4   | 2     | 259 | GLU  | CB-CG-CD  | 7.16  | 124.78      | 112.60   |
| 4   | 2     | 323 | SER  | N-CA-C    | 7.16  | 121.65      | 112.34   |
| 4   | 4     | 259 | GLU  | CB-CG-CD  | 7.16  | 124.78      | 112.60   |
| 4   | Z     | 259 | GLU  | CB-CG-CD  | 7.16  | 124.78      | 112.60   |
| 4   | 9     | 323 | SER  | N-CA-C    | 7.16  | 121.65      | 112.34   |
| 1   | J     | 625 | THR  | CA-CB-CG2 | -7.16 | 98.33       | 110.50   |
| 4   | 5     | 259 | GLU  | CB-CG-CD  | 7.16  | 124.76      | 112.60   |
| 4   | W     | 259 | GLU  | CB-CG-CD  | 7.15  | 124.76      | 112.60   |
| 4   | 4     | 323 | SER  | N-CA-C    | 7.15  | 121.64      | 112.34   |
| 4   | 8     | 259 | GLU  | CB-CG-CD  | 7.15  | 124.76      | 112.60   |
| 4   | 1     | 259 | GLU  | CB-CG-CD  | 7.15  | 124.75      | 112.60   |
| 4   | X     | 259 | GLU  | CB-CG-CD  | 7.15  | 124.75      | 112.60   |
| 4   | Y     | 323 | SER  | N-CA-C    | 7.15  | 121.63      | 112.34   |
| 4   | 9     | 259 | GLU  | CB-CG-CD  | 7.15  | 124.75      | 112.60   |
| 4   | 5     | 323 | SER  | N-CA-C    | 7.14  | 121.63      | 112.34   |
| 4   | V     | 259 | GLU  | CB-CG-CD  | 7.14  | 124.75      | 112.60   |
| 4   | Z     | 323 | SER  | N-CA-C    | 7.14  | 121.62      | 112.34   |
| 4   | 0     | 259 | GLU  | CB-CG-CD  | 7.14  | 124.73      | 112.60   |
| 4   | Y     | 259 | GLU  | CB-CG-CD  | 7.13  | 124.72      | 112.60   |
| 4   | 8     | 323 | SER  | N-CA-C    | 7.13  | 121.61      | 112.34   |
| 1   | D     | 625 | THR  | CA-CB-CG2 | -7.12 | 98.39       | 110.50   |
| 4   | 7     | 259 | GLU  | CB-CG-CD  | 7.12  | 124.71      | 112.60   |
| 4   | 3     | 259 | GLU  | CB-CG-CD  | 7.12  | 124.70      | 112.60   |
| 4   | 0     | 323 | SER  | N-CA-C    | 7.12  | 121.59      | 112.34   |
| 4   | 3     | 323 | SER  | N-CA-C    | 7.11  | 121.58      | 112.34   |
| 4   | 1     | 323 | SER  | N-CA-C    | 7.11  | 121.58      | 112.34   |
| 1   | J     | 652 | LEU  | O-C-N     | 7.07  | 130.31      | 122.11   |
| 4   | X     | 69  | TYR  | CA-C-N    | 7.05  | 126.76      | 119.56   |
| 4   | X     | 69  | TYR  | C-N-CA    | 7.05  | 126.76      | 119.56   |
| 4   | 8     | 69  | TYR  | CA-C-N    | 7.04  | 126.74      | 119.56   |
| 4   | 8     | 69  | TYR  | C-N-CA    | 7.04  | 126.74      | 119.56   |
| 1   | D     | 686 | MET  | CA-C-N    | -7.04 | 111.35      | 121.42   |
| 1   | D     | 686 | MET  | C-N-CA    | -7.04 | 111.35      | 121.42   |
| 4   | Y     | 69  | TYR  | CA-C-N    | 7.03  | 126.73      | 119.56   |
| 4   | Y     | 69  | TYR  | C-N-CA    | 7.03  | 126.73      | 119.56   |
| 4   | 5     | 73  | HIS  | CA-CB-CG  | -7.03 | 106.77      | 113.80   |
| 4   | Z     | 69  | TYR  | CA-C-N    | 7.03  | 126.73      | 119.56   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | Z     | 69  | TYR  | C-N-CA   | 7.03  | 126.73      | 119.56   |
| 4   | V     | 73  | HIS  | CA-CB-CG | -7.01 | 106.79      | 113.80   |
| 4   | V     | 69  | TYR  | CA-C-N   | 7.01  | 126.71      | 119.56   |
| 4   | V     | 69  | TYR  | C-N-CA   | 7.01  | 126.71      | 119.56   |
| 4   | 8     | 73  | HIS  | CA-CB-CG | -7.01 | 106.79      | 113.80   |
| 1   | G     | 652 | LEU  | O-C-N    | 7.01  | 130.24      | 122.11   |
| 4   | 0     | 73  | HIS  | CA-CB-CG | -7.01 | 106.79      | 113.80   |
| 4   | 7     | 73  | HIS  | CA-CB-CG | -7.00 | 106.80      | 113.80   |
| 4   | 2     | 73  | HIS  | CA-CB-CG | -7.00 | 106.80      | 113.80   |
| 4   | 2     | 69  | TYR  | CA-C-N   | 6.99  | 126.69      | 119.56   |
| 4   | 2     | 69  | TYR  | C-N-CA   | 6.99  | 126.69      | 119.56   |
| 4   | W     | 73  | HIS  | CA-CB-CG | -6.99 | 106.81      | 113.80   |
| 4   | 9     | 73  | HIS  | CA-CB-CG | -6.99 | 106.81      | 113.80   |
| 4   | 7     | 69  | TYR  | CA-C-N   | 6.98  | 126.68      | 119.56   |
| 4   | 7     | 69  | TYR  | C-N-CA   | 6.98  | 126.68      | 119.56   |
| 4   | X     | 73  | HIS  | CA-CB-CG | -6.98 | 106.82      | 113.80   |
| 4   | 0     | 69  | TYR  | CA-C-N   | 6.98  | 126.68      | 119.56   |
| 4   | 0     | 69  | TYR  | C-N-CA   | 6.98  | 126.68      | 119.56   |
| 4   | 5     | 287 | ILE  | CB-CA-C  | -6.98 | 102.72      | 112.14   |
| 4   | 4     | 287 | ILE  | CB-CA-C  | -6.97 | 102.72      | 112.14   |
| 4   | 5     | 69  | TYR  | CA-C-N   | 6.97  | 126.67      | 119.56   |
| 4   | 5     | 69  | TYR  | C-N-CA   | 6.97  | 126.67      | 119.56   |
| 4   | 9     | 69  | TYR  | CA-C-N   | 6.97  | 126.67      | 119.56   |
| 4   | 9     | 69  | TYR  | C-N-CA   | 6.97  | 126.67      | 119.56   |
| 4   | 9     | 287 | ILE  | CB-CA-C  | -6.97 | 102.73      | 112.14   |
| 4   | 1     | 287 | ILE  | CB-CA-C  | -6.97 | 102.73      | 112.14   |
| 4   | W     | 69  | TYR  | CA-C-N   | 6.97  | 126.67      | 119.56   |
| 4   | W     | 69  | TYR  | C-N-CA   | 6.97  | 126.67      | 119.56   |
| 4   | X     | 287 | ILE  | CB-CA-C  | -6.97 | 102.73      | 112.14   |
| 1   | A     | 686 | MET  | CA-C-N   | -6.97 | 111.46      | 121.42   |
| 1   | A     | 686 | MET  | C-N-CA   | -6.97 | 111.46      | 121.42   |
| 4   | 0     | 287 | ILE  | CB-CA-C  | -6.97 | 102.73      | 112.14   |
| 4   | 8     | 287 | ILE  | CB-CA-C  | -6.96 | 102.74      | 112.14   |
| 4   | 4     | 73  | HIS  | CA-CB-CG | -6.96 | 106.84      | 113.80   |
| 4   | 3     | 73  | HIS  | CA-CB-CG | -6.96 | 106.84      | 113.80   |
| 4   | V     | 287 | ILE  | CB-CA-C  | -6.96 | 102.74      | 112.14   |
| 4   | 3     | 287 | ILE  | CB-CA-C  | -6.96 | 102.75      | 112.14   |
| 4   | 2     | 287 | ILE  | CB-CA-C  | -6.96 | 102.75      | 112.14   |
| 4   | 3     | 69  | TYR  | CA-C-N   | 6.95  | 126.65      | 119.56   |
| 4   | 3     | 69  | TYR  | C-N-CA   | 6.95  | 126.65      | 119.56   |
| 4   | Z     | 73  | HIS  | CA-CB-CG | -6.95 | 106.85      | 113.80   |
| 4   | Y     | 287 | ILE  | CB-CA-C  | -6.95 | 102.75      | 112.14   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | Y     | 73  | HIS  | CA-CB-CG | -6.95 | 106.85      | 113.80   |
| 4   | 1     | 69  | TYR  | CA-C-N   | 6.95  | 126.64      | 119.56   |
| 4   | 1     | 69  | TYR  | C-N-CA   | 6.95  | 126.64      | 119.56   |
| 4   | 3     | 287 | ILE  | N-CA-C   | 6.95  | 117.70      | 110.62   |
| 4   | 1     | 191 | LYS  | CA-C-O   | -6.94 | 113.55      | 120.70   |
| 4   | X     | 287 | ILE  | N-CA-C   | 6.94  | 117.70      | 110.62   |
| 4   | Z     | 287 | ILE  | CB-CA-C  | -6.94 | 102.77      | 112.14   |
| 1   | D     | 652 | LEU  | O-C-N    | 6.94  | 130.16      | 122.11   |
| 4   | W     | 287 | ILE  | CB-CA-C  | -6.94 | 102.77      | 112.14   |
| 4   | 7     | 287 | ILE  | CB-CA-C  | -6.93 | 102.78      | 112.14   |
| 1   | J     | 686 | MET  | CA-C-N   | -6.93 | 111.51      | 121.42   |
| 1   | J     | 686 | MET  | C-N-CA   | -6.93 | 111.51      | 121.42   |
| 1   | A     | 652 | LEU  | O-C-N    | 6.93  | 130.15      | 122.11   |
| 4   | 1     | 73  | HIS  | CA-CB-CG | -6.92 | 106.88      | 113.80   |
| 4   | 4     | 69  | TYR  | CA-C-N   | 6.92  | 126.62      | 119.56   |
| 4   | 4     | 69  | TYR  | C-N-CA   | 6.92  | 126.62      | 119.56   |
| 4   | W     | 191 | LYS  | CA-C-O   | -6.92 | 113.58      | 120.70   |
| 1   | G     | 686 | MET  | CA-C-N   | -6.90 | 111.55      | 121.42   |
| 1   | G     | 686 | MET  | C-N-CA   | -6.90 | 111.55      | 121.42   |
| 1   | G     | 676 | ILE  | CA-C-N   | 6.90  | 128.46      | 119.84   |
| 1   | G     | 676 | ILE  | C-N-CA   | 6.90  | 128.46      | 119.84   |
| 4   | 0     | 191 | LYS  | CA-C-O   | -6.89 | 113.60      | 120.70   |
| 4   | 4     | 287 | ILE  | N-CA-C   | 6.89  | 117.65      | 110.62   |
| 4   | 7     | 287 | ILE  | N-CA-C   | 6.89  | 117.65      | 110.62   |
| 4   | 2     | 287 | ILE  | N-CA-C   | 6.89  | 117.65      | 110.62   |
| 4   | 5     | 191 | LYS  | CA-C-O   | -6.88 | 113.61      | 120.70   |
| 4   | 5     | 287 | ILE  | N-CA-C   | 6.88  | 117.63      | 110.62   |
| 4   | 8     | 287 | ILE  | N-CA-C   | 6.88  | 117.63      | 110.62   |
| 4   | 1     | 287 | ILE  | N-CA-C   | 6.87  | 117.63      | 110.62   |
| 4   | 7     | 191 | LYS  | CA-C-O   | -6.87 | 113.63      | 120.70   |
| 4   | 8     | 191 | LYS  | CA-C-O   | -6.87 | 113.62      | 120.70   |
| 4   | Z     | 287 | ILE  | N-CA-C   | 6.87  | 117.63      | 110.62   |
| 4   | 2     | 191 | LYS  | CA-C-O   | -6.87 | 113.63      | 120.70   |
| 4   | V     | 191 | LYS  | CA-C-O   | -6.86 | 113.64      | 120.70   |
| 4   | V     | 287 | ILE  | N-CA-C   | 6.86  | 117.62      | 110.62   |
| 1   | G     | 785 | GLU  | O-C-N    | 6.86  | 131.71      | 122.59   |
| 4   | W     | 287 | ILE  | N-CA-C   | 6.86  | 117.61      | 110.62   |
| 4   | X     | 191 | LYS  | CA-C-O   | -6.85 | 113.64      | 120.70   |
| 1   | G     | 578 | HIS  | N-CA-CB  | 6.85  | 122.06      | 110.49   |
| 4   | 4     | 191 | LYS  | CA-C-O   | -6.85 | 113.65      | 120.70   |
| 1   | J     | 218 | LEU  | O-C-N    | 6.84  | 131.37      | 123.29   |
| 4   | 9     | 191 | LYS  | CA-C-O   | -6.84 | 113.65      | 120.70   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 676 | ILE  | CA-C-N   | 6.84  | 128.39      | 119.84   |
| 1   | D     | 676 | ILE  | C-N-CA   | 6.84  | 128.39      | 119.84   |
| 4   | 0     | 287 | ILE  | N-CA-C   | 6.84  | 117.60      | 110.62   |
| 4   | 3     | 191 | LYS  | CA-C-O   | -6.83 | 113.66      | 120.70   |
| 4   | Z     | 191 | LYS  | CA-C-O   | -6.83 | 113.66      | 120.70   |
| 4   | Y     | 287 | ILE  | N-CA-C   | 6.83  | 117.59      | 110.62   |
| 1   | J     | 201 | ALA  | CB-CA-C  | -6.82 | 106.51      | 116.53   |
| 1   | J     | 676 | ILE  | CA-C-N   | 6.82  | 128.36      | 119.84   |
| 1   | J     | 676 | ILE  | C-N-CA   | 6.82  | 128.36      | 119.84   |
| 4   | Y     | 191 | LYS  | CA-C-O   | -6.82 | 113.68      | 120.70   |
| 1   | G     | 529 | PRO  | CA-C-N   | -6.81 | 111.75      | 122.65   |
| 1   | G     | 529 | PRO  | C-N-CA   | -6.81 | 111.75      | 122.65   |
| 1   | A     | 676 | ILE  | CA-C-N   | 6.81  | 128.36      | 119.84   |
| 1   | A     | 676 | ILE  | C-N-CA   | 6.81  | 128.36      | 119.84   |
| 1   | J     | 529 | PRO  | CA-C-N   | -6.81 | 111.75      | 122.65   |
| 1   | J     | 529 | PRO  | C-N-CA   | -6.81 | 111.75      | 122.65   |
| 4   | 9     | 287 | ILE  | N-CA-C   | 6.80  | 117.56      | 110.62   |
| 1   | A     | 529 | PRO  | CA-C-N   | -6.80 | 111.77      | 122.65   |
| 1   | A     | 529 | PRO  | C-N-CA   | -6.80 | 111.77      | 122.65   |
| 2   | E     | 139 | ALA  | N-CA-C   | -6.80 | 104.31      | 114.64   |
| 1   | D     | 146 | LYS  | N-CA-C   | 6.79  | 119.59      | 108.52   |
| 1   | D     | 529 | PRO  | CA-C-N   | -6.79 | 111.78      | 122.65   |
| 1   | D     | 529 | PRO  | C-N-CA   | -6.79 | 111.78      | 122.65   |
| 1   | G     | 218 | LEU  | O-C-N    | 6.79  | 131.31      | 123.29   |
| 4   | 5     | 259 | GLU  | N-CA-C   | -6.79 | 104.09      | 112.38   |
| 1   | G     | 201 | ALA  | CB-CA-C  | -6.79 | 106.55      | 116.53   |
| 1   | J     | 578 | HIS  | N-CA-CB  | 6.79  | 121.96      | 110.49   |
| 1   | D     | 201 | ALA  | CB-CA-C  | -6.78 | 106.57      | 116.53   |
| 1   | D     | 578 | HIS  | N-CA-CB  | 6.76  | 121.92      | 110.49   |
| 2   | B     | 139 | ALA  | N-CA-C   | -6.76 | 104.36      | 114.64   |
| 4   | V     | 214 | GLU  | CB-CG-CD | 6.76  | 124.09      | 112.60   |
| 4   | 8     | 259 | GLU  | N-CA-C   | -6.76 | 104.14      | 112.38   |
| 4   | 3     | 214 | GLU  | CB-CG-CD | 6.75  | 124.08      | 112.60   |
| 4   | X     | 259 | GLU  | N-CA-C   | -6.75 | 104.14      | 112.38   |
| 4   | Z     | 214 | GLU  | CB-CG-CD | 6.75  | 124.08      | 112.60   |
| 4   | 1     | 259 | GLU  | N-CA-C   | -6.75 | 104.15      | 112.38   |
| 1   | A     | 146 | LYS  | N-CA-C   | 6.74  | 119.51      | 108.52   |
| 1   | A     | 578 | HIS  | N-CA-CB  | 6.74  | 121.89      | 110.49   |
| 4   | 0     | 214 | GLU  | CB-CG-CD | 6.74  | 124.06      | 112.60   |
| 4   | 3     | 259 | GLU  | N-CA-C   | -6.74 | 104.15      | 112.38   |
| 4   | 9     | 259 | GLU  | N-CA-C   | -6.74 | 104.15      | 112.38   |
| 4   | 2     | 214 | GLU  | CB-CG-CD | 6.74  | 124.06      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | X     | 214 | GLU  | CB-CG-CD | 6.74  | 124.06      | 112.60   |
| 4   | 0     | 259 | GLU  | N-CA-C   | -6.74 | 104.16      | 112.38   |
| 4   | 7     | 214 | GLU  | CB-CG-CD | 6.74  | 124.05      | 112.60   |
| 1   | A     | 201 | ALA  | CB-CA-C  | -6.73 | 106.64      | 116.53   |
| 4   | 4     | 259 | GLU  | N-CA-C   | -6.73 | 104.17      | 112.38   |
| 4   | 9     | 214 | GLU  | CB-CG-CD | 6.73  | 124.04      | 112.60   |
| 4   | W     | 214 | GLU  | CB-CG-CD | 6.73  | 124.04      | 112.60   |
| 4   | W     | 259 | GLU  | N-CA-C   | -6.72 | 104.18      | 112.38   |
| 4   | Y     | 259 | GLU  | N-CA-C   | -6.72 | 104.18      | 112.38   |
| 4   | 8     | 214 | GLU  | CB-CG-CD | 6.72  | 124.02      | 112.60   |
| 4   | Y     | 214 | GLU  | CB-CG-CD | 6.71  | 124.02      | 112.60   |
| 4   | 1     | 214 | GLU  | CB-CG-CD | 6.71  | 124.01      | 112.60   |
| 4   | 4     | 214 | GLU  | CB-CG-CD | 6.71  | 124.01      | 112.60   |
| 4   | Z     | 259 | GLU  | N-CA-C   | -6.71 | 104.20      | 112.38   |
| 4   | 5     | 214 | GLU  | CB-CG-CD | 6.70  | 123.99      | 112.60   |
| 4   | 2     | 259 | GLU  | N-CA-C   | -6.70 | 104.21      | 112.38   |
| 4   | 7     | 259 | GLU  | N-CA-C   | -6.70 | 104.21      | 112.38   |
| 2   | H     | 139 | ALA  | N-CA-C   | -6.69 | 104.47      | 114.64   |
| 2   | K     | 139 | ALA  | N-CA-C   | -6.69 | 104.47      | 114.64   |
| 4   | V     | 259 | GLU  | N-CA-C   | -6.68 | 104.23      | 112.38   |
| 1   | J     | 146 | LYS  | N-CA-C   | 6.66  | 119.38      | 108.52   |
| 1   | G     | 146 | LYS  | N-CA-C   | 6.65  | 119.36      | 108.52   |
| 1   | A     | 218 | LEU  | O-C-N    | 6.62  | 131.10      | 123.29   |
| 1   | A     | 340 | ILE  | O-C-N    | 6.59  | 128.53      | 121.87   |
| 1   | D     | 218 | LEU  | O-C-N    | 6.59  | 131.06      | 123.29   |
| 1   | J     | 628 | GLY  | O-C-N    | -6.55 | 114.45      | 122.71   |
| 4   | 8     | 371 | HIS  | CA-CB-CG | -6.53 | 107.27      | 113.80   |
| 1   | D     | 82  | PRO  | N-CA-CB  | 6.53  | 109.41      | 103.08   |
| 2   | H     | 141 | PRO  | N-CA-C   | 6.52  | 118.66      | 110.70   |
| 1   | A     | 156 | PHE  | N-CA-C   | -6.52 | 104.59      | 112.54   |
| 1   | J     | 82  | PRO  | N-CA-CB  | 6.52  | 109.40      | 103.08   |
| 4   | 7     | 371 | HIS  | CA-CB-CG | -6.52 | 107.28      | 113.80   |
| 4   | V     | 286 | ASP  | CA-C-N   | 6.51  | 129.38      | 120.46   |
| 4   | V     | 286 | ASP  | C-N-CA   | 6.51  | 129.38      | 120.46   |
| 2   | H     | 139 | ALA  | O-C-N    | 6.51  | 128.83      | 121.93   |
| 4   | 9     | 286 | ASP  | CA-C-N   | 6.51  | 129.37      | 120.46   |
| 4   | 9     | 286 | ASP  | C-N-CA   | 6.51  | 129.37      | 120.46   |
| 2   | E     | 139 | ALA  | O-C-N    | 6.50  | 128.82      | 121.93   |
| 4   | 4     | 371 | HIS  | CA-CB-CG | -6.49 | 107.31      | 113.80   |
| 1   | D     | 156 | PHE  | N-CA-C   | -6.49 | 104.62      | 112.54   |
| 1   | D     | 217 | THR  | N-CA-CB  | 6.49  | 123.60      | 111.53   |
| 1   | D     | 628 | GLY  | O-C-N    | -6.49 | 114.54      | 122.71   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 156 | PHE  | N-CA-C    | -6.49 | 104.63      | 112.54   |
| 2   | H     | 141 | PRO  | N-CD-CG   | -6.49 | 93.47       | 103.20   |
| 2   | E     | 141 | PRO  | N-CA-C    | 6.48  | 118.61      | 110.70   |
| 4   | 2     | 371 | HIS  | CA-CB-CG  | -6.48 | 107.32      | 113.80   |
| 4   | W     | 371 | HIS  | CA-CB-CG  | -6.48 | 107.32      | 113.80   |
| 4   | Y     | 286 | ASP  | CA-C-N    | 6.48  | 129.34      | 120.46   |
| 4   | Y     | 286 | ASP  | C-N-CA    | 6.48  | 129.34      | 120.46   |
| 1   | A     | 217 | THR  | N-CA-CB   | 6.48  | 123.58      | 111.53   |
| 2   | E     | 141 | PRO  | N-CD-CG   | -6.48 | 93.49       | 103.20   |
| 1   | J     | 156 | PHE  | N-CA-C    | -6.48 | 104.64      | 112.54   |
| 4   | 4     | 286 | ASP  | CA-C-N    | 6.47  | 129.33      | 120.46   |
| 4   | 4     | 286 | ASP  | C-N-CA    | 6.47  | 129.33      | 120.46   |
| 4   | 0     | 286 | ASP  | CA-C-N    | 6.47  | 129.33      | 120.46   |
| 4   | 0     | 286 | ASP  | C-N-CA    | 6.47  | 129.33      | 120.46   |
| 2   | B     | 141 | PRO  | N-CA-C    | 6.47  | 118.59      | 110.70   |
| 1   | G     | 217 | THR  | N-CA-CB   | 6.46  | 123.55      | 111.53   |
| 4   | 0     | 371 | HIS  | CA-CB-CG  | -6.46 | 107.34      | 113.80   |
| 4   | 7     | 80  | ASP  | CA-CB-CG  | 6.46  | 119.06      | 112.60   |
| 4   | V     | 80  | ASP  | CA-CB-CG  | 6.46  | 119.06      | 112.60   |
| 4   | V     | 371 | HIS  | CA-CB-CG  | -6.46 | 107.34      | 113.80   |
| 4   | Y     | 371 | HIS  | CA-CB-CG  | -6.46 | 107.34      | 113.80   |
| 4   | 1     | 286 | ASP  | CA-C-N    | 6.46  | 129.31      | 120.46   |
| 4   | 1     | 286 | ASP  | C-N-CA    | 6.46  | 129.31      | 120.46   |
| 4   | 4     | 101 | HIS  | CB-CG-CD2 | -6.46 | 122.80      | 131.20   |
| 4   | X     | 371 | HIS  | CA-CB-CG  | -6.46 | 107.34      | 113.80   |
| 1   | A     | 82  | PRO  | N-CA-CB   | 6.45  | 109.34      | 103.08   |
| 4   | Z     | 371 | HIS  | CA-CB-CG  | -6.45 | 107.35      | 113.80   |
| 4   | 5     | 371 | HIS  | CA-CB-CG  | -6.45 | 107.35      | 113.80   |
| 1   | J     | 217 | THR  | N-CA-CB   | 6.45  | 123.53      | 111.53   |
| 4   | 1     | 371 | HIS  | CA-CB-CG  | -6.45 | 107.35      | 113.80   |
| 4   | 9     | 371 | HIS  | CA-CB-CG  | -6.45 | 107.35      | 113.80   |
| 4   | Z     | 286 | ASP  | CA-C-N    | 6.45  | 129.30      | 120.46   |
| 4   | Z     | 286 | ASP  | C-N-CA    | 6.45  | 129.30      | 120.46   |
| 2   | K     | 139 | ALA  | O-C-N     | 6.45  | 128.76      | 121.93   |
| 1   | J     | 340 | ILE  | O-C-N     | 6.45  | 128.38      | 121.87   |
| 4   | 7     | 286 | ASP  | CA-C-N    | 6.44  | 129.28      | 120.46   |
| 4   | 7     | 286 | ASP  | C-N-CA    | 6.44  | 129.28      | 120.46   |
| 4   | W     | 286 | ASP  | CA-C-N    | 6.44  | 129.29      | 120.46   |
| 4   | W     | 286 | ASP  | C-N-CA    | 6.44  | 129.29      | 120.46   |
| 2   | B     | 139 | ALA  | O-C-N     | 6.44  | 128.76      | 121.93   |
| 1   | D     | 340 | ILE  | O-C-N     | 6.44  | 128.37      | 121.87   |
| 1   | G     | 628 | GLY  | O-C-N     | -6.44 | 114.60      | 122.71   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 8     | 286 | ASP  | CA-C-N    | 6.43  | 129.27      | 120.46   |
| 4   | 8     | 286 | ASP  | C-N-CA    | 6.43  | 129.27      | 120.46   |
| 4   | 3     | 371 | HIS  | CA-CB-CG  | -6.43 | 107.37      | 113.80   |
| 4   | 1     | 101 | HIS  | CB-CG-CD2 | -6.42 | 122.85      | 131.20   |
| 4   | 3     | 80  | ASP  | CA-CB-CG  | 6.42  | 119.02      | 112.60   |
| 4   | 3     | 286 | ASP  | CA-C-N    | 6.42  | 129.26      | 120.46   |
| 4   | 3     | 286 | ASP  | C-N-CA    | 6.42  | 129.26      | 120.46   |
| 4   | 4     | 259 | GLU  | CA-CB-CG  | 6.42  | 126.94      | 114.10   |
| 4   | X     | 286 | ASP  | CA-C-N    | 6.42  | 129.25      | 120.46   |
| 4   | X     | 286 | ASP  | C-N-CA    | 6.42  | 129.25      | 120.46   |
| 1   | D     | 47  | PHE  | CB-CA-C   | -6.41 | 100.88      | 110.24   |
| 4   | 0     | 80  | ASP  | CA-CB-CG  | 6.41  | 119.01      | 112.60   |
| 1   | A     | 628 | GLY  | O-C-N     | -6.41 | 114.64      | 122.71   |
| 4   | W     | 80  | ASP  | CA-CB-CG  | 6.40  | 119.00      | 112.60   |
| 2   | K     | 141 | PRO  | N-CA-C    | 6.40  | 118.51      | 110.70   |
| 4   | 0     | 259 | GLU  | CA-CB-CG  | 6.40  | 126.90      | 114.10   |
| 4   | 2     | 80  | ASP  | CA-CB-CG  | 6.40  | 119.00      | 112.60   |
| 4   | 2     | 286 | ASP  | CA-C-N    | 6.40  | 129.23      | 120.46   |
| 4   | 2     | 286 | ASP  | C-N-CA    | 6.40  | 129.23      | 120.46   |
| 4   | 1     | 80  | ASP  | CA-CB-CG  | 6.40  | 119.00      | 112.60   |
| 4   | 5     | 80  | ASP  | CA-CB-CG  | 6.40  | 119.00      | 112.60   |
| 4   | 5     | 259 | GLU  | CA-CB-CG  | 6.40  | 126.89      | 114.10   |
| 4   | Z     | 80  | ASP  | CA-CB-CG  | 6.39  | 118.99      | 112.60   |
| 1   | D     | 604 | ASN  | CA-C-O    | 6.39  | 128.37      | 121.02   |
| 1   | D     | 688 | HIS  | CA-CB-CG  | -6.39 | 107.41      | 113.80   |
| 4   | W     | 259 | GLU  | CA-CB-CG  | 6.39  | 126.88      | 114.10   |
| 4   | 7     | 101 | HIS  | CB-CG-CD2 | -6.39 | 122.89      | 131.20   |
| 4   | Z     | 101 | HIS  | CB-CG-CD2 | -6.39 | 122.89      | 131.20   |
| 4   | 0     | 47  | MET  | CA-CB-CG  | -6.39 | 101.32      | 114.10   |
| 4   | 3     | 259 | GLU  | CA-CB-CG  | 6.39  | 126.87      | 114.10   |
| 4   | 4     | 47  | MET  | CA-CB-CG  | -6.39 | 101.33      | 114.10   |
| 4   | 5     | 286 | ASP  | CA-C-N    | 6.39  | 129.21      | 120.46   |
| 4   | 5     | 286 | ASP  | C-N-CA    | 6.39  | 129.21      | 120.46   |
| 4   | 8     | 259 | GLU  | CA-CB-CG  | 6.39  | 126.87      | 114.10   |
| 4   | 2     | 259 | GLU  | CA-CB-CG  | 6.38  | 126.87      | 114.10   |
| 4   | 3     | 47  | MET  | CA-CB-CG  | -6.38 | 101.33      | 114.10   |
| 4   | Z     | 259 | GLU  | CA-CB-CG  | 6.38  | 126.87      | 114.10   |
| 4   | 7     | 259 | GLU  | CA-CB-CG  | 6.38  | 126.86      | 114.10   |
| 4   | 2     | 101 | HIS  | CB-CG-CD2 | -6.38 | 122.90      | 131.20   |
| 4   | 9     | 259 | GLU  | CA-CB-CG  | 6.38  | 126.86      | 114.10   |
| 4   | V     | 259 | GLU  | CA-CB-CG  | 6.38  | 126.86      | 114.10   |
| 4   | 9     | 80  | ASP  | CA-CB-CG  | 6.38  | 118.98      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | X     | 80  | ASP  | CA-CB-CG  | 6.38  | 118.98      | 112.60   |
| 4   | 1     | 47  | MET  | CA-CB-CG  | -6.37 | 101.35      | 114.10   |
| 4   | 1     | 259 | GLU  | CA-CB-CG  | 6.37  | 126.85      | 114.10   |
| 4   | 3     | 101 | HIS  | CB-CG-CD2 | -6.37 | 122.91      | 131.20   |
| 4   | X     | 259 | GLU  | CA-CB-CG  | 6.37  | 126.85      | 114.10   |
| 4   | 0     | 101 | HIS  | CB-CG-CD2 | -6.37 | 122.92      | 131.20   |
| 4   | V     | 47  | MET  | CA-CB-CG  | -6.37 | 101.36      | 114.10   |
| 4   | Y     | 259 | GLU  | CA-CB-CG  | 6.37  | 126.84      | 114.10   |
| 2   | B     | 141 | PRO  | N-CD-CG   | -6.37 | 93.65       | 103.20   |
| 1   | G     | 604 | ASN  | CA-C-O    | 6.37  | 128.34      | 121.02   |
| 4   | Y     | 47  | MET  | CA-CB-CG  | -6.37 | 101.37      | 114.10   |
| 1   | G     | 82  | PRO  | N-CA-CB   | 6.36  | 109.25      | 103.08   |
| 4   | 8     | 47  | MET  | CA-CB-CG  | -6.36 | 101.38      | 114.10   |
| 1   | J     | 47  | PHE  | CB-CA-C   | -6.36 | 100.95      | 110.24   |
| 4   | 8     | 101 | HIS  | CB-CG-CD2 | -6.36 | 122.93      | 131.20   |
| 4   | W     | 101 | HIS  | CB-CG-CD2 | -6.36 | 122.93      | 131.20   |
| 4   | X     | 47  | MET  | CA-CB-CG  | -6.36 | 101.38      | 114.10   |
| 1   | G     | 340 | ILE  | O-C-N     | 6.36  | 128.29      | 121.87   |
| 4   | 5     | 47  | MET  | CA-CB-CG  | -6.36 | 101.39      | 114.10   |
| 4   | 7     | 47  | MET  | CA-CB-CG  | -6.35 | 101.39      | 114.10   |
| 4   | 9     | 101 | HIS  | CB-CG-CD2 | -6.35 | 122.94      | 131.20   |
| 4   | 8     | 80  | ASP  | CA-CB-CG  | 6.35  | 118.95      | 112.60   |
| 4   | Y     | 80  | ASP  | CA-CB-CG  | 6.35  | 118.95      | 112.60   |
| 1   | A     | 688 | HIS  | CA-CB-CG  | -6.35 | 107.45      | 113.80   |
| 4   | 2     | 47  | MET  | CA-CB-CG  | -6.35 | 101.40      | 114.10   |
| 4   | 2     | 282 | ILE  | CA-C-O    | -6.35 | 114.00      | 121.05   |
| 4   | X     | 101 | HIS  | CB-CG-CD2 | -6.35 | 122.95      | 131.20   |
| 1   | J     | 604 | ASN  | CA-C-O    | 6.34  | 128.31      | 121.02   |
| 2   | K     | 141 | PRO  | N-CD-CG   | -6.34 | 93.69       | 103.20   |
| 4   | 9     | 47  | MET  | CA-CB-CG  | -6.34 | 101.42      | 114.10   |
| 4   | W     | 47  | MET  | CA-CB-CG  | -6.34 | 101.42      | 114.10   |
| 4   | 9     | 217 | CYS  | N-CA-C    | 6.34  | 119.66      | 110.28   |
| 4   | X     | 282 | ILE  | CA-C-O    | -6.34 | 114.02      | 121.05   |
| 4   | 5     | 282 | ILE  | CA-C-O    | -6.33 | 114.02      | 121.05   |
| 4   | 5     | 101 | HIS  | CB-CG-CD2 | -6.33 | 122.97      | 131.20   |
| 4   | Y     | 101 | HIS  | CB-CG-CD2 | -6.33 | 122.97      | 131.20   |
| 1   | J     | 688 | HIS  | CA-CB-CG  | -6.33 | 107.47      | 113.80   |
| 4   | Z     | 47  | MET  | CA-CB-CG  | -6.33 | 101.45      | 114.10   |
| 4   | V     | 1   | ASP  | CA-CB-CG  | 6.32  | 118.92      | 112.60   |
| 1   | A     | 291 | ILE  | N-CA-C    | 6.32  | 117.00      | 110.36   |
| 1   | D     | 755 | HIS  | CA-CB-CG  | 6.32  | 120.12      | 113.80   |
| 1   | J     | 755 | HIS  | CA-CB-CG  | 6.32  | 120.12      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | V     | 101 | HIS  | CB-CG-CD2  | -6.32 | 122.99      | 131.20   |
| 1   | A     | 47  | PHE  | CB-CA-C    | -6.31 | 101.02      | 110.24   |
| 1   | A     | 755 | HIS  | CA-CB-CG   | 6.31  | 120.11      | 113.80   |
| 4   | 7     | 282 | ILE  | CA-C-O     | -6.31 | 114.05      | 121.05   |
| 4   | Y     | 282 | ILE  | CA-C-O     | -6.31 | 114.05      | 121.05   |
| 1   | D     | 599 | ASN  | OD1-CG-ND2 | -6.30 | 116.30      | 122.60   |
| 4   | 1     | 282 | ILE  | CA-C-O     | -6.30 | 114.06      | 121.05   |
| 4   | 2     | 1   | ASP  | CA-CB-CG   | 6.30  | 118.90      | 112.60   |
| 4   | W     | 282 | ILE  | CA-C-O     | -6.29 | 114.06      | 121.05   |
| 4   | Z     | 1   | ASP  | CA-CB-CG   | 6.29  | 118.89      | 112.60   |
| 4   | 3     | 282 | ILE  | CA-C-O     | -6.29 | 114.07      | 121.05   |
| 4   | 4     | 80  | ASP  | CA-CB-CG   | 6.29  | 118.89      | 112.60   |
| 4   | V     | 282 | ILE  | CA-C-O     | -6.29 | 114.07      | 121.05   |
| 1   | G     | 599 | ASN  | OD1-CG-ND2 | -6.29 | 116.31      | 122.60   |
| 4   | Z     | 282 | ILE  | CA-C-O     | -6.29 | 114.07      | 121.05   |
| 1   | A     | 604 | ASN  | CA-C-O     | 6.29  | 128.25      | 121.02   |
| 4   | 8     | 217 | CYS  | N-CA-C     | 6.29  | 119.58      | 110.28   |
| 4   | 9     | 282 | ILE  | CA-C-O     | -6.29 | 114.07      | 121.05   |
| 4   | W     | 217 | CYS  | N-CA-C     | 6.29  | 119.58      | 110.28   |
| 1   | G     | 47  | PHE  | CB-CA-C    | -6.28 | 101.07      | 110.24   |
| 4   | Y     | 217 | CYS  | N-CA-C     | 6.28  | 119.58      | 110.28   |
| 4   | 4     | 217 | CYS  | N-CA-C     | 6.28  | 119.58      | 110.28   |
| 1   | A     | 599 | ASN  | OD1-CG-ND2 | -6.28 | 116.32      | 122.60   |
| 4   | 7     | 217 | CYS  | N-CA-C     | 6.28  | 119.57      | 110.28   |
| 4   | 9     | 1   | ASP  | CA-CB-CG   | 6.28  | 118.88      | 112.60   |
| 4   | 0     | 217 | CYS  | N-CA-C     | 6.27  | 119.57      | 110.28   |
| 4   | 8     | 282 | ILE  | CA-C-O     | -6.27 | 114.09      | 121.05   |
| 4   | 1     | 217 | CYS  | N-CA-C     | 6.27  | 119.56      | 110.28   |
| 4   | V     | 217 | CYS  | N-CA-C     | 6.27  | 119.56      | 110.28   |
| 1   | G     | 524 | GLU  | N-CA-CB    | 6.26  | 119.46      | 110.06   |
| 4   | 4     | 1   | ASP  | CA-CB-CG   | 6.26  | 118.86      | 112.60   |
| 1   | A     | 524 | GLU  | N-CA-CB    | 6.26  | 119.45      | 110.06   |
| 1   | D     | 443 | ILE  | CB-CA-C    | -6.26 | 103.87      | 111.88   |
| 4   | 4     | 282 | ILE  | CA-C-O     | -6.25 | 114.11      | 121.05   |
| 1   | G     | 688 | HIS  | CA-CB-CG   | -6.25 | 107.55      | 113.80   |
| 4   | 7     | 1   | ASP  | CA-CB-CG   | 6.25  | 118.85      | 112.60   |
| 4   | 0     | 282 | ILE  | CA-C-O     | -6.24 | 114.12      | 121.05   |
| 4   | 3     | 217 | CYS  | N-CA-C     | 6.24  | 119.52      | 110.28   |
| 1   | J     | 443 | ILE  | CB-CA-C    | -6.24 | 103.89      | 111.88   |
| 4   | 8     | 1   | ASP  | CA-CB-CG   | 6.24  | 118.84      | 112.60   |
| 4   | 5     | 217 | CYS  | N-CA-C     | 6.24  | 119.51      | 110.28   |
| 4   | Z     | 217 | CYS  | N-CA-C     | 6.24  | 119.51      | 110.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | X     | 217 | CYS  | N-CA-C     | 6.23  | 119.50      | 110.28   |
| 4   | 2     | 217 | CYS  | N-CA-C     | 6.23  | 119.50      | 110.28   |
| 4   | 1     | 1   | ASP  | CA-CB-CG   | 6.23  | 118.83      | 112.60   |
| 1   | D     | 524 | GLU  | N-CA-CB    | 6.22  | 119.39      | 110.06   |
| 1   | J     | 599 | ASN  | OD1-CG-ND2 | -6.22 | 116.38      | 122.60   |
| 1   | G     | 755 | HIS  | CA-CB-CG   | 6.21  | 120.02      | 113.80   |
| 1   | A     | 443 | ILE  | CB-CA-C    | -6.21 | 103.93      | 111.88   |
| 1   | D     | 631 | GLU  | CA-C-N     | 6.21  | 131.84      | 120.79   |
| 1   | D     | 631 | GLU  | C-N-CA     | 6.21  | 131.84      | 120.79   |
| 1   | J     | 631 | GLU  | CA-C-N     | 6.21  | 131.84      | 120.79   |
| 1   | J     | 631 | GLU  | C-N-CA     | 6.21  | 131.84      | 120.79   |
| 1   | G     | 341 | LEU  | CB-CA-C    | 6.20  | 122.30      | 110.27   |
| 4   | 3     | 1   | ASP  | CA-CB-CG   | 6.20  | 118.80      | 112.60   |
| 4   | 5     | 1   | ASP  | CA-CB-CG   | 6.20  | 118.80      | 112.60   |
| 1   | A     | 341 | LEU  | CB-CA-C    | 6.20  | 122.29      | 110.27   |
| 1   | J     | 524 | GLU  | N-CA-CB    | 6.19  | 119.34      | 110.06   |
| 4   | 2     | 219 | VAL  | CB-CA-C    | -6.19 | 102.95      | 110.99   |
| 4   | X     | 1   | ASP  | CA-CB-CG   | 6.18  | 118.78      | 112.60   |
| 4   | 4     | 219 | VAL  | N-CA-CB    | 6.18  | 119.69      | 111.90   |
| 1   | G     | 443 | ILE  | CB-CA-C    | -6.18 | 103.97      | 111.88   |
| 1   | J     | 341 | LEU  | CB-CA-C    | 6.18  | 122.26      | 110.27   |
| 1   | A     | 22  | LYS  | N-CA-C     | -6.17 | 106.35      | 114.31   |
| 4   | 9     | 219 | VAL  | CB-CA-C    | -6.17 | 102.97      | 110.99   |
| 4   | 8     | 219 | VAL  | CB-CA-C    | -6.17 | 102.97      | 110.99   |
| 4   | V     | 219 | VAL  | N-CA-CB    | 6.17  | 119.67      | 111.90   |
| 4   | 0     | 1   | ASP  | CA-CB-CG   | 6.16  | 118.76      | 112.60   |
| 4   | 5     | 219 | VAL  | CB-CA-C    | -6.16 | 102.98      | 110.99   |
| 4   | 7     | 219 | VAL  | CB-CA-C    | -6.16 | 102.98      | 110.99   |
| 4   | Y     | 1   | ASP  | CA-CB-CG   | 6.16  | 118.76      | 112.60   |
| 4   | Z     | 219 | VAL  | CB-CA-C    | -6.16 | 102.99      | 110.99   |
| 4   | 0     | 219 | VAL  | N-CA-CB    | 6.16  | 119.66      | 111.90   |
| 4   | 3     | 219 | VAL  | CB-CA-C    | -6.16 | 102.99      | 110.99   |
| 2   | E     | 129 | THR  | CA-CB-CG2  | 6.15  | 120.96      | 110.50   |
| 4   | 1     | 219 | VAL  | CB-CA-C    | -6.15 | 103.00      | 110.99   |
| 4   | 7     | 219 | VAL  | N-CA-CB    | 6.15  | 119.65      | 111.90   |
| 1   | A     | 631 | GLU  | CA-C-N     | 6.15  | 131.74      | 120.79   |
| 1   | A     | 631 | GLU  | C-N-CA     | 6.15  | 131.74      | 120.79   |
| 1   | G     | 363 | ASN  | OD1-CG-ND2 | 6.15  | 128.75      | 122.60   |
| 4   | 2     | 219 | VAL  | N-CA-CB    | 6.15  | 119.65      | 111.90   |
| 4   | W     | 219 | VAL  | N-CA-CB    | 6.15  | 119.64      | 111.90   |
| 4   | 3     | 219 | VAL  | N-CA-CB    | 6.15  | 119.64      | 111.90   |
| 4   | W     | 1   | ASP  | CA-CB-CG   | 6.15  | 118.75      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | V     | 219 | VAL  | CB-CA-C    | -6.14 | 103.01      | 110.99   |
| 4   | X     | 219 | VAL  | CB-CA-C    | -6.14 | 103.01      | 110.99   |
| 1   | A     | 363 | ASN  | OD1-CG-ND2 | 6.14  | 128.74      | 122.60   |
| 4   | 0     | 219 | VAL  | CB-CA-C    | -6.14 | 103.01      | 110.99   |
| 4   | 4     | 128 | ASN  | N-CA-CB    | -6.13 | 102.59      | 111.91   |
| 4   | 4     | 219 | VAL  | CB-CA-C    | -6.13 | 103.02      | 110.99   |
| 4   | 5     | 128 | ASN  | N-CA-CB    | -6.13 | 102.59      | 111.91   |
| 4   | Y     | 219 | VAL  | CB-CA-C    | -6.13 | 103.02      | 110.99   |
| 4   | 2     | 128 | ASN  | N-CA-CB    | -6.13 | 102.59      | 111.91   |
| 4   | 3     | 128 | ASN  | N-CA-CB    | -6.13 | 102.59      | 111.91   |
| 4   | 5     | 205 | GLU  | N-CA-C     | -6.13 | 104.53      | 112.68   |
| 4   | X     | 128 | ASN  | N-CA-CB    | -6.13 | 102.60      | 111.91   |
| 4   | Z     | 219 | VAL  | N-CA-CB    | 6.13  | 119.62      | 111.90   |
| 4   | W     | 205 | GLU  | N-CA-C     | -6.13 | 104.53      | 112.68   |
| 4   | 4     | 205 | GLU  | N-CA-C     | -6.12 | 104.54      | 112.68   |
| 1   | G     | 631 | GLU  | CA-C-N     | 6.12  | 131.68      | 120.79   |
| 1   | G     | 631 | GLU  | C-N-CA     | 6.12  | 131.68      | 120.79   |
| 4   | 1     | 128 | ASN  | N-CA-CB    | -6.12 | 102.61      | 111.91   |
| 4   | 9     | 128 | ASN  | N-CA-CB    | -6.12 | 102.61      | 111.91   |
| 4   | 9     | 205 | GLU  | N-CA-C     | -6.11 | 104.55      | 112.68   |
| 1   | D     | 22  | LYS  | N-CA-C     | -6.11 | 106.43      | 114.31   |
| 4   | 3     | 205 | GLU  | N-CA-C     | -6.11 | 104.55      | 112.68   |
| 4   | 8     | 219 | VAL  | N-CA-CB    | 6.11  | 119.60      | 111.90   |
| 4   | W     | 128 | ASN  | N-CA-CB    | -6.11 | 102.62      | 111.91   |
| 4   | 1     | 219 | VAL  | N-CA-CB    | 6.11  | 119.59      | 111.90   |
| 4   | 7     | 128 | ASN  | N-CA-CB    | -6.11 | 102.63      | 111.91   |
| 4   | 0     | 128 | ASN  | N-CA-CB    | -6.11 | 102.63      | 111.91   |
| 4   | 8     | 128 | ASN  | N-CA-CB    | -6.11 | 102.63      | 111.91   |
| 4   | V     | 128 | ASN  | N-CA-CB    | -6.11 | 102.63      | 111.91   |
| 4   | W     | 219 | VAL  | CB-CA-C    | -6.10 | 103.06      | 110.99   |
| 4   | Y     | 128 | ASN  | N-CA-CB    | -6.10 | 102.64      | 111.91   |
| 2   | H     | 129 | THR  | CA-CB-CG2  | 6.10  | 120.87      | 110.50   |
| 4   | X     | 219 | VAL  | N-CA-CB    | 6.10  | 119.59      | 111.90   |
| 1   | D     | 352 | TYR  | N-CA-CB    | 6.10  | 120.87      | 110.50   |
| 1   | J     | 22  | LYS  | N-CA-C     | -6.10 | 106.44      | 114.31   |
| 1   | D     | 341 | LEU  | CB-CA-C    | 6.09  | 122.09      | 110.27   |
| 4   | Z     | 205 | GLU  | N-CA-C     | -6.09 | 104.58      | 112.68   |
| 4   | V     | 205 | GLU  | N-CA-C     | -6.09 | 104.58      | 112.68   |
| 1   | G     | 352 | TYR  | N-CA-CB    | 6.09  | 120.85      | 110.50   |
| 4   | Y     | 219 | VAL  | N-CA-CB    | 6.09  | 119.57      | 111.90   |
| 4   | X     | 205 | GLU  | N-CA-C     | -6.08 | 104.59      | 112.68   |
| 4   | Z     | 59  | GLN  | OE1-CD-NE2 | -6.08 | 116.52      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | J     | 479 | CYS  | N-CA-CB    | 6.08  | 119.00      | 109.94   |
| 1   | J     | 279 | LEU  | CA-C-N     | 6.08  | 125.96      | 119.28   |
| 1   | J     | 279 | LEU  | C-N-CA     | 6.08  | 125.96      | 119.28   |
| 2   | K     | 129 | THR  | CA-CB-CG2  | 6.07  | 120.82      | 110.50   |
| 4   | 2     | 205 | GLU  | N-CA-C     | -6.07 | 104.61      | 112.68   |
| 2   | B     | 129 | THR  | CA-CB-CG2  | 6.07  | 120.82      | 110.50   |
| 1   | J     | 686 | MET  | N-CA-CB    | -6.07 | 100.58      | 110.59   |
| 4   | 9     | 219 | VAL  | N-CA-CB    | 6.07  | 119.54      | 111.90   |
| 4   | Z     | 128 | ASN  | N-CA-CB    | -6.07 | 102.69      | 111.91   |
| 1   | G     | 592 | ILE  | CA-C-N     | -6.06 | 113.38      | 122.47   |
| 1   | G     | 592 | ILE  | C-N-CA     | -6.06 | 113.38      | 122.47   |
| 1   | G     | 686 | MET  | N-CA-CB    | -6.06 | 100.59      | 110.59   |
| 1   | J     | 136 | ASN  | CA-C-O     | 6.06  | 124.80      | 119.71   |
| 4   | 1     | 205 | GLU  | N-CA-C     | -6.06 | 104.62      | 112.68   |
| 4   | 5     | 219 | VAL  | N-CA-CB    | 6.05  | 119.53      | 111.90   |
| 4   | Y     | 205 | GLU  | N-CA-C     | -6.05 | 104.63      | 112.68   |
| 1   | D     | 279 | LEU  | CA-C-N     | 6.05  | 125.93      | 119.28   |
| 1   | D     | 279 | LEU  | C-N-CA     | 6.05  | 125.93      | 119.28   |
| 4   | 0     | 95  | ARG  | CA-CB-CG   | 6.05  | 126.20      | 114.10   |
| 4   | Y     | 95  | ARG  | CA-CB-CG   | 6.05  | 126.20      | 114.10   |
| 4   | 7     | 205 | GLU  | N-CA-C     | -6.05 | 104.64      | 112.68   |
| 1   | D     | 363 | ASN  | OD1-CG-ND2 | 6.05  | 128.65      | 122.60   |
| 4   | V     | 95  | ARG  | CA-CB-CG   | 6.05  | 126.19      | 114.10   |
| 4   | 0     | 205 | GLU  | N-CA-C     | -6.04 | 104.64      | 112.68   |
| 1   | J     | 165 | PHE  | N-CA-CB    | -6.04 | 100.28      | 110.49   |
| 4   | 8     | 59  | GLN  | OE1-CD-NE2 | -6.04 | 116.56      | 122.60   |
| 1   | A     | 279 | LEU  | CA-C-N     | 6.04  | 125.92      | 119.28   |
| 1   | A     | 279 | LEU  | C-N-CA     | 6.04  | 125.92      | 119.28   |
| 1   | G     | 165 | PHE  | N-CA-CB    | -6.04 | 100.29      | 110.49   |
| 1   | D     | 136 | ASN  | CA-C-O     | 6.03  | 124.78      | 119.71   |
| 1   | D     | 686 | MET  | N-CA-CB    | -6.03 | 100.64      | 110.59   |
| 1   | G     | 22  | LYS  | N-CA-C     | -6.03 | 106.54      | 114.31   |
| 4   | 5     | 59  | GLN  | OE1-CD-NE2 | -6.03 | 116.57      | 122.60   |
| 1   | A     | 686 | MET  | N-CA-CB    | -6.02 | 100.65      | 110.59   |
| 4   | 2     | 95  | ARG  | CA-CB-CG   | 6.02  | 126.15      | 114.10   |
| 4   | Z     | 95  | ARG  | CA-CB-CG   | 6.02  | 126.15      | 114.10   |
| 1   | A     | 165 | PHE  | N-CA-CB    | -6.02 | 100.31      | 110.49   |
| 4   | 3     | 95  | ARG  | CA-CB-CG   | 6.02  | 126.14      | 114.10   |
| 1   | J     | 180 | GLU  | N-CA-CB    | 6.02  | 118.63      | 110.38   |
| 4   | 1     | 95  | ARG  | CA-CB-CG   | 6.02  | 126.14      | 114.10   |
| 4   | 8     | 205 | GLU  | N-CA-C     | -6.02 | 104.68      | 112.68   |
| 4   | 9     | 252 | ASN  | CA-CB-CG   | 6.01  | 118.61      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 308 | ASN  | CA-C-N     | 6.01  | 125.63      | 119.56   |
| 1   | A     | 308 | ASN  | C-N-CA     | 6.01  | 125.63      | 119.56   |
| 4   | W     | 95  | ARG  | CA-CB-CG   | 6.01  | 126.12      | 114.10   |
| 1   | D     | 576 | GLU  | CA-CB-CG   | -6.01 | 102.08      | 114.10   |
| 1   | G     | 279 | LEU  | CA-C-N     | 6.01  | 125.89      | 119.28   |
| 1   | G     | 279 | LEU  | C-N-CA     | 6.01  | 125.89      | 119.28   |
| 4   | 2     | 59  | GLN  | OE1-CD-NE2 | -6.01 | 116.59      | 122.60   |
| 4   | 7     | 59  | GLN  | OE1-CD-NE2 | -6.01 | 116.59      | 122.60   |
| 4   | 7     | 95  | ARG  | CA-CB-CG   | 6.01  | 126.12      | 114.10   |
| 4   | 4     | 95  | ARG  | CA-CB-CG   | 6.01  | 126.12      | 114.10   |
| 4   | 5     | 95  | ARG  | CA-CB-CG   | 6.01  | 126.12      | 114.10   |
| 4   | 3     | 252 | ASN  | CA-CB-CG   | 6.01  | 118.61      | 112.60   |
| 1   | J     | 352 | TYR  | N-CA-CB    | 6.00  | 120.71      | 110.50   |
| 4   | 8     | 5   | THR  | CA-C-N     | 6.00  | 130.74      | 120.72   |
| 4   | 8     | 5   | THR  | C-N-CA     | 6.00  | 130.74      | 120.72   |
| 4   | W     | 59  | GLN  | OE1-CD-NE2 | -6.00 | 116.60      | 122.60   |
| 4   | 8     | 95  | ARG  | CA-CB-CG   | 6.00  | 126.10      | 114.10   |
| 1   | G     | 308 | ASN  | CA-C-N     | 6.00  | 125.62      | 119.56   |
| 1   | G     | 308 | ASN  | C-N-CA     | 6.00  | 125.62      | 119.56   |
| 4   | 1     | 252 | ASN  | CA-CB-CG   | 6.00  | 118.60      | 112.60   |
| 4   | X     | 59  | GLN  | OE1-CD-NE2 | -6.00 | 116.60      | 122.60   |
| 1   | D     | 180 | GLU  | N-CA-CB    | 6.00  | 118.59      | 110.38   |
| 1   | D     | 231 | ALA  | O-C-N      | 5.99  | 129.64      | 122.27   |
| 4   | 9     | 95  | ARG  | CA-CB-CG   | 5.99  | 126.09      | 114.10   |
| 1   | A     | 231 | ALA  | O-C-N      | 5.99  | 129.64      | 122.27   |
| 1   | J     | 747 | LEU  | N-CA-CB    | 5.99  | 118.87      | 109.94   |
| 1   | A     | 576 | GLU  | CA-CB-CG   | -5.99 | 102.12      | 114.10   |
| 4   | V     | 5   | THR  | CA-C-N     | 5.99  | 130.72      | 120.72   |
| 4   | V     | 5   | THR  | C-N-CA     | 5.99  | 130.72      | 120.72   |
| 4   | X     | 95  | ARG  | CA-CB-CG   | 5.99  | 126.08      | 114.10   |
| 1   | D     | 790 | THR  | CA-C-O     | 5.99  | 126.74      | 119.31   |
| 1   | J     | 231 | ALA  | O-C-N      | 5.99  | 129.64      | 122.27   |
| 4   | V     | 231 | ALA  | N-CA-C     | 5.99  | 117.47      | 111.07   |
| 1   | G     | 231 | ALA  | O-C-N      | 5.98  | 129.63      | 122.27   |
| 1   | G     | 576 | GLU  | CA-CB-CG   | -5.98 | 102.14      | 114.10   |
| 4   | 0     | 5   | THR  | CA-C-N     | 5.98  | 130.71      | 120.72   |
| 4   | 0     | 5   | THR  | C-N-CA     | 5.98  | 130.71      | 120.72   |
| 4   | Y     | 252 | ASN  | CA-CB-CG   | 5.98  | 118.58      | 112.60   |
| 1   | D     | 479 | CYS  | N-CA-CB    | 5.98  | 119.03      | 110.06   |
| 1   | J     | 576 | GLU  | CA-CB-CG   | -5.97 | 102.15      | 114.10   |
| 4   | 5     | 231 | ALA  | N-CA-C     | 5.97  | 117.46      | 111.07   |
| 4   | 9     | 59  | GLN  | OE1-CD-NE2 | -5.97 | 116.63      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Y     | 5   | THR  | CA-C-N     | 5.97  | 130.69      | 120.72   |
| 4   | Y     | 5   | THR  | C-N-CA     | 5.97  | 130.69      | 120.72   |
| 4   | X     | 5   | THR  | CA-C-N     | 5.97  | 130.69      | 120.72   |
| 4   | X     | 5   | THR  | C-N-CA     | 5.97  | 130.69      | 120.72   |
| 4   | X     | 252 | ASN  | CA-CB-CG   | 5.97  | 118.57      | 112.60   |
| 1   | A     | 352 | TYR  | N-CA-CB    | 5.97  | 120.64      | 110.50   |
| 4   | 4     | 252 | ASN  | CA-CB-CG   | 5.97  | 118.57      | 112.60   |
| 4   | Z     | 231 | ALA  | N-CA-C     | 5.97  | 117.45      | 111.07   |
| 1   | J     | 363 | ASN  | OD1-CG-ND2 | 5.96  | 128.56      | 122.60   |
| 1   | G     | 717 | TYR  | N-CA-C     | 5.96  | 121.21      | 111.37   |
| 4   | 4     | 5   | THR  | CA-C-N     | 5.96  | 130.68      | 120.72   |
| 4   | 4     | 5   | THR  | C-N-CA     | 5.96  | 130.68      | 120.72   |
| 4   | Z     | 252 | ASN  | CA-CB-CG   | 5.96  | 118.56      | 112.60   |
| 1   | A     | 632 | GLY  | O-C-N      | 5.96  | 129.41      | 122.68   |
| 1   | D     | 165 | PHE  | N-CA-CB    | -5.96 | 100.42      | 110.49   |
| 4   | 1     | 5   | THR  | CA-C-N     | 5.96  | 130.67      | 120.72   |
| 4   | 1     | 5   | THR  | C-N-CA     | 5.96  | 130.67      | 120.72   |
| 4   | 5     | 5   | THR  | CA-C-N     | 5.96  | 130.67      | 120.72   |
| 4   | 5     | 5   | THR  | C-N-CA     | 5.96  | 130.67      | 120.72   |
| 4   | W     | 231 | ALA  | N-CA-C     | 5.96  | 117.44      | 111.07   |
| 4   | 0     | 231 | ALA  | N-CA-C     | 5.96  | 117.44      | 111.07   |
| 4   | 8     | 231 | ALA  | N-CA-C     | 5.96  | 117.44      | 111.07   |
| 4   | W     | 252 | ASN  | CA-CB-CG   | 5.96  | 118.56      | 112.60   |
| 4   | W     | 5   | THR  | CA-C-N     | 5.95  | 130.66      | 120.72   |
| 4   | W     | 5   | THR  | C-N-CA     | 5.95  | 130.66      | 120.72   |
| 4   | 2     | 5   | THR  | CA-C-N     | 5.95  | 130.66      | 120.72   |
| 4   | 2     | 5   | THR  | C-N-CA     | 5.95  | 130.66      | 120.72   |
| 4   | 3     | 5   | THR  | CA-C-N     | 5.95  | 130.65      | 120.72   |
| 4   | 3     | 5   | THR  | C-N-CA     | 5.95  | 130.65      | 120.72   |
| 4   | 0     | 335 | ARG  | CA-CB-CG   | 5.95  | 125.99      | 114.10   |
| 4   | 8     | 34  | ILE  | CB-CA-C    | -5.95 | 102.34      | 110.90   |
| 4   | 7     | 231 | ALA  | N-CA-C     | 5.95  | 117.43      | 111.07   |
| 4   | 9     | 231 | ALA  | N-CA-C     | 5.95  | 117.43      | 111.07   |
| 1   | D     | 717 | TYR  | N-CA-C     | 5.94  | 121.18      | 111.37   |
| 4   | 0     | 252 | ASN  | CA-CB-CG   | 5.94  | 118.54      | 112.60   |
| 4   | Y     | 97  | ALA  | N-CA-C     | -5.94 | 102.29      | 109.72   |
| 4   | 4     | 59  | GLN  | OE1-CD-NE2 | -5.94 | 116.66      | 122.60   |
| 4   | 7     | 252 | ASN  | CA-CB-CG   | 5.94  | 118.54      | 112.60   |
| 4   | X     | 97  | ALA  | N-CA-C     | -5.93 | 102.30      | 109.72   |
| 4   | Z     | 5   | THR  | CA-C-N     | 5.93  | 130.63      | 120.72   |
| 4   | Z     | 5   | THR  | C-N-CA     | 5.93  | 130.63      | 120.72   |
| 1   | G     | 632 | GLY  | O-C-N      | 5.93  | 129.38      | 122.68   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 2     | 231 | ALA  | N-CA-C     | 5.93  | 117.42      | 111.07   |
| 4   | V     | 335 | ARG  | CA-CB-CG   | 5.93  | 125.97      | 114.10   |
| 1   | G     | 136 | ASN  | CA-C-O     | 5.93  | 124.69      | 119.71   |
| 4   | 3     | 231 | ALA  | N-CA-C     | 5.93  | 117.42      | 111.07   |
| 4   | 4     | 335 | ARG  | CA-CB-CG   | 5.93  | 125.96      | 114.10   |
| 4   | W     | 335 | ARG  | CA-CB-CG   | 5.92  | 125.95      | 114.10   |
| 4   | V     | 59  | GLN  | OE1-CD-NE2 | -5.92 | 116.68      | 122.60   |
| 4   | V     | 257 | CYS  | O-C-N      | -5.92 | 116.18      | 120.27   |
| 1   | G     | 88  | ILE  | CB-CG1-CD1 | -5.92 | 101.36      | 113.80   |
| 1   | G     | 479 | CYS  | N-CA-CB    | 5.92  | 118.94      | 110.06   |
| 4   | X     | 231 | ALA  | N-CA-C     | 5.92  | 117.41      | 111.07   |
| 1   | J     | 753 | VAL  | N-CA-C     | 5.92  | 118.47      | 109.12   |
| 4   | 5     | 233 | SER  | CA-C-O     | 5.92  | 128.98      | 120.51   |
| 4   | 7     | 5   | THR  | CA-C-N     | 5.92  | 130.61      | 120.72   |
| 4   | 7     | 5   | THR  | C-N-CA     | 5.92  | 130.61      | 120.72   |
| 4   | 8     | 252 | ASN  | CA-CB-CG   | 5.92  | 118.52      | 112.60   |
| 4   | 9     | 5   | THR  | CA-C-N     | 5.92  | 130.61      | 120.72   |
| 4   | 9     | 5   | THR  | C-N-CA     | 5.92  | 130.61      | 120.72   |
| 1   | A     | 747 | LEU  | N-CA-CB    | 5.92  | 118.76      | 109.94   |
| 1   | D     | 747 | LEU  | N-CA-CB    | 5.92  | 118.76      | 109.94   |
| 4   | 3     | 59  | GLN  | OE1-CD-NE2 | -5.92 | 116.68      | 122.60   |
| 4   | 4     | 97  | ALA  | N-CA-C     | -5.92 | 102.32      | 109.72   |
| 4   | 5     | 335 | ARG  | CA-CB-CG   | 5.92  | 125.94      | 114.10   |
| 4   | 7     | 233 | SER  | CA-C-O     | 5.92  | 128.97      | 120.51   |
| 4   | 0     | 34  | ILE  | CB-CA-C    | -5.92 | 102.38      | 110.90   |
| 4   | 2     | 335 | ARG  | CA-CB-CG   | 5.92  | 125.93      | 114.10   |
| 4   | 4     | 231 | ALA  | N-CA-C     | 5.92  | 117.40      | 111.07   |
| 4   | 5     | 252 | ASN  | CA-CB-CG   | 5.92  | 118.52      | 112.60   |
| 4   | Y     | 59  | GLN  | OE1-CD-NE2 | -5.92 | 116.68      | 122.60   |
| 1   | D     | 592 | ILE  | CA-C-N     | -5.92 | 113.60      | 122.47   |
| 1   | D     | 592 | ILE  | C-N-CA     | -5.92 | 113.60      | 122.47   |
| 4   | Y     | 335 | ARG  | CA-CB-CG   | 5.91  | 125.93      | 114.10   |
| 4   | Z     | 335 | ARG  | CA-CB-CG   | 5.91  | 125.92      | 114.10   |
| 1   | D     | 308 | ASN  | CA-C-N     | 5.91  | 125.53      | 119.56   |
| 1   | D     | 308 | ASN  | C-N-CA     | 5.91  | 125.53      | 119.56   |
| 1   | J     | 88  | ILE  | CB-CG1-CD1 | -5.91 | 101.38      | 113.80   |
| 4   | 8     | 233 | SER  | CA-C-O     | 5.91  | 128.96      | 120.51   |
| 1   | J     | 308 | ASN  | CA-C-N     | 5.91  | 125.53      | 119.56   |
| 1   | J     | 308 | ASN  | C-N-CA     | 5.91  | 125.53      | 119.56   |
| 1   | J     | 632 | GLY  | O-C-N      | 5.91  | 129.36      | 122.68   |
| 4   | 2     | 233 | SER  | CA-C-O     | 5.91  | 128.96      | 120.51   |
| 4   | 3     | 335 | ARG  | CA-CB-CG   | 5.91  | 125.92      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 8     | 335 | ARG  | CA-CB-CG   | 5.91  | 125.92      | 114.10   |
| 4   | 9     | 263 | GLN  | CA-C-N     | 5.91  | 125.53      | 119.56   |
| 4   | 9     | 263 | GLN  | C-N-CA     | 5.91  | 125.53      | 119.56   |
| 4   | 7     | 335 | ARG  | CA-CB-CG   | 5.91  | 125.91      | 114.10   |
| 4   | 9     | 335 | ARG  | CA-CB-CG   | 5.91  | 125.91      | 114.10   |
| 4   | 1     | 34  | ILE  | CB-CA-C    | -5.91 | 102.39      | 110.90   |
| 4   | 1     | 231 | ALA  | N-CA-C     | 5.91  | 117.39      | 111.07   |
| 4   | 0     | 233 | SER  | CA-C-O     | 5.90  | 128.95      | 120.51   |
| 1   | A     | 180 | GLU  | N-CA-CB    | 5.90  | 118.47      | 110.38   |
| 1   | G     | 136 | ASN  | O-C-N      | 5.90  | 126.22      | 121.38   |
| 4   | 0     | 257 | CYS  | O-C-N      | -5.90 | 116.20      | 120.27   |
| 4   | 2     | 97  | ALA  | N-CA-C     | -5.90 | 102.34      | 109.72   |
| 4   | 5     | 34  | ILE  | CB-CA-C    | -5.90 | 102.40      | 110.90   |
| 4   | V     | 34  | ILE  | CB-CA-C    | -5.90 | 102.40      | 110.90   |
| 4   | V     | 252 | ASN  | CA-CB-CG   | 5.90  | 118.50      | 112.60   |
| 4   | W     | 34  | ILE  | CB-CA-C    | -5.90 | 102.40      | 110.90   |
| 4   | X     | 335 | ARG  | CA-CB-CG   | 5.90  | 125.90      | 114.10   |
| 4   | Y     | 34  | ILE  | CB-CA-C    | -5.90 | 102.40      | 110.90   |
| 4   | 1     | 59  | GLN  | OE1-CD-NE2 | -5.90 | 116.70      | 122.60   |
| 1   | A     | 592 | ILE  | CA-C-N     | -5.90 | 113.62      | 122.47   |
| 1   | A     | 592 | ILE  | C-N-CA     | -5.90 | 113.62      | 122.47   |
| 1   | G     | 180 | GLU  | N-CA-CB    | 5.90  | 118.46      | 110.38   |
| 4   | 2     | 252 | ASN  | CA-CB-CG   | 5.90  | 118.50      | 112.60   |
| 4   | 2     | 263 | GLN  | CA-C-N     | 5.90  | 125.52      | 119.56   |
| 4   | 2     | 263 | GLN  | C-N-CA     | 5.90  | 125.52      | 119.56   |
| 4   | 5     | 263 | GLN  | CA-C-N     | 5.90  | 125.52      | 119.56   |
| 4   | 5     | 263 | GLN  | C-N-CA     | 5.90  | 125.52      | 119.56   |
| 4   | Z     | 233 | SER  | CA-C-O     | 5.90  | 128.94      | 120.51   |
| 1   | D     | 136 | ASN  | O-C-N      | 5.89  | 126.21      | 121.38   |
| 1   | G     | 753 | VAL  | N-CA-C     | 5.89  | 118.43      | 109.12   |
| 1   | J     | 717 | TYR  | N-CA-C     | 5.89  | 121.10      | 111.37   |
| 4   | 2     | 34  | ILE  | CB-CA-C    | -5.89 | 102.41      | 110.90   |
| 1   | A     | 136 | ASN  | O-C-N      | 5.89  | 126.21      | 121.38   |
| 4   | 3     | 34  | ILE  | CB-CA-C    | -5.89 | 102.42      | 110.90   |
| 4   | Y     | 231 | ALA  | N-CA-C     | 5.89  | 117.37      | 111.07   |
| 4   | X     | 257 | CYS  | O-C-N      | -5.89 | 116.21      | 120.27   |
| 1   | A     | 717 | TYR  | N-CA-C     | 5.89  | 121.09      | 111.37   |
| 4   | 5     | 97  | ALA  | N-CA-C     | -5.89 | 102.36      | 109.72   |
| 4   | 7     | 34  | ILE  | CB-CA-C    | -5.89 | 102.42      | 110.90   |
| 4   | 9     | 97  | ALA  | N-CA-C     | -5.89 | 102.36      | 109.72   |
| 4   | V     | 233 | SER  | CA-C-O     | 5.89  | 128.93      | 120.51   |
| 4   | W     | 97  | ALA  | N-CA-C     | -5.89 | 102.36      | 109.72   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Z     | 263 | GLN  | CA-C-N     | 5.89  | 125.51      | 119.56   |
| 4   | Z     | 263 | GLN  | C-N-CA     | 5.89  | 125.51      | 119.56   |
| 4   | 1     | 335 | ARG  | CA-CB-CG   | 5.89  | 125.88      | 114.10   |
| 4   | X     | 34  | ILE  | CB-CA-C    | -5.89 | 102.42      | 110.90   |
| 4   | Y     | 263 | GLN  | CA-C-N     | 5.89  | 125.50      | 119.56   |
| 4   | Y     | 263 | GLN  | C-N-CA     | 5.89  | 125.50      | 119.56   |
| 4   | 4     | 263 | GLN  | CA-C-N     | 5.88  | 125.50      | 119.56   |
| 4   | 4     | 263 | GLN  | C-N-CA     | 5.88  | 125.50      | 119.56   |
| 4   | W     | 263 | GLN  | CA-C-N     | 5.88  | 125.50      | 119.56   |
| 4   | W     | 263 | GLN  | C-N-CA     | 5.88  | 125.50      | 119.56   |
| 4   | 1     | 97  | ALA  | N-CA-C     | -5.88 | 102.37      | 109.72   |
| 1   | A     | 136 | ASN  | CA-C-O     | 5.88  | 124.65      | 119.71   |
| 4   | 4     | 34  | ILE  | CB-CA-C    | -5.88 | 102.43      | 110.90   |
| 4   | V     | 263 | GLN  | CA-C-N     | 5.88  | 125.50      | 119.56   |
| 4   | V     | 263 | GLN  | C-N-CA     | 5.88  | 125.50      | 119.56   |
| 4   | V     | 97  | ALA  | N-CA-C     | -5.88 | 102.37      | 109.72   |
| 1   | D     | 88  | ILE  | CB-CG1-CD1 | -5.88 | 101.45      | 113.80   |
| 4   | 2     | 257 | CYS  | O-C-N      | -5.88 | 116.21      | 120.27   |
| 4   | 1     | 233 | SER  | CA-C-O     | 5.88  | 128.91      | 120.51   |
| 4   | Z     | 34  | ILE  | CB-CA-C    | -5.88 | 102.44      | 110.90   |
| 4   | X     | 263 | GLN  | CA-C-N     | 5.87  | 125.49      | 119.56   |
| 4   | X     | 263 | GLN  | C-N-CA     | 5.87  | 125.49      | 119.56   |
| 1   | A     | 479 | CYS  | N-CA-CB    | 5.87  | 118.87      | 110.06   |
| 1   | D     | 718 | ALA  | O-C-N      | 5.87  | 128.84      | 122.15   |
| 4   | 0     | 97  | ALA  | N-CA-C     | -5.87 | 102.38      | 109.72   |
| 4   | 0     | 263 | GLN  | CA-C-N     | 5.87  | 125.49      | 119.56   |
| 4   | 0     | 263 | GLN  | C-N-CA     | 5.87  | 125.49      | 119.56   |
| 4   | 8     | 97  | ALA  | N-CA-C     | -5.87 | 102.38      | 109.72   |
| 1   | G     | 687 | GLU  | N-CA-CB    | 5.87  | 118.92      | 110.06   |
| 4   | 3     | 233 | SER  | CA-C-O     | 5.87  | 128.90      | 120.51   |
| 1   | A     | 88  | ILE  | CB-CG1-CD1 | -5.87 | 101.48      | 113.80   |
| 1   | D     | 632 | GLY  | O-C-N      | 5.87  | 129.31      | 122.68   |
| 4   | 7     | 97  | ALA  | N-CA-C     | -5.87 | 102.38      | 109.72   |
| 1   | A     | 753 | VAL  | N-CA-C     | 5.87  | 118.39      | 109.12   |
| 4   | 1     | 257 | CYS  | O-C-N      | -5.86 | 116.22      | 120.27   |
| 4   | 7     | 263 | GLN  | CA-C-N     | 5.86  | 125.48      | 119.56   |
| 4   | 7     | 263 | GLN  | C-N-CA     | 5.86  | 125.48      | 119.56   |
| 4   | 8     | 263 | GLN  | CA-C-N     | 5.86  | 125.48      | 119.56   |
| 4   | 8     | 263 | GLN  | C-N-CA     | 5.86  | 125.48      | 119.56   |
| 1   | J     | 136 | ASN  | O-C-N      | 5.86  | 126.18      | 121.38   |
| 1   | D     | 753 | VAL  | N-CA-C     | 5.86  | 118.37      | 109.12   |
| 1   | J     | 592 | ILE  | CA-C-N     | -5.86 | 113.68      | 122.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | J     | 592 | ILE  | C-N-CA     | -5.86 | 113.68      | 122.47   |
| 1   | A     | 23  | GLU  | N-CA-C     | -5.86 | 104.98      | 111.71   |
| 1   | D     | 786 | ILE  | CB-CA-C    | -5.86 | 104.37      | 112.04   |
| 4   | 9     | 34  | ILE  | CB-CA-C    | -5.86 | 102.47      | 110.90   |
| 4   | 9     | 254 | ARG  | N-CA-CB    | -5.86 | 100.59      | 110.49   |
| 4   | X     | 233 | SER  | CA-C-O     | 5.86  | 128.88      | 120.51   |
| 4   | 1     | 263 | GLN  | CA-C-N     | 5.85  | 125.47      | 119.56   |
| 4   | 1     | 263 | GLN  | C-N-CA     | 5.85  | 125.47      | 119.56   |
| 1   | J     | 463 | ASP  | CA-CB-CG   | 5.85  | 118.45      | 112.60   |
| 4   | 1     | 254 | ARG  | N-CA-CB    | -5.85 | 100.60      | 110.49   |
| 1   | D     | 23  | GLU  | N-CA-C     | -5.85 | 104.98      | 111.71   |
| 4   | Z     | 97  | ALA  | N-CA-C     | -5.85 | 102.41      | 109.72   |
| 4   | W     | 257 | CYS  | O-C-N      | -5.85 | 116.23      | 120.27   |
| 4   | Y     | 257 | CYS  | O-C-N      | -5.85 | 116.23      | 120.27   |
| 4   | 0     | 59  | GLN  | OE1-CD-NE2 | -5.84 | 116.75      | 122.60   |
| 4   | 3     | 97  | ALA  | N-CA-C     | -5.84 | 102.42      | 109.72   |
| 4   | 9     | 233 | SER  | CA-C-O     | 5.84  | 128.86      | 120.51   |
| 1   | D     | 463 | ASP  | CA-CB-CG   | 5.84  | 118.44      | 112.60   |
| 4   | V     | 254 | ARG  | N-CA-CB    | -5.84 | 100.62      | 110.49   |
| 4   | Z     | 257 | CYS  | O-C-N      | -5.84 | 116.24      | 120.27   |
| 4   | 3     | 254 | ARG  | N-CA-CB    | -5.84 | 100.62      | 110.49   |
| 4   | 5     | 254 | ARG  | N-CA-CB    | -5.84 | 100.63      | 110.49   |
| 4   | 9     | 113 | LYS  | CA-CB-CG   | 5.83  | 125.77      | 114.10   |
| 4   | 9     | 257 | CYS  | O-C-N      | -5.83 | 116.25      | 120.27   |
| 4   | 0     | 113 | LYS  | CA-CB-CG   | 5.83  | 125.76      | 114.10   |
| 4   | W     | 233 | SER  | CA-C-O     | 5.83  | 128.85      | 120.51   |
| 4   | 8     | 113 | LYS  | CA-CB-CG   | 5.83  | 125.76      | 114.10   |
| 1   | J     | 739 | ASP  | N-CA-CB    | 5.83  | 119.62      | 110.71   |
| 4   | 4     | 257 | CYS  | O-C-N      | -5.83 | 116.25      | 120.27   |
| 4   | 7     | 257 | CYS  | O-C-N      | -5.82 | 116.25      | 120.27   |
| 1   | G     | 217 | THR  | O-C-N      | 5.82  | 130.02      | 123.27   |
| 1   | G     | 278 | GLN  | OE1-CD-NE2 | 5.82  | 128.42      | 122.60   |
| 1   | G     | 747 | LEU  | N-CA-CB    | 5.82  | 118.61      | 109.94   |
| 4   | 0     | 254 | ARG  | N-CA-CB    | -5.82 | 100.66      | 110.49   |
| 4   | 3     | 263 | GLN  | CA-C-N     | 5.82  | 125.44      | 119.56   |
| 4   | 3     | 263 | GLN  | C-N-CA     | 5.82  | 125.44      | 119.56   |
| 1   | D     | 739 | ASP  | N-CA-CB    | 5.82  | 119.61      | 110.71   |
| 4   | 1     | 113 | LYS  | CA-CB-CG   | 5.82  | 125.73      | 114.10   |
| 4   | W     | 254 | ARG  | N-CA-CB    | -5.82 | 100.66      | 110.49   |
| 4   | 3     | 257 | CYS  | O-C-N      | -5.82 | 116.26      | 120.27   |
| 4   | 7     | 254 | ARG  | N-CA-CB    | -5.82 | 100.66      | 110.49   |
| 4   | Y     | 233 | SER  | CA-C-O     | 5.82  | 128.83      | 120.51   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 2     | 254 | ARG  | N-CA-CB    | -5.81 | 100.67      | 110.49   |
| 4   | 3     | 113 | LYS  | CA-CB-CG   | 5.81  | 125.72      | 114.10   |
| 4   | 8     | 257 | CYS  | O-C-N      | -5.81 | 116.26      | 120.27   |
| 1   | J     | 687 | GLU  | N-CA-CB    | 5.81  | 118.83      | 110.06   |
| 4   | 4     | 233 | SER  | CA-C-O     | 5.81  | 128.81      | 120.51   |
| 4   | Z     | 113 | LYS  | CA-CB-CG   | 5.80  | 125.71      | 114.10   |
| 4   | W     | 113 | LYS  | CA-CB-CG   | 5.80  | 125.71      | 114.10   |
| 4   | 8     | 254 | ARG  | N-CA-CB    | -5.80 | 100.69      | 110.49   |
| 4   | V     | 113 | LYS  | CA-CB-CG   | 5.80  | 125.70      | 114.10   |
| 4   | Y     | 254 | ARG  | N-CA-CB    | -5.80 | 100.69      | 110.49   |
| 1   | A     | 278 | GLN  | OE1-CD-NE2 | 5.80  | 128.40      | 122.60   |
| 4   | Y     | 113 | LYS  | CA-CB-CG   | 5.80  | 125.70      | 114.10   |
| 1   | D     | 278 | GLN  | OE1-CD-NE2 | 5.80  | 128.40      | 122.60   |
| 1   | G     | 463 | ASP  | CA-CB-CG   | 5.80  | 118.40      | 112.60   |
| 4   | 0     | 161 | HIS  | CB-CG-CD2  | -5.80 | 123.66      | 131.20   |
| 4   | 7     | 113 | LYS  | CA-CB-CG   | 5.80  | 125.69      | 114.10   |
| 4   | X     | 113 | LYS  | CA-CB-CG   | 5.80  | 125.69      | 114.10   |
| 1   | J     | 23  | GLU  | N-CA-C     | -5.79 | 105.05      | 111.71   |
| 4   | 2     | 113 | LYS  | CA-CB-CG   | 5.79  | 125.68      | 114.10   |
| 1   | A     | 687 | GLU  | N-CA-CB    | 5.79  | 118.80      | 110.06   |
| 4   | 5     | 113 | LYS  | CA-CB-CG   | 5.79  | 125.68      | 114.10   |
| 4   | V     | 161 | HIS  | CB-CG-CD2  | -5.79 | 123.67      | 131.20   |
| 4   | W     | 161 | HIS  | CB-CG-CD2  | -5.79 | 123.67      | 131.20   |
| 4   | 4     | 254 | ARG  | N-CA-CB    | -5.79 | 100.71      | 110.49   |
| 4   | 0     | 335 | ARG  | N-CA-C     | 5.79  | 123.12      | 110.80   |
| 4   | X     | 254 | ARG  | N-CA-CB    | -5.78 | 100.72      | 110.49   |
| 4   | Y     | 161 | HIS  | CB-CG-CD2  | -5.78 | 123.69      | 131.20   |
| 4   | Z     | 254 | ARG  | N-CA-CB    | -5.78 | 100.72      | 110.49   |
| 1   | A     | 718 | ALA  | O-C-N      | 5.78  | 128.74      | 122.15   |
| 1   | G     | 739 | ASP  | N-CA-CB    | 5.78  | 119.55      | 110.71   |
| 1   | J     | 790 | THR  | CA-C-O     | 5.77  | 126.47      | 119.31   |
| 4   | 4     | 113 | LYS  | CA-CB-CG   | 5.77  | 125.65      | 114.10   |
| 1   | J     | 217 | THR  | O-C-N      | 5.77  | 129.96      | 123.27   |
| 4   | 4     | 161 | HIS  | CB-CG-CD2  | -5.77 | 123.70      | 131.20   |
| 4   | X     | 161 | HIS  | CB-CG-CD2  | -5.77 | 123.70      | 131.20   |
| 1   | G     | 828 | HIS  | CA-C-N     | 5.77  | 129.27      | 121.20   |
| 1   | G     | 828 | HIS  | C-N-CA     | 5.77  | 129.27      | 121.20   |
| 1   | J     | 828 | HIS  | CA-C-N     | 5.77  | 129.27      | 121.20   |
| 1   | J     | 828 | HIS  | C-N-CA     | 5.77  | 129.27      | 121.20   |
| 4   | 1     | 161 | HIS  | CB-CG-CD2  | -5.77 | 123.70      | 131.20   |
| 4   | 5     | 161 | HIS  | CB-CG-CD2  | -5.77 | 123.70      | 131.20   |
| 4   | 9     | 161 | HIS  | CB-CG-CD2  | -5.77 | 123.70      | 131.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 739 | ASP  | N-CA-CB    | 5.76  | 119.53      | 110.71   |
| 1   | D     | 687 | GLU  | N-CA-CB    | 5.76  | 118.77      | 110.06   |
| 2   | E     | 138 | ALA  | CA-C-N     | -5.76 | 110.86      | 121.41   |
| 2   | E     | 138 | ALA  | C-N-CA     | -5.76 | 110.86      | 121.41   |
| 1   | A     | 790 | THR  | CA-C-O     | 5.76  | 126.45      | 119.31   |
| 4   | 7     | 161 | HIS  | CB-CG-CD2  | -5.76 | 123.71      | 131.20   |
| 4   | 2     | 161 | HIS  | CB-CG-CD2  | -5.76 | 123.72      | 131.20   |
| 4   | 4     | 335 | ARG  | N-CA-C     | 5.76  | 123.06      | 110.80   |
| 4   | 5     | 335 | ARG  | N-CA-C     | 5.76  | 123.06      | 110.80   |
| 4   | 8     | 161 | HIS  | CB-CG-CD2  | -5.76 | 123.72      | 131.20   |
| 4   | 3     | 335 | ARG  | N-CA-C     | 5.75  | 123.06      | 110.80   |
| 2   | H     | 138 | ALA  | CA-C-N     | -5.75 | 110.89      | 121.41   |
| 2   | H     | 138 | ALA  | C-N-CA     | -5.75 | 110.89      | 121.41   |
| 4   | 8     | 335 | ARG  | N-CA-C     | 5.75  | 123.04      | 110.80   |
| 4   | 9     | 335 | ARG  | N-CA-C     | 5.75  | 123.04      | 110.80   |
| 4   | W     | 335 | ARG  | N-CA-C     | 5.75  | 123.04      | 110.80   |
| 4   | Z     | 335 | ARG  | N-CA-C     | 5.75  | 123.04      | 110.80   |
| 1   | J     | 718 | ALA  | O-C-N      | 5.74  | 128.70      | 122.15   |
| 4   | V     | 185 | LEU  | N-CA-C     | 5.74  | 118.48      | 111.82   |
| 1   | G     | 739 | ASP  | CB-CA-C    | -5.74 | 102.81      | 110.79   |
| 4   | 2     | 335 | ARG  | N-CA-C     | 5.74  | 123.03      | 110.80   |
| 4   | 8     | 263 | GLN  | OE1-CD-NE2 | -5.74 | 116.86      | 122.60   |
| 2   | B     | 138 | ALA  | CA-C-N     | -5.74 | 110.91      | 121.41   |
| 2   | B     | 138 | ALA  | C-N-CA     | -5.74 | 110.91      | 121.41   |
| 4   | 0     | 135 | ALA  | O-C-N      | -5.74 | 116.64      | 123.06   |
| 4   | 5     | 257 | CYS  | O-C-N      | -5.73 | 116.31      | 120.27   |
| 4   | 9     | 263 | GLN  | OE1-CD-NE2 | -5.73 | 116.87      | 122.60   |
| 1   | G     | 23  | GLU  | N-CA-C     | -5.73 | 105.12      | 111.71   |
| 4   | 3     | 161 | HIS  | CB-CG-CD2  | -5.73 | 123.75      | 131.20   |
| 4   | 4     | 263 | GLN  | OE1-CD-NE2 | -5.73 | 116.87      | 122.60   |
| 4   | V     | 263 | GLN  | OE1-CD-NE2 | -5.73 | 116.87      | 122.60   |
| 1   | J     | 278 | GLN  | OE1-CD-NE2 | 5.73  | 128.33      | 122.60   |
| 4   | 1     | 335 | ARG  | N-CA-C     | 5.73  | 123.00      | 110.80   |
| 4   | V     | 335 | ARG  | N-CA-C     | 5.73  | 123.00      | 110.80   |
| 4   | W     | 263 | GLN  | OE1-CD-NE2 | -5.73 | 116.87      | 122.60   |
| 4   | 7     | 135 | ALA  | O-C-N      | -5.73 | 116.65      | 123.06   |
| 4   | Y     | 335 | ARG  | N-CA-C     | 5.73  | 123.00      | 110.80   |
| 1   | A     | 217 | THR  | O-C-N      | 5.72  | 129.91      | 123.27   |
| 4   | 2     | 185 | LEU  | N-CA-C     | 5.72  | 118.46      | 111.82   |
| 4   | 7     | 335 | ARG  | N-CA-C     | 5.72  | 122.98      | 110.80   |
| 4   | Z     | 161 | HIS  | CB-CG-CD2  | -5.72 | 123.77      | 131.20   |
| 4   | X     | 335 | ARG  | N-CA-C     | 5.71  | 122.97      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 786 | ILE  | CB-CA-C    | -5.71 | 104.56      | 112.04   |
| 4   | X     | 185 | LEU  | N-CA-C     | 5.71  | 118.45      | 111.82   |
| 4   | Z     | 135 | ALA  | O-C-N      | -5.71 | 116.66      | 123.06   |
| 1   | G     | 790 | THR  | CA-C-O     | 5.71  | 126.39      | 119.31   |
| 1   | D     | 828 | HIS  | CA-C-N     | 5.71  | 129.19      | 121.20   |
| 1   | D     | 828 | HIS  | C-N-CA     | 5.71  | 129.19      | 121.20   |
| 4   | W     | 135 | ALA  | O-C-N      | -5.71 | 116.67      | 123.06   |
| 1   | A     | 463 | ASP  | CA-CB-CG   | 5.71  | 118.31      | 112.60   |
| 4   | Z     | 185 | LEU  | N-CA-C     | 5.70  | 118.44      | 111.82   |
| 4   | 0     | 263 | GLN  | OE1-CD-NE2 | -5.70 | 116.90      | 122.60   |
| 3   | I     | 63  | ILE  | CB-CA-C    | 5.70  | 120.74      | 110.48   |
| 1   | D     | 739 | ASP  | CB-CA-C    | -5.69 | 102.88      | 110.79   |
| 1   | J     | 433 | VAL  | N-CA-C     | 5.69  | 115.88      | 110.42   |
| 2   | K     | 138 | ALA  | CA-C-N     | -5.69 | 111.00      | 121.41   |
| 2   | K     | 138 | ALA  | C-N-CA     | -5.69 | 111.00      | 121.41   |
| 4   | 0     | 262 | PHE  | CA-CB-CG   | -5.69 | 108.11      | 113.80   |
| 4   | 1     | 185 | LEU  | N-CA-C     | 5.69  | 118.42      | 111.82   |
| 4   | V     | 135 | ALA  | O-C-N      | -5.68 | 116.69      | 123.06   |
| 4   | 2     | 262 | PHE  | CA-CB-CG   | -5.68 | 108.12      | 113.80   |
| 4   | 3     | 185 | LEU  | N-CA-C     | 5.68  | 118.41      | 111.82   |
| 4   | 9     | 135 | ALA  | O-C-N      | -5.68 | 116.70      | 123.06   |
| 4   | Y     | 135 | ALA  | O-C-N      | -5.68 | 116.70      | 123.06   |
| 4   | Y     | 262 | PHE  | CA-CB-CG   | -5.68 | 108.12      | 113.80   |
| 4   | Z     | 262 | PHE  | CA-CB-CG   | -5.68 | 108.12      | 113.80   |
| 4   | 5     | 263 | GLN  | OE1-CD-NE2 | -5.67 | 116.93      | 122.60   |
| 4   | V     | 262 | PHE  | CA-CB-CG   | -5.67 | 108.12      | 113.80   |
| 1   | A     | 351 | ILE  | CB-CA-C    | -5.67 | 104.63      | 111.88   |
| 1   | J     | 739 | ASP  | CB-CA-C    | -5.67 | 102.91      | 110.79   |
| 4   | 3     | 263 | GLN  | OE1-CD-NE2 | -5.67 | 116.93      | 122.60   |
| 4   | 8     | 135 | ALA  | O-C-N      | -5.67 | 116.71      | 123.06   |
| 1   | A     | 739 | ASP  | CB-CA-C    | -5.66 | 102.92      | 110.79   |
| 3   | F     | 63  | ILE  | CB-CA-C    | 5.66  | 120.68      | 110.48   |
| 1   | G     | 433 | VAL  | N-CA-C     | 5.66  | 115.86      | 110.42   |
| 4   | Z     | 263 | GLN  | OE1-CD-NE2 | -5.66 | 116.94      | 122.60   |
| 4   | 5     | 185 | LEU  | N-CA-C     | 5.66  | 118.39      | 111.82   |
| 3   | C     | 63  | ILE  | CB-CA-C    | 5.66  | 120.66      | 110.48   |
| 4   | 2     | 263 | GLN  | OE1-CD-NE2 | -5.66 | 116.94      | 122.60   |
| 4   | 4     | 135 | ALA  | O-C-N      | -5.65 | 116.73      | 123.06   |
| 1   | D     | 22  | LYS  | CB-CA-C    | 5.65  | 118.52      | 109.02   |
| 4   | 7     | 185 | LEU  | N-CA-C     | 5.65  | 118.38      | 111.82   |
| 1   | A     | 346 | ASP  | N-CA-CB    | -5.65 | 101.23      | 109.82   |
| 1   | D     | 217 | THR  | O-C-N      | 5.65  | 129.82      | 123.27   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 1     | 263 | GLN  | OE1-CD-NE2 | -5.65 | 116.95      | 122.60   |
| 4   | 4     | 185 | LEU  | N-CA-C     | 5.65  | 118.37      | 111.82   |
| 4   | 9     | 185 | LEU  | N-CA-C     | 5.65  | 118.38      | 111.82   |
| 4   | X     | 135 | ALA  | O-C-N      | -5.65 | 116.73      | 123.06   |
| 4   | X     | 262 | PHE  | CA-CB-CG   | -5.65 | 108.15      | 113.80   |
| 1   | D     | 433 | VAL  | N-CA-C     | 5.65  | 115.84      | 110.42   |
| 4   | 1     | 135 | ALA  | O-C-N      | -5.65 | 116.73      | 123.06   |
| 4   | Y     | 185 | LEU  | N-CA-C     | 5.65  | 118.37      | 111.82   |
| 4   | 2     | 135 | ALA  | O-C-N      | -5.64 | 116.74      | 123.06   |
| 1   | D     | 196 | PHE  | CA-CB-CG   | -5.64 | 108.16      | 113.80   |
| 1   | D     | 351 | ILE  | CB-CA-C    | -5.64 | 104.66      | 111.88   |
| 4   | 3     | 135 | ALA  | O-C-N      | -5.64 | 116.75      | 123.06   |
| 4   | X     | 263 | GLN  | OE1-CD-NE2 | -5.64 | 116.96      | 122.60   |
| 1   | J     | 22  | LYS  | CB-CA-C    | 5.64  | 118.49      | 109.02   |
| 4   | 9     | 262 | PHE  | CA-CB-CG   | -5.64 | 108.16      | 113.80   |
| 1   | A     | 22  | LYS  | CB-CA-C    | 5.63  | 118.49      | 109.02   |
| 1   | G     | 22  | LYS  | CB-CA-C    | 5.63  | 118.49      | 109.02   |
| 1   | J     | 351 | ILE  | CB-CA-C    | -5.63 | 104.67      | 111.88   |
| 1   | J     | 346 | ASP  | N-CA-CB    | -5.63 | 101.26      | 109.82   |
| 1   | J     | 291 | ILE  | N-CA-C     | 5.63  | 117.04      | 110.62   |
| 4   | 5     | 135 | ALA  | O-C-N      | -5.63 | 116.76      | 123.06   |
| 1   | D     | 291 | ILE  | N-CA-C     | 5.62  | 117.03      | 110.62   |
| 4   | W     | 185 | LEU  | N-CA-C     | 5.62  | 118.34      | 111.82   |
| 1   | D     | 346 | ASP  | N-CA-CB    | -5.62 | 101.27      | 109.82   |
| 1   | J     | 568 | PRO  | CB-CA-C    | -5.62 | 104.03      | 111.23   |
| 4   | 7     | 262 | PHE  | CA-CB-CG   | -5.62 | 108.18      | 113.80   |
| 1   | G     | 351 | ILE  | CB-CA-C    | -5.62 | 104.69      | 111.88   |
| 1   | D     | 755 | HIS  | CA-C-N     | 5.61  | 129.51      | 121.71   |
| 1   | D     | 755 | HIS  | C-N-CA     | 5.61  | 129.51      | 121.71   |
| 1   | A     | 755 | HIS  | CA-C-N     | 5.61  | 129.51      | 121.71   |
| 1   | A     | 755 | HIS  | C-N-CA     | 5.61  | 129.51      | 121.71   |
| 1   | J     | 309 | PRO  | CB-CA-C    | -5.61 | 103.49      | 111.68   |
| 3   | L     | 63  | ILE  | CB-CA-C    | 5.61  | 120.58      | 110.48   |
| 4   | 0     | 185 | LEU  | N-CA-C     | 5.61  | 118.33      | 111.82   |
| 1   | A     | 433 | VAL  | N-CA-C     | 5.61  | 115.80      | 110.42   |
| 1   | A     | 568 | PRO  | CB-CA-C    | -5.60 | 104.06      | 111.23   |
| 4   | 3     | 262 | PHE  | CA-CB-CG   | -5.60 | 108.20      | 113.80   |
| 4   | Y     | 263 | GLN  | OE1-CD-NE2 | -5.60 | 117.00      | 122.60   |
| 1   | A     | 623 | PHE  | CB-CG-CD2  | -5.59 | 111.19      | 120.70   |
| 1   | A     | 828 | HIS  | CA-C-N     | 5.59  | 129.03      | 121.20   |
| 1   | A     | 828 | HIS  | C-N-CA     | 5.59  | 129.03      | 121.20   |
| 1   | G     | 623 | PHE  | CB-CG-CD2  | -5.59 | 111.19      | 120.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 8     | 185 | LEU  | N-CA-C     | 5.59  | 118.31      | 111.82   |
| 1   | J     | 257 | THR  | N-CA-C     | -5.59 | 104.87      | 110.97   |
| 4   | 7     | 263 | GLN  | OE1-CD-NE2 | -5.59 | 117.01      | 122.60   |
| 4   | V     | 137 | GLN  | CA-C-O     | -5.59 | 115.13      | 121.00   |
| 4   | 4     | 262 | PHE  | CA-CB-CG   | -5.59 | 108.21      | 113.80   |
| 4   | 1     | 262 | PHE  | CA-CB-CG   | -5.59 | 108.21      | 113.80   |
| 4   | 8     | 262 | PHE  | CA-CB-CG   | -5.58 | 108.22      | 113.80   |
| 4   | Z     | 137 | GLN  | CA-C-O     | -5.58 | 115.14      | 121.00   |
| 1   | J     | 755 | HIS  | CA-C-N     | 5.58  | 129.47      | 121.71   |
| 1   | J     | 755 | HIS  | C-N-CA     | 5.58  | 129.47      | 121.71   |
| 4   | 7     | 349 | LEU  | CA-C-N     | 5.58  | 127.75      | 120.28   |
| 4   | 7     | 349 | LEU  | C-N-CA     | 5.58  | 127.75      | 120.28   |
| 1   | D     | 309 | PRO  | CB-CA-C    | -5.58 | 103.54      | 111.68   |
| 1   | G     | 346 | ASP  | N-CA-CB    | -5.58 | 101.34      | 109.82   |
| 4   | W     | 262 | PHE  | CA-CB-CG   | -5.58 | 108.22      | 113.80   |
| 1   | D     | 257 | THR  | N-CA-C     | -5.57 | 104.90      | 110.97   |
| 1   | G     | 671 | PHE  | N-CA-C     | 5.56  | 118.88      | 109.76   |
| 1   | G     | 718 | ALA  | O-C-N      | 5.56  | 128.49      | 122.15   |
| 1   | D     | 671 | PHE  | N-CA-C     | 5.56  | 118.88      | 109.76   |
| 1   | A     | 257 | THR  | N-CA-C     | -5.55 | 104.92      | 110.97   |
| 1   | D     | 623 | PHE  | CB-CG-CD2  | -5.55 | 111.26      | 120.70   |
| 1   | J     | 623 | PHE  | CB-CG-CD2  | -5.55 | 111.26      | 120.70   |
| 1   | G     | 291 | ILE  | N-CA-C     | 5.55  | 116.95      | 110.62   |
| 1   | G     | 309 | PRO  | CB-CA-C    | -5.55 | 103.58      | 111.68   |
| 1   | J     | 671 | PHE  | N-CA-C     | 5.55  | 118.86      | 109.76   |
| 4   | X     | 275 | HIS  | CB-CG-CD2  | -5.55 | 123.99      | 131.20   |
| 1   | G     | 568 | PRO  | CB-CA-C    | -5.54 | 104.14      | 111.23   |
| 4   | Y     | 275 | HIS  | CB-CG-CD2  | -5.54 | 124.00      | 131.20   |
| 1   | A     | 196 | PHE  | CA-CB-CG   | -5.54 | 108.26      | 113.80   |
| 4   | 9     | 137 | GLN  | CA-C-O     | -5.54 | 115.18      | 121.00   |
| 4   | W     | 275 | HIS  | CB-CG-CD2  | -5.54 | 124.00      | 131.20   |
| 4   | 9     | 44  | MET  | N-CA-C     | -5.54 | 102.33      | 110.52   |
| 4   | 3     | 349 | LEU  | CA-C-N     | 5.54  | 127.70      | 120.28   |
| 4   | 3     | 349 | LEU  | C-N-CA     | 5.54  | 127.70      | 120.28   |
| 4   | 0     | 275 | HIS  | CB-CG-CD2  | -5.53 | 124.01      | 131.20   |
| 4   | 4     | 275 | HIS  | CB-CG-CD2  | -5.53 | 124.01      | 131.20   |
| 1   | G     | 333 | ALA  | CA-C-O     | 5.53  | 126.82      | 120.90   |
| 4   | 0     | 312 | ARG  | NE-CZ-NH2  | 5.53  | 124.18      | 119.20   |
| 4   | 5     | 262 | PHE  | CA-CB-CG   | -5.53 | 108.27      | 113.80   |
| 4   | 8     | 312 | ARG  | NE-CZ-NH2  | 5.53  | 124.18      | 119.20   |
| 4   | 2     | 44  | MET  | N-CA-C     | -5.53 | 102.34      | 110.52   |
| 4   | Y     | 44  | MET  | N-CA-C     | -5.53 | 102.34      | 110.52   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 8     | 275 | HIS  | CB-CG-CD2 | -5.53 | 124.02      | 131.20   |
| 4   | 5     | 44  | MET  | N-CA-C    | -5.52 | 102.34      | 110.52   |
| 4   | 1     | 275 | HIS  | CB-CG-CD2 | -5.52 | 124.02      | 131.20   |
| 4   | X     | 349 | LEU  | CA-C-N    | 5.52  | 127.68      | 120.28   |
| 4   | X     | 349 | LEU  | C-N-CA    | 5.52  | 127.68      | 120.28   |
| 4   | 9     | 275 | HIS  | CB-CG-CD2 | -5.52 | 124.02      | 131.20   |
| 1   | G     | 755 | HIS  | CA-C-N    | 5.52  | 129.38      | 121.71   |
| 1   | G     | 755 | HIS  | C-N-CA    | 5.52  | 129.38      | 121.71   |
| 4   | 2     | 275 | HIS  | CB-CG-CD2 | -5.52 | 124.03      | 131.20   |
| 4   | 7     | 44  | MET  | N-CA-C    | -5.52 | 102.35      | 110.52   |
| 4   | 5     | 137 | GLN  | CA-C-O    | -5.51 | 115.21      | 121.00   |
| 4   | 8     | 349 | LEU  | CA-C-N    | 5.51  | 127.67      | 120.28   |
| 4   | 8     | 349 | LEU  | C-N-CA    | 5.51  | 127.67      | 120.28   |
| 4   | 2     | 349 | LEU  | CA-C-N    | 5.51  | 127.66      | 120.28   |
| 4   | 2     | 349 | LEU  | C-N-CA    | 5.51  | 127.66      | 120.28   |
| 4   | 4     | 44  | MET  | N-CA-C    | -5.51 | 102.36      | 110.52   |
| 4   | W     | 44  | MET  | N-CA-C    | -5.51 | 102.36      | 110.52   |
| 4   | Z     | 44  | MET  | N-CA-C    | -5.51 | 102.36      | 110.52   |
| 4   | X     | 44  | MET  | N-CA-C    | -5.51 | 102.36      | 110.52   |
| 1   | G     | 785 | GLU  | CA-C-N    | -5.51 | 112.06      | 121.97   |
| 1   | G     | 785 | GLU  | C-N-CA    | -5.51 | 112.06      | 121.97   |
| 4   | 0     | 349 | LEU  | CA-C-N    | 5.50  | 127.66      | 120.28   |
| 4   | 0     | 349 | LEU  | C-N-CA    | 5.50  | 127.66      | 120.28   |
| 4   | 1     | 116 | ARG  | N-CA-C    | -5.50 | 105.28      | 111.28   |
| 4   | 3     | 44  | MET  | N-CA-C    | -5.50 | 102.38      | 110.52   |
| 4   | V     | 275 | HIS  | CB-CG-CD2 | -5.50 | 124.05      | 131.20   |
| 1   | G     | 257 | THR  | N-CA-C    | -5.50 | 104.98      | 110.97   |
| 4   | 2     | 312 | ARG  | NE-CZ-NH2 | 5.50  | 124.15      | 119.20   |
| 4   | 9     | 349 | LEU  | CA-C-N    | 5.50  | 127.65      | 120.28   |
| 4   | 9     | 349 | LEU  | C-N-CA    | 5.50  | 127.65      | 120.28   |
| 4   | 0     | 44  | MET  | N-CA-C    | -5.50 | 102.39      | 110.52   |
| 4   | Z     | 275 | HIS  | CB-CG-CD2 | -5.50 | 124.06      | 131.20   |
| 4   | 3     | 137 | GLN  | CA-C-O    | -5.50 | 115.23      | 121.00   |
| 4   | V     | 44  | MET  | N-CA-C    | -5.50 | 102.39      | 110.52   |
| 4   | 5     | 349 | LEU  | CA-C-N    | 5.49  | 127.64      | 120.28   |
| 4   | 5     | 349 | LEU  | C-N-CA    | 5.49  | 127.64      | 120.28   |
| 4   | W     | 349 | LEU  | CA-C-N    | 5.49  | 127.64      | 120.28   |
| 4   | W     | 349 | LEU  | C-N-CA    | 5.49  | 127.64      | 120.28   |
| 4   | W     | 200 | PHE  | CA-C-O    | 5.49  | 127.86      | 121.11   |
| 4   | 3     | 275 | HIS  | CB-CG-CD2 | -5.49 | 124.07      | 131.20   |
| 1   | D     | 305 | ILE  | CB-CA-C   | -5.49 | 103.66      | 111.34   |
| 4   | 7     | 137 | GLN  | CA-C-O    | -5.49 | 115.24      | 121.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 9     | 200 | PHE  | CA-C-O    | 5.49  | 127.86      | 121.11   |
| 4   | 7     | 275 | HIS  | CB-CG-CD2 | -5.48 | 124.07      | 131.20   |
| 4   | W     | 137 | GLN  | CA-C-O    | -5.48 | 115.24      | 121.00   |
| 1   | J     | 196 | PHE  | CA-CB-CG  | -5.48 | 108.32      | 113.80   |
| 4   | 0     | 226 | GLU  | N-CA-C    | -5.48 | 107.24      | 114.04   |
| 4   | X     | 200 | PHE  | CA-C-O    | 5.48  | 127.85      | 121.11   |
| 4   | 3     | 200 | PHE  | CA-C-O    | 5.48  | 127.85      | 121.11   |
| 1   | G     | 632 | GLY  | N-CA-C    | 5.48  | 120.79      | 114.16   |
| 4   | 1     | 349 | LEU  | CA-C-N    | 5.48  | 127.62      | 120.28   |
| 4   | 1     | 349 | LEU  | C-N-CA    | 5.48  | 127.62      | 120.28   |
| 4   | Z     | 312 | ARG  | NE-CZ-NH2 | 5.48  | 124.13      | 119.20   |
| 1   | D     | 333 | ALA  | CA-C-O    | 5.48  | 126.76      | 120.90   |
| 4   | 4     | 200 | PHE  | CA-C-O    | 5.47  | 127.84      | 121.11   |
| 1   | G     | 203 | GLY  | N-CA-C    | -5.47 | 106.26      | 115.62   |
| 4   | 4     | 226 | GLU  | N-CA-C    | -5.47 | 107.25      | 114.04   |
| 1   | A     | 305 | ILE  | CB-CA-C   | -5.47 | 103.68      | 111.34   |
| 1   | D     | 568 | PRO  | CB-CA-C   | -5.47 | 104.23      | 111.23   |
| 4   | 2     | 200 | PHE  | CA-C-O    | 5.47  | 127.84      | 121.11   |
| 4   | 8     | 44  | MET  | N-CA-C    | -5.47 | 102.43      | 110.52   |
| 4   | 8     | 226 | GLU  | N-CA-C    | -5.47 | 107.26      | 114.04   |
| 1   | G     | 173 | GLN  | N-CA-CB   | -5.46 | 102.86      | 111.05   |
| 4   | 2     | 137 | GLN  | CA-C-O    | -5.46 | 115.26      | 121.00   |
| 4   | W     | 116 | ARG  | N-CA-C    | -5.46 | 105.32      | 111.28   |
| 1   | A     | 309 | PRO  | CB-CA-C   | -5.46 | 103.70      | 111.68   |
| 4   | 1     | 200 | PHE  | CA-C-O    | 5.46  | 127.83      | 121.11   |
| 4   | Y     | 116 | ARG  | N-CA-C    | -5.46 | 105.33      | 111.28   |
| 4   | 5     | 275 | HIS  | CB-CG-CD2 | -5.46 | 124.10      | 131.20   |
| 4   | 7     | 200 | PHE  | CA-C-O    | 5.46  | 127.83      | 121.11   |
| 1   | J     | 333 | ALA  | CA-C-O    | 5.46  | 126.74      | 120.90   |
| 4   | Y     | 349 | LEU  | CA-C-N    | 5.46  | 127.59      | 120.28   |
| 4   | Y     | 349 | LEU  | C-N-CA    | 5.46  | 127.59      | 120.28   |
| 4   | V     | 200 | PHE  | CA-C-O    | 5.46  | 127.82      | 121.11   |
| 4   | 1     | 44  | MET  | N-CA-C    | -5.46 | 102.45      | 110.52   |
| 4   | 4     | 349 | LEU  | CA-C-N    | 5.45  | 127.59      | 120.28   |
| 4   | 4     | 349 | LEU  | C-N-CA    | 5.45  | 127.59      | 120.28   |
| 4   | 4     | 257 | CYS  | N-CA-CB   | -5.45 | 105.21      | 110.39   |
| 4   | 5     | 200 | PHE  | CA-C-O    | 5.45  | 127.81      | 121.11   |
| 4   | Y     | 200 | PHE  | CA-C-O    | 5.45  | 127.81      | 121.11   |
| 1   | A     | 671 | PHE  | N-CA-C    | 5.45  | 118.69      | 109.76   |
| 4   | 0     | 116 | ARG  | N-CA-C    | -5.45 | 105.34      | 111.28   |
| 4   | Y     | 137 | GLN  | CA-C-O    | -5.45 | 115.28      | 121.00   |
| 4   | 4     | 137 | GLN  | CA-C-O    | -5.45 | 115.28      | 121.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 0     | 31  | PHE  | CA-CB-CG  | 5.45  | 119.25      | 113.80   |
| 4   | 7     | 312 | ARG  | NE-CZ-NH2 | 5.45  | 124.10      | 119.20   |
| 4   | 9     | 116 | ARG  | N-CA-C    | -5.45 | 105.34      | 111.28   |
| 4   | V     | 312 | ARG  | NE-CZ-NH2 | 5.45  | 124.10      | 119.20   |
| 4   | X     | 137 | GLN  | CA-C-O    | -5.45 | 115.28      | 121.00   |
| 4   | Z     | 200 | PHE  | CA-C-O    | 5.45  | 127.81      | 121.11   |
| 1   | D     | 203 | GLY  | N-CA-C    | -5.44 | 106.31      | 115.62   |
| 1   | G     | 196 | PHE  | CA-CB-CG  | -5.44 | 108.36      | 113.80   |
| 4   | 8     | 200 | PHE  | CA-C-O    | 5.44  | 127.80      | 121.11   |
| 4   | Y     | 312 | ARG  | NE-CZ-NH2 | 5.44  | 124.10      | 119.20   |
| 4   | Z     | 116 | ARG  | N-CA-C    | -5.44 | 105.35      | 111.28   |
| 1   | D     | 173 | GLN  | N-CA-CB   | -5.44 | 102.89      | 111.05   |
| 4   | 0     | 200 | PHE  | CA-C-O    | 5.44  | 127.80      | 121.11   |
| 1   | J     | 173 | GLN  | N-CA-CB   | -5.43 | 102.90      | 111.05   |
| 4   | 2     | 116 | ARG  | N-CA-C    | -5.43 | 105.36      | 111.28   |
| 4   | 1     | 237 | GLU  | N-CA-C    | 5.43  | 117.30      | 110.24   |
| 4   | 5     | 116 | ARG  | N-CA-C    | -5.43 | 105.36      | 111.28   |
| 4   | X     | 116 | ARG  | N-CA-C    | -5.43 | 105.36      | 111.28   |
| 4   | V     | 349 | LEU  | CA-C-N    | 5.43  | 127.55      | 120.28   |
| 4   | V     | 349 | LEU  | C-N-CA    | 5.43  | 127.55      | 120.28   |
| 4   | 1     | 137 | GLN  | CA-C-O    | -5.42 | 115.31      | 121.00   |
| 4   | 3     | 31  | PHE  | CA-CB-CG  | 5.42  | 119.22      | 113.80   |
| 4   | V     | 116 | ARG  | N-CA-C    | -5.42 | 105.37      | 111.28   |
| 4   | 1     | 31  | PHE  | CA-CB-CG  | 5.42  | 119.22      | 113.80   |
| 1   | A     | 173 | GLN  | N-CA-CB   | -5.42 | 102.92      | 111.05   |
| 4   | 4     | 31  | PHE  | CA-CB-CG  | 5.42  | 119.22      | 113.80   |
| 1   | D     | 632 | GLY  | N-CA-C    | 5.42  | 120.72      | 114.16   |
| 4   | 8     | 257 | CYS  | N-CA-CB   | -5.42 | 105.24      | 110.39   |
| 4   | 9     | 226 | GLU  | N-CA-C    | -5.42 | 107.32      | 114.04   |
| 4   | 0     | 137 | GLN  | CA-C-O    | -5.42 | 115.31      | 121.00   |
| 4   | Z     | 349 | LEU  | CA-C-N    | 5.42  | 127.54      | 120.28   |
| 4   | Z     | 349 | LEU  | C-N-CA    | 5.42  | 127.54      | 120.28   |
| 1   | J     | 203 | GLY  | N-CA-C    | -5.41 | 106.36      | 115.62   |
| 4   | X     | 312 | ARG  | NE-CZ-NH2 | 5.41  | 124.07      | 119.20   |
| 4   | Z     | 31  | PHE  | CA-CB-CG  | 5.41  | 119.21      | 113.80   |
| 4   | X     | 31  | PHE  | CA-CB-CG  | 5.41  | 119.21      | 113.80   |
| 4   | X     | 257 | CYS  | N-CA-CB   | -5.41 | 105.25      | 110.39   |
| 1   | A     | 632 | GLY  | N-CA-C    | 5.41  | 120.71      | 114.16   |
| 1   | J     | 632 | GLY  | N-CA-C    | 5.41  | 120.70      | 114.16   |
| 4   | 1     | 312 | ARG  | NE-CZ-NH2 | 5.41  | 124.07      | 119.20   |
| 4   | 7     | 31  | PHE  | CA-CB-CG  | 5.41  | 119.21      | 113.80   |
| 4   | 9     | 312 | ARG  | NE-CZ-NH2 | 5.41  | 124.07      | 119.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 203 | GLY  | N-CA-C    | -5.41 | 106.37      | 115.62   |
| 4   | 5     | 31  | PHE  | CA-CB-CG  | 5.41  | 119.21      | 113.80   |
| 4   | 5     | 226 | GLU  | N-CA-C    | -5.41 | 107.34      | 114.04   |
| 1   | G     | 305 | ILE  | CB-CA-C   | -5.41 | 103.77      | 111.34   |
| 4   | 4     | 91  | TYR  | N-CA-C    | 5.41  | 119.04      | 112.23   |
| 4   | 8     | 31  | PHE  | CA-CB-CG  | 5.41  | 119.20      | 113.80   |
| 4   | 9     | 257 | CYS  | N-CA-CB   | -5.40 | 105.26      | 110.39   |
| 4   | 2     | 31  | PHE  | CA-CB-CG  | 5.40  | 119.20      | 113.80   |
| 4   | 8     | 137 | GLN  | CA-C-O    | -5.40 | 115.33      | 121.00   |
| 4   | W     | 237 | GLU  | N-CA-C    | 5.40  | 117.26      | 110.24   |
| 4   | 5     | 237 | GLU  | N-CA-C    | 5.40  | 117.26      | 110.24   |
| 4   | 7     | 257 | CYS  | N-CA-CB   | -5.40 | 105.26      | 110.39   |
| 4   | V     | 31  | PHE  | CA-CB-CG  | 5.40  | 119.20      | 113.80   |
| 1   | A     | 333 | ALA  | CA-C-O    | 5.40  | 126.68      | 120.90   |
| 4   | 2     | 237 | GLU  | N-CA-C    | 5.40  | 117.26      | 110.24   |
| 4   | Z     | 237 | GLU  | N-CA-C    | 5.40  | 117.25      | 110.24   |
| 1   | J     | 305 | ILE  | CB-CA-C   | -5.39 | 103.79      | 111.34   |
| 4   | Y     | 226 | GLU  | N-CA-C    | -5.39 | 107.35      | 114.04   |
| 4   | W     | 312 | ARG  | NE-CZ-NH2 | 5.39  | 124.05      | 119.20   |
| 4   | 7     | 237 | GLU  | N-CA-C    | 5.39  | 117.25      | 110.24   |
| 4   | W     | 31  | PHE  | CA-CB-CG  | 5.39  | 119.19      | 113.80   |
| 4   | Z     | 226 | GLU  | N-CA-C    | -5.39 | 107.36      | 114.04   |
| 4   | 0     | 257 | CYS  | N-CA-CB   | -5.39 | 105.27      | 110.39   |
| 4   | 1     | 226 | GLU  | N-CA-C    | -5.39 | 107.36      | 114.04   |
| 4   | W     | 257 | CYS  | N-CA-CB   | -5.39 | 105.27      | 110.39   |
| 4   | 2     | 226 | GLU  | N-CA-C    | -5.38 | 107.36      | 114.04   |
| 4   | 3     | 226 | GLU  | N-CA-C    | -5.38 | 107.36      | 114.04   |
| 4   | 3     | 237 | GLU  | N-CA-C    | 5.38  | 117.24      | 110.24   |
| 4   | 9     | 31  | PHE  | CA-CB-CG  | 5.38  | 119.18      | 113.80   |
| 4   | 4     | 116 | ARG  | N-CA-C    | -5.38 | 105.42      | 111.28   |
| 4   | 9     | 91  | TYR  | N-CA-C    | 5.38  | 119.01      | 112.23   |
| 4   | 3     | 312 | ARG  | NE-CZ-NH2 | 5.38  | 124.04      | 119.20   |
| 4   | X     | 237 | GLU  | N-CA-C    | 5.38  | 117.23      | 110.24   |
| 4   | Y     | 237 | GLU  | N-CA-C    | 5.38  | 117.23      | 110.24   |
| 4   | Y     | 257 | CYS  | N-CA-CB   | -5.38 | 105.28      | 110.39   |
| 4   | 1     | 257 | CYS  | N-CA-CB   | -5.38 | 105.28      | 110.39   |
| 4   | 4     | 237 | GLU  | N-CA-C    | 5.38  | 117.23      | 110.24   |
| 4   | V     | 226 | GLU  | N-CA-C    | -5.38 | 107.37      | 114.04   |
| 4   | 2     | 332 | PRO  | CA-C-N    | 5.38  | 124.71      | 118.85   |
| 4   | 2     | 332 | PRO  | C-N-CA    | 5.38  | 124.71      | 118.85   |
| 4   | 7     | 116 | ARG  | N-CA-C    | -5.37 | 105.43      | 111.28   |
| 4   | 7     | 226 | GLU  | N-CA-C    | -5.37 | 107.38      | 114.04   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | W     | 332 | PRO  | CA-C-N     | 5.37  | 124.70      | 118.85   |
| 4   | W     | 332 | PRO  | C-N-CA     | 5.37  | 124.70      | 118.85   |
| 4   | 5     | 312 | ARG  | NE-CZ-NH2  | 5.37  | 124.03      | 119.20   |
| 1   | G     | 291 | ILE  | CB-CA-C    | -5.37 | 105.01      | 112.04   |
| 1   | G     | 772 | LEU  | N-CA-C     | -5.37 | 104.88      | 111.75   |
| 4   | 3     | 116 | ARG  | N-CA-C     | -5.37 | 105.43      | 111.28   |
| 4   | 0     | 91  | TYR  | N-CA-C     | 5.37  | 118.99      | 112.23   |
| 4   | 8     | 237 | GLU  | N-CA-C     | 5.37  | 117.21      | 110.24   |
| 2   | K     | 129 | THR  | O-C-N      | -5.36 | 115.15      | 121.32   |
| 4   | Y     | 31  | PHE  | CA-CB-CG   | 5.36  | 119.16      | 113.80   |
| 4   | Y     | 91  | TYR  | N-CA-C     | 5.36  | 118.99      | 112.23   |
| 4   | 2     | 77  | THR  | N-CA-CB    | -5.36 | 102.64      | 110.47   |
| 4   | 4     | 79  | TRP  | CG-CD2-CE3 | 5.36  | 139.26      | 133.90   |
| 4   | 5     | 257 | CYS  | N-CA-CB    | -5.36 | 105.30      | 110.39   |
| 4   | X     | 77  | THR  | N-CA-CB    | -5.36 | 102.64      | 110.47   |
| 1   | J     | 291 | ILE  | CB-CA-C    | -5.36 | 105.02      | 112.04   |
| 4   | 0     | 237 | GLU  | N-CA-C     | 5.36  | 117.20      | 110.24   |
| 4   | X     | 91  | TYR  | N-CA-C     | 5.36  | 118.98      | 112.23   |
| 1   | D     | 720 | PHE  | CA-CB-CG   | -5.36 | 108.44      | 113.80   |
| 4   | V     | 237 | GLU  | N-CA-C     | 5.36  | 117.20      | 110.24   |
| 4   | 8     | 77  | THR  | N-CA-CB    | -5.35 | 102.65      | 110.47   |
| 4   | 8     | 116 | ARG  | N-CA-C     | -5.35 | 105.44      | 111.28   |
| 1   | A     | 329 | GLU  | CA-C-O     | 5.35  | 126.09      | 120.42   |
| 4   | 1     | 332 | PRO  | CA-C-N     | 5.35  | 124.68      | 118.85   |
| 4   | 1     | 332 | PRO  | C-N-CA     | 5.35  | 124.68      | 118.85   |
| 4   | X     | 226 | GLU  | N-CA-C     | -5.35 | 107.41      | 114.04   |
| 4   | 9     | 237 | GLU  | N-CA-C     | 5.34  | 117.19      | 110.24   |
| 4   | X     | 332 | PRO  | CA-C-N     | 5.34  | 124.67      | 118.85   |
| 4   | X     | 332 | PRO  | C-N-CA     | 5.34  | 124.67      | 118.85   |
| 4   | V     | 349 | LEU  | O-C-N      | 5.34  | 129.44      | 122.87   |
| 1   | A     | 654 | ARG  | CA-C-N     | 5.34  | 127.44      | 120.28   |
| 1   | A     | 654 | ARG  | C-N-CA     | 5.34  | 127.44      | 120.28   |
| 4   | 2     | 91  | TYR  | N-CA-C     | 5.34  | 118.96      | 112.23   |
| 4   | 3     | 257 | CYS  | N-CA-CB    | -5.34 | 105.32      | 110.39   |
| 4   | V     | 257 | CYS  | N-CA-CB    | -5.34 | 105.31      | 110.39   |
| 4   | 3     | 77  | THR  | N-CA-CB    | -5.34 | 102.67      | 110.47   |
| 4   | 5     | 77  | THR  | N-CA-CB    | -5.34 | 102.67      | 110.47   |
| 4   | 1     | 77  | THR  | N-CA-CB    | -5.34 | 102.68      | 110.47   |
| 4   | 5     | 251 | GLY  | O-C-N      | 5.34  | 129.64      | 122.70   |
| 4   | W     | 226 | GLU  | N-CA-C     | -5.34 | 107.42      | 114.04   |
| 4   | Y     | 349 | LEU  | O-C-N      | 5.34  | 129.44      | 122.87   |
| 1   | D     | 447 | GLN  | CB-CA-C    | 5.34  | 119.65      | 110.79   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 127 | ARG  | NE-CZ-NH2  | 5.33  | 124.00      | 119.20   |
| 1   | D     | 291 | ILE  | CB-CA-C    | -5.33 | 105.05      | 112.04   |
| 4   | V     | 332 | PRO  | CA-C-N     | 5.33  | 124.66      | 118.85   |
| 4   | V     | 332 | PRO  | C-N-CA     | 5.33  | 124.66      | 118.85   |
| 4   | 4     | 312 | ARG  | NE-CZ-NH2  | 5.33  | 124.00      | 119.20   |
| 4   | 8     | 79  | TRP  | CG-CD2-CE3 | 5.33  | 139.23      | 133.90   |
| 4   | 8     | 91  | TYR  | N-CA-C     | 5.33  | 118.95      | 112.23   |
| 1   | G     | 329 | GLU  | CA-C-O     | 5.33  | 126.07      | 120.42   |
| 4   | 4     | 332 | PRO  | CA-C-N     | 5.33  | 124.66      | 118.85   |
| 4   | 4     | 332 | PRO  | C-N-CA     | 5.33  | 124.66      | 118.85   |
| 4   | Z     | 257 | CYS  | N-CA-CB    | -5.33 | 105.33      | 110.39   |
| 1   | G     | 649 | VAL  | CA-C-N     | 5.33  | 131.72      | 121.54   |
| 1   | G     | 649 | VAL  | C-N-CA     | 5.33  | 131.72      | 121.54   |
| 2   | H     | 129 | THR  | N-CA-CB    | 5.33  | 119.86      | 110.37   |
| 4   | V     | 77  | THR  | N-CA-CB    | -5.33 | 102.69      | 110.47   |
| 4   | V     | 91  | TYR  | N-CA-C     | 5.33  | 118.94      | 112.23   |
| 4   | 0     | 332 | PRO  | CA-C-N     | 5.33  | 124.66      | 118.85   |
| 4   | 0     | 332 | PRO  | C-N-CA     | 5.33  | 124.66      | 118.85   |
| 4   | 2     | 257 | CYS  | N-CA-CB    | -5.33 | 105.33      | 110.39   |
| 4   | W     | 91  | TYR  | N-CA-C     | 5.33  | 118.94      | 112.23   |
| 4   | Z     | 349 | LEU  | O-C-N      | 5.33  | 129.42      | 122.87   |
| 1   | D     | 649 | VAL  | CA-C-N     | 5.32  | 131.71      | 121.54   |
| 1   | D     | 649 | VAL  | C-N-CA     | 5.32  | 131.71      | 121.54   |
| 1   | J     | 447 | GLN  | CB-CA-C    | 5.32  | 119.63      | 110.79   |
| 4   | Y     | 77  | THR  | N-CA-CB    | -5.32 | 102.70      | 110.47   |
| 2   | E     | 127 | ARG  | NE-CZ-NH2  | 5.32  | 123.99      | 119.20   |
| 4   | 4     | 251 | GLY  | O-C-N      | 5.32  | 129.62      | 122.70   |
| 4   | W     | 77  | THR  | N-CA-CB    | -5.32 | 102.70      | 110.47   |
| 1   | A     | 720 | PHE  | CA-CB-CG   | -5.32 | 108.48      | 113.80   |
| 4   | 4     | 349 | LEU  | O-C-N      | 5.32  | 129.41      | 122.87   |
| 1   | G     | 447 | GLN  | CB-CA-C    | 5.32  | 119.61      | 110.79   |
| 4   | 2     | 349 | LEU  | O-C-N      | 5.32  | 129.41      | 122.87   |
| 4   | 7     | 251 | GLY  | O-C-N      | 5.32  | 129.61      | 122.70   |
| 4   | 9     | 77  | THR  | N-CA-CB    | -5.32 | 102.71      | 110.47   |
| 4   | Z     | 332 | PRO  | CA-C-N     | 5.31  | 124.64      | 118.85   |
| 4   | Z     | 332 | PRO  | C-N-CA     | 5.31  | 124.64      | 118.85   |
| 4   | 7     | 332 | PRO  | CA-C-N     | 5.31  | 124.64      | 118.85   |
| 4   | 7     | 332 | PRO  | C-N-CA     | 5.31  | 124.64      | 118.85   |
| 4   | W     | 251 | GLY  | O-C-N      | 5.31  | 129.60      | 122.70   |
| 4   | 5     | 332 | PRO  | CA-C-N     | 5.31  | 124.64      | 118.85   |
| 4   | 5     | 332 | PRO  | C-N-CA     | 5.31  | 124.64      | 118.85   |
| 4   | 9     | 349 | LEU  | O-C-N      | 5.31  | 129.40      | 122.87   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Z     | 91  | TYR  | N-CA-C     | 5.31  | 118.92      | 112.23   |
| 1   | A     | 592 | ILE  | N-CA-CB    | -5.31 | 102.47      | 111.23   |
| 4   | 0     | 251 | GLY  | O-C-N      | 5.31  | 129.60      | 122.70   |
| 1   | J     | 592 | ILE  | N-CA-CB    | -5.30 | 102.48      | 111.23   |
| 4   | 5     | 91  | TYR  | N-CA-C     | 5.30  | 118.91      | 112.23   |
| 4   | Y     | 79  | TRP  | CG-CD2-CE3 | 5.30  | 139.20      | 133.90   |
| 1   | A     | 649 | VAL  | CA-C-N     | 5.30  | 131.66      | 121.54   |
| 1   | A     | 649 | VAL  | C-N-CA     | 5.30  | 131.66      | 121.54   |
| 4   | 2     | 251 | GLY  | O-C-N      | 5.30  | 129.59      | 122.70   |
| 4   | 9     | 332 | PRO  | CA-C-N     | 5.30  | 124.62      | 118.85   |
| 4   | 9     | 332 | PRO  | C-N-CA     | 5.30  | 124.62      | 118.85   |
| 4   | X     | 349 | LEU  | O-C-N      | 5.30  | 129.39      | 122.87   |
| 4   | 3     | 349 | LEU  | O-C-N      | 5.30  | 129.38      | 122.87   |
| 4   | 9     | 251 | GLY  | O-C-N      | 5.30  | 129.59      | 122.70   |
| 1   | G     | 592 | ILE  | N-CA-CB    | -5.29 | 102.49      | 111.23   |
| 4   | 1     | 251 | GLY  | O-C-N      | 5.29  | 129.58      | 122.70   |
| 4   | X     | 251 | GLY  | O-C-N      | 5.29  | 129.58      | 122.70   |
| 1   | D     | 772 | LEU  | N-CA-C     | -5.29 | 104.98      | 111.75   |
| 4   | 4     | 77  | THR  | N-CA-CB    | -5.29 | 102.75      | 110.47   |
| 3   | C     | 63  | ILE  | CG1-CB-CG2 | -5.29 | 94.83       | 110.70   |
| 4   | 7     | 91  | TYR  | N-CA-C     | 5.29  | 118.89      | 112.23   |
| 4   | W     | 349 | LEU  | O-C-N      | 5.29  | 129.37      | 122.87   |
| 4   | Z     | 77  | THR  | N-CA-CB    | -5.29 | 102.75      | 110.47   |
| 4   | 8     | 349 | LEU  | O-C-N      | 5.29  | 129.37      | 122.87   |
| 4   | 3     | 332 | PRO  | CA-C-N     | 5.29  | 124.61      | 118.85   |
| 4   | 3     | 332 | PRO  | C-N-CA     | 5.29  | 124.61      | 118.85   |
| 4   | X     | 79  | TRP  | CG-CD2-CE3 | 5.29  | 139.19      | 133.90   |
| 4   | X     | 101 | HIS  | CA-C-O     | -5.29 | 114.79      | 119.86   |
| 1   | D     | 329 | GLU  | CA-C-O     | 5.28  | 126.02      | 120.42   |
| 4   | 3     | 91  | TYR  | N-CA-C     | 5.28  | 118.89      | 112.23   |
| 4   | 8     | 251 | GLY  | O-C-N      | 5.28  | 129.57      | 122.70   |
| 1   | A     | 447 | GLN  | CB-CA-C    | 5.28  | 119.56      | 110.79   |
| 4   | 5     | 79  | TRP  | CG-CD2-CE3 | 5.28  | 139.18      | 133.90   |
| 4   | Z     | 251 | GLY  | O-C-N      | 5.28  | 129.57      | 122.70   |
| 2   | E     | 129 | THR  | O-C-N      | -5.28 | 115.25      | 121.32   |
| 1   | A     | 291 | ILE  | CB-CA-C    | -5.28 | 105.12      | 111.88   |
| 4   | 3     | 251 | GLY  | O-C-N      | 5.28  | 129.56      | 122.70   |
| 4   | Y     | 251 | GLY  | O-C-N      | 5.28  | 129.56      | 122.70   |
| 1   | A     | 772 | LEU  | N-CA-C     | -5.28 | 105.00      | 111.75   |
| 4   | Z     | 79  | TRP  | CG-CD2-CE3 | 5.28  | 139.18      | 133.90   |
| 4   | 1     | 91  | TYR  | N-CA-C     | 5.27  | 118.87      | 112.23   |
| 4   | V     | 251 | GLY  | O-C-N      | 5.27  | 129.55      | 122.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Y     | 332 | PRO  | CA-C-N     | 5.27  | 124.59      | 118.85   |
| 4   | Y     | 332 | PRO  | C-N-CA     | 5.27  | 124.59      | 118.85   |
| 1   | D     | 564 | ASN  | CA-CB-CG   | -5.27 | 107.33      | 112.60   |
| 1   | J     | 669 | PRO  | N-CA-CB    | 5.27  | 108.01      | 103.27   |
| 1   | A     | 669 | PRO  | N-CA-CB    | 5.27  | 108.01      | 103.27   |
| 4   | 0     | 79  | TRP  | CG-CD2-CE3 | 5.27  | 139.17      | 133.90   |
| 4   | 0     | 77  | THR  | N-CA-CB    | -5.26 | 102.79      | 110.47   |
| 3   | F     | 63  | ILE  | CG1-CB-CG2 | -5.26 | 94.92       | 110.70   |
| 1   | G     | 564 | ASN  | CA-CB-CG   | -5.26 | 107.34      | 112.60   |
| 1   | G     | 654 | ARG  | CA-C-N     | 5.26  | 127.33      | 120.28   |
| 1   | G     | 654 | ARG  | C-N-CA     | 5.26  | 127.33      | 120.28   |
| 1   | D     | 601 | ASP  | CA-CB-CG   | -5.26 | 107.34      | 112.60   |
| 1   | J     | 720 | PHE  | CA-CB-CG   | -5.26 | 108.54      | 113.80   |
| 1   | D     | 654 | ARG  | CA-C-N     | 5.26  | 127.33      | 120.28   |
| 1   | D     | 654 | ARG  | C-N-CA     | 5.26  | 127.33      | 120.28   |
| 1   | G     | 267 | THR  | OG1-CB-CG2 | 5.26  | 119.81      | 109.30   |
| 4   | 5     | 349 | LEU  | O-C-N      | 5.26  | 129.34      | 122.87   |
| 1   | D     | 267 | THR  | OG1-CB-CG2 | 5.25  | 119.81      | 109.30   |
| 4   | 2     | 62  | ARG  | CA-CB-CG   | 5.25  | 124.61      | 114.10   |
| 4   | 3     | 79  | TRP  | CG-CD2-CE3 | 5.25  | 139.15      | 133.90   |
| 4   | 7     | 77  | THR  | N-CA-CB    | -5.25 | 102.80      | 110.47   |
| 1   | D     | 592 | ILE  | N-CA-CB    | -5.25 | 102.57      | 111.23   |
| 3   | L     | 63  | ILE  | CG1-CB-CG2 | -5.25 | 94.95       | 110.70   |
| 4   | 1     | 79  | TRP  | CG-CD2-CE3 | 5.25  | 139.15      | 133.90   |
| 4   | V     | 62  | ARG  | CA-CB-CG   | 5.25  | 124.60      | 114.10   |
| 4   | 0     | 349 | LEU  | O-C-N      | 5.25  | 129.33      | 122.87   |
| 4   | 1     | 349 | LEU  | O-C-N      | 5.25  | 129.33      | 122.87   |
| 1   | J     | 649 | VAL  | CA-C-N     | 5.25  | 131.56      | 121.54   |
| 1   | J     | 649 | VAL  | C-N-CA     | 5.25  | 131.56      | 121.54   |
| 4   | V     | 79  | TRP  | CG-CD2-CE3 | 5.25  | 139.15      | 133.90   |
| 1   | D     | 663 | ASN  | N-CA-C     | -5.25 | 105.73      | 111.82   |
| 1   | G     | 663 | ASN  | N-CA-C     | -5.25 | 105.73      | 111.82   |
| 1   | J     | 564 | ASN  | CA-CB-CG   | -5.25 | 107.35      | 112.60   |
| 4   | 1     | 101 | HIS  | CA-C-O     | -5.25 | 114.82      | 119.86   |
| 4   | Z     | 62  | ARG  | CA-CB-CG   | 5.25  | 124.59      | 114.10   |
| 4   | Y     | 356 | TRP  | CE2-CD2-CG | -5.25 | 100.91      | 107.20   |
| 4   | 5     | 62  | ARG  | CA-CB-CG   | 5.24  | 124.58      | 114.10   |
| 1   | A     | 267 | THR  | OG1-CB-CG2 | 5.24  | 119.78      | 109.30   |
| 1   | J     | 654 | ARG  | CA-C-N     | 5.24  | 127.30      | 120.28   |
| 1   | J     | 654 | ARG  | C-N-CA     | 5.24  | 127.30      | 120.28   |
| 4   | 3     | 356 | TRP  | CE2-CD2-CG | -5.24 | 100.91      | 107.20   |
| 4   | 8     | 332 | PRO  | CA-C-N     | 5.24  | 124.56      | 118.85   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 8     | 332 | PRO  | C-N-CA     | 5.24  | 124.56      | 118.85   |
| 4   | 9     | 62  | ARG  | CA-CB-CG   | 5.24  | 124.58      | 114.10   |
| 3   | I     | 63  | ILE  | CG1-CB-CG2 | -5.24 | 94.98       | 110.70   |
| 4   | W     | 62  | ARG  | CA-CB-CG   | 5.24  | 124.58      | 114.10   |
| 1   | A     | 601 | ASP  | CA-CB-CG   | -5.24 | 107.36      | 112.60   |
| 2   | H     | 129 | THR  | O-C-N      | -5.24 | 115.30      | 121.32   |
| 4   | 1     | 62  | ARG  | CA-CB-CG   | 5.24  | 124.57      | 114.10   |
| 4   | 4     | 62  | ARG  | CA-CB-CG   | 5.24  | 124.57      | 114.10   |
| 1   | J     | 601 | ASP  | CA-CB-CG   | -5.24 | 107.36      | 112.60   |
| 1   | G     | 720 | PHE  | CA-CB-CG   | -5.23 | 108.57      | 113.80   |
| 1   | J     | 329 | GLU  | CA-C-O     | 5.23  | 125.97      | 120.42   |
| 4   | 7     | 62  | ARG  | CA-CB-CG   | 5.23  | 124.57      | 114.10   |
| 1   | D     | 157 | SER  | O-C-N      | 5.23  | 127.74      | 122.09   |
| 4   | 7     | 356 | TRP  | CE2-CD2-CG | -5.23 | 100.92      | 107.20   |
| 4   | 2     | 79  | TRP  | CG-CD2-CE3 | 5.23  | 139.13      | 133.90   |
| 4   | 3     | 62  | ARG  | CA-CB-CG   | 5.23  | 124.56      | 114.10   |
| 4   | X     | 62  | ARG  | CA-CB-CG   | 5.23  | 124.56      | 114.10   |
| 1   | J     | 267 | THR  | OG1-CB-CG2 | 5.22  | 119.75      | 109.30   |
| 1   | J     | 663 | ASN  | N-CA-C     | -5.22 | 105.76      | 111.82   |
| 1   | J     | 772 | LEU  | N-CA-C     | -5.22 | 105.06      | 111.75   |
| 4   | 1     | 356 | TRP  | CE2-CD2-CG | -5.22 | 100.93      | 107.20   |
| 1   | D     | 401 | LEU  | CD1-CG-CD2 | -5.22 | 99.31       | 110.80   |
| 4   | 0     | 62  | ARG  | CA-CB-CG   | 5.22  | 124.55      | 114.10   |
| 4   | 9     | 79  | TRP  | CG-CD2-CE3 | 5.22  | 139.12      | 133.90   |
| 4   | W     | 101 | HIS  | CA-C-O     | -5.22 | 114.85      | 119.86   |
| 4   | X     | 356 | TRP  | CE2-CD2-CG | -5.22 | 100.93      | 107.20   |
| 4   | 8     | 62  | ARG  | CA-CB-CG   | 5.22  | 124.54      | 114.10   |
| 4   | W     | 356 | TRP  | CE2-CD2-CG | -5.22 | 100.94      | 107.20   |
| 1   | A     | 663 | ASN  | N-CA-C     | -5.22 | 105.77      | 111.82   |
| 4   | 2     | 101 | HIS  | CA-C-O     | -5.22 | 114.85      | 119.86   |
| 4   | 9     | 274 | ILE  | N-CA-CB    | -5.22 | 102.62      | 111.23   |
| 4   | Y     | 62  | ARG  | CA-CB-CG   | 5.21  | 124.53      | 114.10   |
| 4   | Z     | 101 | HIS  | CA-C-O     | -5.21 | 114.86      | 119.86   |
| 4   | 5     | 356 | TRP  | CE2-CD2-CG | -5.21 | 100.95      | 107.20   |
| 4   | Y     | 274 | ILE  | N-CA-CB    | -5.21 | 102.63      | 111.23   |
| 2   | B     | 129 | THR  | N-CA-CB    | 5.21  | 119.64      | 110.37   |
| 1   | J     | 38  | VAL  | N-CA-CB    | -5.21 | 102.64      | 111.23   |
| 4   | 9     | 22  | ALA  | N-CA-C     | -5.21 | 102.34      | 110.10   |
| 4   | 7     | 349 | LEU  | O-C-N      | 5.21  | 129.27      | 122.87   |
| 4   | 9     | 356 | TRP  | CE2-CD2-CG | -5.21 | 100.95      | 107.20   |
| 4   | 8     | 356 | TRP  | CE2-CD2-CG | -5.21 | 100.95      | 107.20   |
| 4   | W     | 79  | TRP  | CG-CD2-CE3 | 5.21  | 139.10      | 133.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 1     | 274 | ILE  | N-CA-CB    | -5.20 | 102.64      | 111.23   |
| 4   | V     | 356 | TRP  | CE2-CD2-CG | -5.20 | 100.95      | 107.20   |
| 4   | 5     | 22  | ALA  | N-CA-C     | -5.20 | 102.35      | 110.10   |
| 4   | 8     | 274 | ILE  | N-CA-CB    | -5.20 | 102.65      | 111.23   |
| 4   | V     | 252 | ASN  | CB-CG-ND2  | 5.20  | 124.20      | 116.40   |
| 1   | G     | 669 | PRO  | N-CA-CB    | 5.20  | 107.95      | 103.27   |
| 4   | 0     | 274 | ILE  | N-CA-CB    | -5.20 | 102.65      | 111.23   |
| 4   | 3     | 248 | ILE  | N-CA-CB    | -5.20 | 103.39      | 110.56   |
| 4   | 3     | 274 | ILE  | N-CA-CB    | -5.20 | 102.65      | 111.23   |
| 4   | V     | 101 | HIS  | CA-C-O     | -5.20 | 114.87      | 119.86   |
| 1   | A     | 401 | LEU  | CD1-CG-CD2 | -5.20 | 99.37       | 110.80   |
| 1   | G     | 623 | PHE  | CB-CG-CD1  | 5.20  | 129.53      | 120.70   |
| 4   | 1     | 22  | ALA  | N-CA-C     | -5.20 | 102.36      | 110.10   |
| 4   | 8     | 22  | ALA  | N-CA-C     | -5.20 | 102.36      | 110.10   |
| 4   | Z     | 274 | ILE  | N-CA-CB    | -5.20 | 102.66      | 111.23   |
| 1   | G     | 401 | LEU  | CD1-CG-CD2 | -5.19 | 99.37       | 110.80   |
| 2   | K     | 129 | THR  | N-CA-CB    | 5.19  | 119.61      | 110.37   |
| 4   | 0     | 22  | ALA  | N-CA-C     | -5.19 | 102.36      | 110.10   |
| 4   | 3     | 22  | ALA  | N-CA-C     | -5.19 | 102.36      | 110.10   |
| 4   | 5     | 274 | ILE  | N-CA-CB    | -5.19 | 102.66      | 111.23   |
| 4   | W     | 22  | ALA  | N-CA-C     | -5.19 | 102.36      | 110.10   |
| 4   | X     | 22  | ALA  | N-CA-C     | -5.19 | 102.36      | 110.10   |
| 1   | A     | 564 | ASN  | CA-CB-CG   | -5.19 | 107.41      | 112.60   |
| 4   | 2     | 252 | ASN  | CB-CG-ND2  | 5.19  | 124.19      | 116.40   |
| 4   | 7     | 22  | ALA  | N-CA-C     | -5.19 | 102.37      | 110.10   |
| 4   | 7     | 79  | TRP  | CG-CD2-CE3 | 5.19  | 139.09      | 133.90   |
| 4   | 2     | 274 | ILE  | N-CA-CB    | -5.19 | 102.67      | 111.23   |
| 4   | Y     | 22  | ALA  | N-CA-C     | -5.19 | 102.37      | 110.10   |
| 2   | B     | 129 | THR  | O-C-N      | -5.19 | 115.35      | 121.32   |
| 4   | 1     | 50  | LYS  | CB-CG-CD   | -5.19 | 99.37       | 111.30   |
| 4   | 4     | 233 | SER  | O-C-N      | 5.19  | 129.49      | 122.59   |
| 4   | 7     | 274 | ILE  | N-CA-CB    | -5.19 | 102.67      | 111.23   |
| 1   | A     | 623 | PHE  | CB-CG-CD1  | 5.19  | 129.51      | 120.70   |
| 4   | 0     | 356 | TRP  | CE2-CD2-CG | -5.19 | 100.98      | 107.20   |
| 4   | 2     | 22  | ALA  | N-CA-C     | -5.19 | 102.37      | 110.10   |
| 4   | 4     | 101 | HIS  | CA-C-O     | -5.19 | 114.88      | 119.86   |
| 1   | G     | 157 | SER  | O-C-N      | 5.18  | 127.69      | 122.09   |
| 4   | 0     | 40  | HIS  | CB-CG-CD2  | -5.18 | 124.46      | 131.20   |
| 4   | 5     | 34  | ILE  | CA-CB-CG1  | 5.18  | 119.22      | 110.40   |
| 4   | V     | 274 | ILE  | N-CA-CB    | -5.18 | 102.68      | 111.23   |
| 4   | W     | 274 | ILE  | N-CA-CB    | -5.18 | 102.67      | 111.23   |
| 4   | Y     | 252 | ASN  | CB-CG-ND2  | 5.18  | 124.18      | 116.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 38  | VAL  | N-CA-CB    | -5.18 | 102.68      | 111.23   |
| 1   | G     | 38  | VAL  | N-CA-CB    | -5.18 | 102.68      | 111.23   |
| 4   | 1     | 252 | ASN  | CB-CG-ND2  | 5.18  | 124.17      | 116.40   |
| 4   | 4     | 252 | ASN  | CB-CG-ND2  | 5.18  | 124.17      | 116.40   |
| 4   | 4     | 274 | ILE  | N-CA-CB    | -5.18 | 102.68      | 111.23   |
| 4   | 5     | 252 | ASN  | CB-CG-ND2  | 5.18  | 124.17      | 116.40   |
| 4   | X     | 274 | ILE  | N-CA-CB    | -5.18 | 102.68      | 111.23   |
| 1   | J     | 401 | LEU  | CD1-CG-CD2 | -5.18 | 99.40       | 110.80   |
| 4   | 0     | 252 | ASN  | CB-CG-ND2  | 5.18  | 124.17      | 116.40   |
| 4   | 4     | 22  | ALA  | N-CA-C     | -5.18 | 102.38      | 110.10   |
| 4   | 4     | 34  | ILE  | CA-CB-CG1  | 5.18  | 119.21      | 110.40   |
| 1   | A     | 322 | VAL  | O-C-N      | 5.18  | 125.67      | 120.59   |
| 4   | 2     | 356 | TRP  | CE2-CD2-CG | -5.18 | 100.98      | 107.20   |
| 4   | 8     | 360 | GLN  | CB-CG-CD   | 5.18  | 121.40      | 112.60   |
| 4   | 9     | 34  | ILE  | CA-CB-CG1  | 5.18  | 119.20      | 110.40   |
| 1   | A     | 38  | VAL  | N-CA-CB    | -5.18 | 102.69      | 111.23   |
| 4   | 1     | 248 | ILE  | N-CA-CB    | -5.18 | 103.42      | 110.56   |
| 4   | V     | 22  | ALA  | N-CA-C     | -5.18 | 102.39      | 110.10   |
| 2   | E     | 129 | THR  | N-CA-CB    | 5.17  | 119.58      | 110.37   |
| 4   | 9     | 40  | HIS  | CB-CG-CD2  | -5.17 | 124.47      | 131.20   |
| 4   | V     | 40  | HIS  | CB-CG-CD2  | -5.17 | 124.47      | 131.20   |
| 4   | 1     | 71  | ILE  | N-CA-CB    | -5.17 | 105.89      | 112.15   |
| 4   | 4     | 71  | ILE  | N-CA-CB    | -5.17 | 105.89      | 112.15   |
| 4   | 5     | 71  | ILE  | N-CA-CB    | -5.17 | 105.89      | 112.15   |
| 4   | 8     | 40  | HIS  | CB-CG-CD2  | -5.17 | 124.48      | 131.20   |
| 4   | Y     | 71  | ILE  | N-CA-CB    | -5.17 | 105.89      | 112.15   |
| 4   | 3     | 252 | ASN  | CB-CG-ND2  | 5.17  | 124.15      | 116.40   |
| 4   | 8     | 101 | HIS  | CA-C-O     | -5.17 | 114.90      | 119.86   |
| 4   | 9     | 50  | LYS  | CB-CG-CD   | -5.17 | 99.41       | 111.30   |
| 4   | W     | 252 | ASN  | CB-CG-ND2  | 5.17  | 124.15      | 116.40   |
| 4   | X     | 248 | ILE  | N-CA-CB    | -5.17 | 103.43      | 110.56   |
| 4   | Z     | 360 | GLN  | CB-CG-CD   | 5.17  | 121.39      | 112.60   |
| 4   | 4     | 50  | LYS  | CB-CG-CD   | -5.17 | 99.42       | 111.30   |
| 4   | Y     | 34  | ILE  | CA-CB-CG1  | 5.17  | 119.18      | 110.40   |
| 4   | Z     | 34  | ILE  | CA-CB-CG1  | 5.17  | 119.18      | 110.40   |
| 4   | Z     | 22  | ALA  | N-CA-C     | -5.17 | 102.41      | 110.10   |
| 4   | 7     | 252 | ASN  | CB-CG-ND2  | 5.16  | 124.14      | 116.40   |
| 4   | Y     | 40  | HIS  | CB-CG-CD2  | -5.16 | 124.49      | 131.20   |
| 4   | 8     | 34  | ILE  | CA-CB-CG1  | 5.16  | 119.17      | 110.40   |
| 4   | W     | 40  | HIS  | CB-CG-CD2  | -5.16 | 124.49      | 131.20   |
| 4   | 0     | 50  | LYS  | CB-CG-CD   | -5.16 | 99.44       | 111.30   |
| 4   | 7     | 34  | ILE  | CA-CB-CG1  | 5.16  | 119.17      | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 8     | 252 | ASN  | CB-CG-ND2  | 5.16  | 124.14      | 116.40   |
| 1   | A     | 157 | SER  | O-C-N      | 5.16  | 127.66      | 122.09   |
| 4   | Z     | 356 | TRP  | CE2-CD2-CG | -5.16 | 101.01      | 107.20   |
| 1   | D     | 254 | PHE  | CA-CB-CG   | -5.16 | 108.64      | 113.80   |
| 4   | 9     | 248 | ILE  | N-CA-CB    | -5.16 | 103.45      | 110.56   |
| 1   | J     | 623 | PHE  | CB-CG-CD1  | 5.15  | 129.46      | 120.70   |
| 4   | 1     | 34  | ILE  | CA-CB-CG1  | 5.15  | 119.16      | 110.40   |
| 4   | 9     | 71  | ILE  | N-CA-CB    | -5.15 | 105.92      | 112.15   |
| 4   | 3     | 34  | ILE  | CA-CB-CG1  | 5.15  | 119.16      | 110.40   |
| 4   | 3     | 50  | LYS  | CB-CG-CD   | -5.15 | 99.46       | 111.30   |
| 4   | 3     | 71  | ILE  | N-CA-CB    | -5.15 | 105.92      | 112.15   |
| 4   | W     | 50  | LYS  | CB-CG-CD   | -5.15 | 99.45       | 111.30   |
| 4   | X     | 252 | ASN  | CB-CG-ND2  | 5.15  | 124.13      | 116.40   |
| 4   | Y     | 101 | HIS  | CA-C-O     | -5.15 | 114.92      | 119.86   |
| 1   | G     | 601 | ASP  | CA-CB-CG   | -5.15 | 107.45      | 112.60   |
| 4   | 2     | 248 | ILE  | N-CA-CB    | -5.15 | 103.45      | 110.56   |
| 4   | 3     | 40  | HIS  | CB-CG-CD2  | -5.15 | 124.51      | 131.20   |
| 4   | 2     | 360 | GLN  | CB-CG-CD   | 5.15  | 121.35      | 112.60   |
| 4   | X     | 71  | ILE  | N-CA-CB    | -5.15 | 105.92      | 112.15   |
| 4   | Y     | 360 | GLN  | CB-CG-CD   | 5.15  | 121.35      | 112.60   |
| 4   | V     | 34  | ILE  | CA-CB-CG1  | 5.15  | 119.15      | 110.40   |
| 4   | 4     | 356 | TRP  | CE2-CD2-CG | -5.14 | 101.03      | 107.20   |
| 4   | Z     | 50  | LYS  | CB-CG-CD   | -5.14 | 99.47       | 111.30   |
| 1   | J     | 652 | LEU  | CB-CA-C    | -5.14 | 102.38      | 110.86   |
| 4   | 5     | 360 | GLN  | CB-CG-CD   | 5.14  | 121.34      | 112.60   |
| 4   | 8     | 248 | ILE  | N-CA-CB    | -5.14 | 103.46      | 110.56   |
| 4   | V     | 50  | LYS  | CB-CG-CD   | -5.14 | 99.47       | 111.30   |
| 4   | Y     | 233 | SER  | O-C-N      | 5.14  | 129.43      | 122.59   |
| 4   | W     | 71  | ILE  | N-CA-CB    | -5.14 | 105.93      | 112.15   |
| 4   | X     | 360 | GLN  | CB-CG-CD   | 5.14  | 121.34      | 112.60   |
| 4   | 2     | 50  | LYS  | CB-CG-CD   | -5.14 | 99.48       | 111.30   |
| 4   | 7     | 50  | LYS  | CB-CG-CD   | -5.14 | 99.48       | 111.30   |
| 4   | 5     | 50  | LYS  | CB-CG-CD   | -5.14 | 99.48       | 111.30   |
| 4   | V     | 248 | ILE  | N-CA-CB    | -5.14 | 103.47      | 110.56   |
| 4   | Z     | 252 | ASN  | CB-CG-ND2  | 5.14  | 124.11      | 116.40   |
| 1   | J     | 576 | GLU  | N-CA-CB    | 5.14  | 118.98      | 110.97   |
| 4   | 2     | 34  | ILE  | CA-CB-CG1  | 5.14  | 119.13      | 110.40   |
| 4   | 7     | 40  | HIS  | CB-CG-CD2  | -5.14 | 124.52      | 131.20   |
| 4   | 9     | 252 | ASN  | CB-CG-ND2  | 5.14  | 124.11      | 116.40   |
| 4   | 8     | 50  | LYS  | CB-CG-CD   | -5.13 | 99.49       | 111.30   |
| 4   | 0     | 34  | ILE  | CA-CB-CG1  | 5.13  | 119.12      | 110.40   |
| 4   | Y     | 50  | LYS  | CB-CG-CD   | -5.13 | 99.50       | 111.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | W     | 248 | ILE  | N-CA-CB   | -5.13 | 103.48      | 110.56   |
| 1   | J     | 157 | SER  | O-C-N     | 5.13  | 127.63      | 122.09   |
| 4   | 3     | 233 | SER  | O-C-N     | 5.13  | 129.41      | 122.59   |
| 4   | 3     | 360 | GLN  | CB-CG-CD  | 5.13  | 121.32      | 112.60   |
| 4   | 5     | 40  | HIS  | CB-CG-CD2 | -5.13 | 124.53      | 131.20   |
| 4   | 9     | 233 | SER  | O-C-N     | 5.13  | 129.41      | 122.59   |
| 4   | X     | 50  | LYS  | CB-CG-CD  | -5.13 | 99.50       | 111.30   |
| 1   | G     | 652 | LEU  | CB-CA-C   | -5.13 | 102.40      | 110.86   |
| 4   | 0     | 71  | ILE  | N-CA-CB   | -5.13 | 105.95      | 112.15   |
| 4   | V     | 360 | GLN  | CB-CG-CD  | 5.13  | 121.31      | 112.60   |
| 4   | Z     | 71  | ILE  | N-CA-CB   | -5.13 | 105.95      | 112.15   |
| 4   | 1     | 217 | CYS  | CA-CB-SG  | -5.12 | 102.61      | 114.40   |
| 4   | 9     | 360 | GLN  | CB-CG-CD  | 5.12  | 121.31      | 112.60   |
| 4   | 1     | 360 | GLN  | CB-CG-CD  | 5.12  | 121.31      | 112.60   |
| 4   | 2     | 71  | ILE  | N-CA-CB   | -5.12 | 105.95      | 112.15   |
| 4   | 7     | 360 | GLN  | CB-CG-CD  | 5.12  | 121.31      | 112.60   |
| 4   | W     | 34  | ILE  | CA-CB-CG1 | 5.12  | 119.11      | 110.40   |
| 4   | Y     | 248 | ILE  | N-CA-CB   | -5.12 | 103.49      | 110.56   |
| 4   | 0     | 248 | ILE  | N-CA-CB   | -5.12 | 103.49      | 110.56   |
| 1   | A     | 652 | LEU  | CB-CA-C   | -5.12 | 102.42      | 110.86   |
| 1   | G     | 172 | ASN  | N-CA-CB   | 5.12  | 118.23      | 110.45   |
| 1   | G     | 254 | PHE  | CA-CB-CG  | -5.12 | 108.68      | 113.80   |
| 4   | 2     | 233 | SER  | O-C-N     | 5.12  | 129.40      | 122.59   |
| 4   | 8     | 71  | ILE  | N-CA-CB   | -5.12 | 105.96      | 112.15   |
| 4   | W     | 233 | SER  | O-C-N     | 5.12  | 129.39      | 122.59   |
| 1   | G     | 332 | MET  | CB-CA-C   | -5.11 | 102.16      | 110.85   |
| 4   | X     | 34  | ILE  | CA-CB-CG1 | 5.11  | 119.09      | 110.40   |
| 4   | 4     | 360 | GLN  | CB-CG-CD  | 5.11  | 121.29      | 112.60   |
| 4   | 5     | 248 | ILE  | N-CA-CB   | -5.11 | 103.51      | 110.56   |
| 4   | W     | 360 | GLN  | CB-CG-CD  | 5.11  | 121.29      | 112.60   |
| 1   | D     | 669 | PRO  | N-CA-CB   | 5.11  | 107.87      | 103.27   |
| 4   | 0     | 217 | CYS  | CA-CB-SG  | -5.11 | 102.65      | 114.40   |
| 4   | 1     | 40  | HIS  | CB-CG-CD2 | -5.11 | 124.56      | 131.20   |
| 4   | 4     | 40  | HIS  | CB-CG-CD2 | -5.11 | 124.56      | 131.20   |
| 1   | J     | 424 | ASN  | CA-CB-CG  | 5.11  | 117.71      | 112.60   |
| 4   | 2     | 217 | CYS  | CA-CB-SG  | -5.11 | 102.65      | 114.40   |
| 4   | W     | 149 | THR  | CA-CB-OG1 | -5.11 | 101.94      | 109.60   |
| 4   | X     | 40  | HIS  | CB-CG-CD2 | -5.11 | 124.56      | 131.20   |
| 3   | C     | 64  | THR  | O-C-N     | 5.11  | 129.52      | 123.24   |
| 4   | 5     | 217 | CYS  | CA-CB-SG  | -5.11 | 102.66      | 114.40   |
| 4   | W     | 217 | CYS  | CA-CB-SG  | -5.11 | 102.66      | 114.40   |
| 4   | Z     | 40  | HIS  | CB-CG-CD2 | -5.11 | 124.56      | 131.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 172 | ASN  | N-CA-CB   | 5.10  | 118.21      | 110.45   |
| 4   | 2     | 40  | HIS  | CB-CG-CD2 | -5.10 | 124.56      | 131.20   |
| 4   | V     | 233 | SER  | O-C-N     | 5.10  | 129.38      | 122.59   |
| 4   | Z     | 248 | ILE  | N-CA-CB   | -5.10 | 103.52      | 110.56   |
| 1   | A     | 332 | MET  | CG-SD-CE  | -5.10 | 89.68       | 100.90   |
| 4   | 4     | 248 | ILE  | N-CA-CB   | -5.10 | 103.52      | 110.56   |
| 1   | D     | 576 | GLU  | N-CA-CB   | 5.10  | 118.93      | 110.97   |
| 4   | V     | 227 | MET  | N-CA-C    | -5.10 | 105.63      | 111.14   |
| 1   | G     | 322 | VAL  | O-C-N     | 5.10  | 125.59      | 120.59   |
| 4   | 0     | 360 | GLN  | CB-CG-CD  | 5.10  | 121.27      | 112.60   |
| 4   | 5     | 227 | MET  | N-CA-C    | -5.10 | 105.63      | 111.14   |
| 4   | Z     | 217 | CYS  | CA-CB-SG  | -5.10 | 102.67      | 114.40   |
| 1   | A     | 576 | GLU  | N-CA-CB   | 5.10  | 118.92      | 110.97   |
| 1   | G     | 576 | GLU  | N-CA-CB   | 5.10  | 118.92      | 110.97   |
| 4   | 7     | 233 | SER  | O-C-N     | 5.10  | 129.37      | 122.59   |
| 1   | J     | 322 | VAL  | O-C-N     | 5.10  | 125.58      | 120.59   |
| 4   | 4     | 227 | MET  | N-CA-C    | -5.10 | 105.64      | 111.14   |
| 4   | 8     | 227 | MET  | N-CA-C    | -5.10 | 105.64      | 111.14   |
| 1   | A     | 76  | GLN  | CA-C-O    | 5.09  | 125.19      | 119.18   |
| 4   | 4     | 217 | CYS  | CA-CB-SG  | -5.09 | 102.69      | 114.40   |
| 4   | X     | 217 | CYS  | CA-CB-SG  | -5.09 | 102.68      | 114.40   |
| 2   | H     | 127 | ARG  | NE-CZ-NH2 | 5.09  | 123.78      | 119.20   |
| 1   | J     | 425 | SER  | N-CA-CB   | 5.09  | 117.69      | 110.16   |
| 4   | 0     | 149 | THR  | CA-CB-OG1 | -5.09 | 101.96      | 109.60   |
| 4   | 7     | 217 | CYS  | CA-CB-SG  | -5.09 | 102.69      | 114.40   |
| 4   | 8     | 217 | CYS  | CA-CB-SG  | -5.09 | 102.69      | 114.40   |
| 1   | A     | 424 | ASN  | CA-CB-CG  | 5.09  | 117.69      | 112.60   |
| 4   | 3     | 217 | CYS  | CA-CB-SG  | -5.09 | 102.69      | 114.40   |
| 4   | V     | 217 | CYS  | CA-CB-SG  | -5.09 | 102.69      | 114.40   |
| 1   | A     | 425 | SER  | N-CA-CB   | 5.09  | 117.69      | 110.16   |
| 1   | D     | 595 | TRP  | O-C-N     | 5.09  | 127.38      | 122.09   |
| 2   | K     | 127 | ARG  | NE-CZ-NH2 | 5.09  | 123.78      | 119.20   |
| 4   | 2     | 371 | HIS  | CB-CG-CD2 | -5.09 | 124.59      | 131.20   |
| 4   | 3     | 149 | THR  | CA-CB-OG1 | -5.09 | 101.97      | 109.60   |
| 4   | 7     | 248 | ILE  | N-CA-CB   | -5.08 | 103.54      | 110.56   |
| 4   | 7     | 371 | HIS  | CB-CG-CD2 | -5.08 | 124.59      | 131.20   |
| 4   | V     | 71  | ILE  | N-CA-CB   | -5.08 | 106.00      | 112.15   |
| 4   | X     | 233 | SER  | O-C-N     | 5.08  | 129.35      | 122.59   |
| 1   | D     | 332 | MET  | CG-SD-CE  | -5.08 | 89.72       | 100.90   |
| 1   | G     | 332 | MET  | CG-SD-CE  | -5.08 | 89.72       | 100.90   |
| 1   | J     | 278 | GLN  | CA-C-O    | 5.08  | 127.78      | 120.51   |
| 4   | 9     | 217 | CYS  | CA-CB-SG  | -5.08 | 102.71      | 114.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | W     | 227 | MET  | N-CA-C     | -5.08 | 105.65      | 111.14   |
| 4   | 4     | 266 | PHE  | CA-CB-CG   | 5.08  | 118.88      | 113.80   |
| 4   | 7     | 71  | ILE  | N-CA-CB    | -5.08 | 106.00      | 112.15   |
| 1   | G     | 359 | MET  | O-C-N      | 5.08  | 127.30      | 122.07   |
| 4   | 0     | 371 | HIS  | CB-CG-CD2  | -5.08 | 124.60      | 131.20   |
| 4   | 7     | 227 | MET  | N-CA-C     | -5.08 | 105.66      | 111.14   |
| 4   | 3     | 227 | MET  | N-CA-C     | -5.08 | 105.66      | 111.14   |
| 4   | 1     | 371 | HIS  | CB-CG-CD2  | -5.08 | 124.60      | 131.20   |
| 4   | 5     | 371 | HIS  | CB-CG-CD2  | -5.08 | 124.60      | 131.20   |
| 4   | Y     | 149 | THR  | CA-CB-OG1  | -5.08 | 101.98      | 109.60   |
| 4   | Y     | 217 | CYS  | CA-CB-SG   | -5.08 | 102.73      | 114.40   |
| 4   | Z     | 233 | SER  | O-C-N      | 5.08  | 129.34      | 122.59   |
| 1   | J     | 694 | GLN  | CA-C-O     | 5.07  | 126.11      | 120.63   |
| 4   | 0     | 233 | SER  | O-C-N      | 5.07  | 129.34      | 122.59   |
| 4   | 8     | 233 | SER  | O-C-N      | 5.07  | 129.34      | 122.59   |
| 4   | V     | 371 | HIS  | CB-CG-CD2  | -5.07 | 124.61      | 131.20   |
| 1   | D     | 425 | SER  | N-CA-CB    | 5.07  | 117.66      | 110.16   |
| 1   | J     | 332 | MET  | CG-SD-CE   | -5.07 | 89.74       | 100.90   |
| 1   | A     | 172 | ASN  | N-CA-CB    | 5.07  | 118.15      | 110.45   |
| 4   | 8     | 359 | LYS  | CB-CG-CD   | 5.07  | 122.95      | 111.30   |
| 4   | 7     | 149 | THR  | CA-CB-OG1  | -5.07 | 102.00      | 109.60   |
| 4   | 8     | 371 | HIS  | CB-CG-CD2  | -5.07 | 124.61      | 131.20   |
| 4   | X     | 149 | THR  | CA-CB-OG1  | -5.07 | 102.00      | 109.60   |
| 1   | A     | 694 | GLN  | CA-C-O     | 5.06  | 126.10      | 120.63   |
| 1   | D     | 172 | ASN  | N-CA-CB    | 5.06  | 118.15      | 110.45   |
| 1   | A     | 359 | MET  | O-C-N      | 5.06  | 127.28      | 122.07   |
| 4   | 1     | 149 | THR  | CA-CB-OG1  | -5.06 | 102.01      | 109.60   |
| 4   | Y     | 371 | HIS  | CB-CG-CD2  | -5.06 | 124.62      | 131.20   |
| 4   | V     | 149 | THR  | CA-CB-OG1  | -5.06 | 102.01      | 109.60   |
| 1   | G     | 513 | ILE  | N-CA-CB    | -5.06 | 101.64      | 110.49   |
| 4   | 5     | 149 | THR  | CA-CB-OG1  | -5.06 | 102.01      | 109.60   |
| 4   | 7     | 356 | TRP  | CG-CD2-CE3 | 5.06  | 138.96      | 133.90   |
| 4   | X     | 359 | LYS  | CB-CG-CD   | 5.05  | 122.92      | 111.30   |
| 4   | Z     | 227 | MET  | N-CA-C     | -5.05 | 105.68      | 111.14   |
| 4   | Z     | 371 | HIS  | CB-CG-CD2  | -5.05 | 124.63      | 131.20   |
| 4   | 1     | 233 | SER  | O-C-N      | 5.05  | 129.31      | 122.59   |
| 4   | V     | 142 | LEU  | CA-C-O     | 5.05  | 126.13      | 120.82   |
| 4   | Z     | 149 | THR  | CA-CB-OG1  | -5.05 | 102.02      | 109.60   |
| 1   | A     | 221 | GLN  | O-C-N      | 5.05  | 127.34      | 122.09   |
| 1   | A     | 621 | LEU  | N-CA-C     | 5.05  | 116.47      | 110.97   |
| 1   | J     | 332 | MET  | CB-CA-C    | -5.05 | 102.27      | 110.85   |
| 4   | W     | 371 | HIS  | CB-CG-CD2  | -5.05 | 124.64      | 131.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 9     | 149 | THR  | CA-CB-OG1  | -5.05 | 102.03      | 109.60   |
| 1   | A     | 332 | MET  | CB-CA-C    | -5.05 | 102.27      | 110.85   |
| 1   | D     | 76  | GLN  | CA-C-O     | 5.05  | 125.14      | 119.18   |
| 1   | G     | 76  | GLN  | CA-C-O     | 5.05  | 125.13      | 119.18   |
| 4   | 2     | 227 | MET  | N-CA-C     | -5.05 | 105.69      | 111.14   |
| 4   | 5     | 233 | SER  | O-C-N      | 5.05  | 129.30      | 122.59   |
| 4   | 5     | 359 | LYS  | CB-CG-CD   | 5.05  | 122.91      | 111.30   |
| 4   | W     | 359 | LYS  | CB-CG-CD   | 5.05  | 122.91      | 111.30   |
| 4   | 8     | 149 | THR  | CA-CB-OG1  | -5.04 | 102.03      | 109.60   |
| 4   | 3     | 88  | HIS  | CB-CG-CD2  | -5.04 | 124.64      | 131.20   |
| 4   | 3     | 266 | PHE  | CA-CB-CG   | 5.04  | 118.84      | 113.80   |
| 4   | 9     | 227 | MET  | N-CA-C     | -5.04 | 105.69      | 111.14   |
| 4   | 0     | 266 | PHE  | CA-CB-CG   | 5.04  | 118.84      | 113.80   |
| 4   | V     | 359 | LYS  | CB-CG-CD   | 5.04  | 122.89      | 111.30   |
| 4   | Y     | 356 | TRP  | CG-CD2-CE3 | 5.04  | 138.94      | 133.90   |
| 4   | 0     | 359 | LYS  | CB-CG-CD   | 5.04  | 122.89      | 111.30   |
| 4   | Y     | 227 | MET  | N-CA-C     | -5.04 | 105.70      | 111.14   |
| 1   | D     | 652 | LEU  | CB-CA-C    | -5.04 | 102.55      | 110.86   |
| 4   | 1     | 88  | HIS  | CB-CG-CD2  | -5.04 | 124.65      | 131.20   |
| 4   | W     | 88  | HIS  | CB-CG-CD2  | -5.04 | 124.65      | 131.20   |
| 1   | D     | 675 | ILE  | N-CA-C     | 5.04  | 116.61      | 108.85   |
| 1   | G     | 424 | ASN  | CA-CB-CG   | 5.04  | 117.64      | 112.60   |
| 1   | A     | 254 | PHE  | CA-CB-CG   | -5.03 | 108.77      | 113.80   |
| 1   | D     | 332 | MET  | CB-CA-C    | -5.03 | 102.29      | 110.85   |
| 4   | X     | 88  | HIS  | CB-CG-CD2  | -5.03 | 124.66      | 131.20   |
| 1   | D     | 513 | ILE  | N-CA-CB    | -5.03 | 101.69      | 110.49   |
| 4   | 2     | 149 | THR  | CA-CB-OG1  | -5.03 | 102.06      | 109.60   |
| 4   | 4     | 88  | HIS  | CB-CG-CD2  | -5.03 | 124.66      | 131.20   |
| 1   | D     | 278 | GLN  | CA-C-O     | 5.03  | 127.70      | 120.51   |
| 4   | 1     | 266 | PHE  | CA-CB-CG   | 5.03  | 118.83      | 113.80   |
| 4   | 3     | 359 | LYS  | CB-CG-CD   | 5.03  | 122.86      | 111.30   |
| 4   | 3     | 371 | HIS  | CB-CG-CD2  | -5.03 | 124.67      | 131.20   |
| 4   | 4     | 149 | THR  | CA-CB-OG1  | -5.03 | 102.06      | 109.60   |
| 4   | 9     | 359 | LYS  | CB-CG-CD   | 5.03  | 122.86      | 111.30   |
| 4   | Y     | 88  | HIS  | CB-CG-CD2  | -5.03 | 124.67      | 131.20   |
| 1   | G     | 221 | GLN  | O-C-N      | 5.02  | 127.31      | 122.09   |
| 4   | 2     | 359 | LYS  | CB-CG-CD   | 5.02  | 122.86      | 111.30   |
| 4   | 5     | 88  | HIS  | CB-CG-CD2  | -5.02 | 124.67      | 131.20   |
| 1   | D     | 434 | TYR  | CB-CA-C    | -5.02 | 102.77      | 110.81   |
| 1   | D     | 623 | PHE  | CB-CG-CD1  | 5.02  | 129.24      | 120.70   |
| 4   | Z     | 349 | LEU  | CA-C-O     | 5.02  | 126.72      | 121.19   |
| 1   | D     | 424 | ASN  | CA-CB-CG   | 5.02  | 117.62      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Z     | 88  | HIS  | CB-CG-CD2  | -5.02 | 124.68      | 131.20   |
| 1   | G     | 511 | GLU  | N-CA-CB    | 5.02  | 118.77      | 110.69   |
| 4   | 1     | 227 | MET  | N-CA-C     | -5.02 | 105.72      | 111.14   |
| 4   | 1     | 349 | LEU  | CA-C-O     | 5.02  | 126.71      | 121.19   |
| 4   | 7     | 359 | LYS  | CB-CG-CD   | 5.02  | 122.84      | 111.30   |
| 4   | 9     | 88  | HIS  | CB-CG-CD2  | -5.02 | 124.68      | 131.20   |
| 4   | Y     | 359 | LYS  | CB-CG-CD   | 5.02  | 122.84      | 111.30   |
| 4   | Z     | 359 | LYS  | CB-CG-CD   | 5.02  | 122.84      | 111.30   |
| 3   | F     | 64  | THR  | O-C-N      | 5.01  | 129.39      | 123.27   |
| 4   | X     | 266 | PHE  | CA-CB-CG   | 5.01  | 118.81      | 113.80   |
| 4   | 4     | 43  | VAL  | N-CA-C     | 5.01  | 117.22      | 108.90   |
| 4   | 4     | 371 | HIS  | CB-CG-CD2  | -5.01 | 124.69      | 131.20   |
| 4   | 7     | 266 | PHE  | CA-CB-CG   | 5.01  | 118.81      | 113.80   |
| 1   | A     | 513 | ILE  | N-CA-CB    | -5.01 | 101.72      | 110.49   |
| 4   | 1     | 356 | TRP  | CG-CD2-CE3 | 5.01  | 138.91      | 133.90   |
| 1   | A     | 434 | TYR  | CB-CA-C    | -5.01 | 102.80      | 110.81   |
| 4   | 1     | 359 | LYS  | CB-CG-CD   | 5.01  | 122.82      | 111.30   |
| 4   | X     | 227 | MET  | N-CA-C     | -5.01 | 105.73      | 111.14   |
| 1   | G     | 434 | TYR  | CB-CA-C    | -5.00 | 102.80      | 110.81   |
| 1   | G     | 762 | HIS  | N-CA-C     | 5.00  | 121.46      | 110.80   |
| 4   | 4     | 359 | LYS  | CB-CG-CD   | 5.00  | 122.81      | 111.30   |
| 1   | D     | 694 | GLN  | CA-C-O     | 5.00  | 126.03      | 120.63   |
| 1   | G     | 425 | SER  | N-CA-CB    | 5.00  | 117.57      | 110.16   |
| 1   | J     | 359 | MET  | O-C-N      | 5.00  | 127.22      | 122.07   |
| 4   | 2     | 88  | HIS  | CB-CG-CD2  | -5.00 | 124.69      | 131.20   |
| 4   | 7     | 88  | HIS  | CB-CG-CD2  | -5.00 | 124.69      | 131.20   |
| 4   | 9     | 266 | PHE  | CA-CB-CG   | 5.00  | 118.80      | 113.80   |
| 4   | 9     | 371 | HIS  | CB-CG-CD2  | -5.00 | 124.69      | 131.20   |
| 1   | G     | 278 | GLN  | CA-C-O     | 5.00  | 127.66      | 120.51   |
| 1   | G     | 829 | TRP  | N-CA-C     | 5.00  | 116.82      | 109.42   |
| 4   | 5     | 349 | LEU  | CA-C-O     | 5.00  | 126.69      | 121.19   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 648 | THR  | CB   |
| 1   | D     | 648 | THR  | CB   |
| 1   | G     | 648 | THR  | CB   |
| 1   | J     | 648 | THR  | CB   |

All (52) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 4   | 0     | 62  | ARG  | Sidechain         |
| 4   | 1     | 62  | ARG  | Sidechain         |
| 4   | 2     | 62  | ARG  | Sidechain         |
| 4   | 3     | 62  | ARG  | Sidechain         |
| 4   | 4     | 62  | ARG  | Sidechain         |
| 4   | 5     | 62  | ARG  | Sidechain         |
| 4   | 7     | 62  | ARG  | Sidechain         |
| 4   | 8     | 62  | ARG  | Sidechain         |
| 4   | 9     | 62  | ARG  | Sidechain         |
| 1   | A     | 623 | PHE  | Sidechain         |
| 1   | A     | 637 | LYS  | Mainchain         |
| 1   | A     | 649 | VAL  | Mainchain         |
| 1   | A     | 98  | HIS  | Mainchain         |
| 2   | B     | 150 | TYR  | Sidechain         |
| 2   | B     | 155 | TYR  | Mainchain         |
| 2   | B     | 22  | THR  | Mainchain         |
| 3   | C     | 75  | ALA  | Mainchain         |
| 3   | C     | 85  | GLU  | Mainchain         |
| 1   | D     | 623 | PHE  | Sidechain         |
| 1   | D     | 637 | LYS  | Mainchain         |
| 1   | D     | 649 | VAL  | Mainchain         |
| 1   | D     | 98  | HIS  | Mainchain         |
| 2   | E     | 150 | TYR  | Sidechain         |
| 2   | E     | 155 | TYR  | Mainchain         |
| 2   | E     | 22  | THR  | Mainchain         |
| 3   | F     | 75  | ALA  | Mainchain         |
| 3   | F     | 85  | GLU  | Mainchain         |
| 1   | G     | 623 | PHE  | Sidechain         |
| 1   | G     | 637 | LYS  | Mainchain         |
| 1   | G     | 649 | VAL  | Mainchain         |
| 1   | G     | 98  | HIS  | Mainchain         |
| 2   | H     | 150 | TYR  | Sidechain         |
| 2   | H     | 155 | TYR  | Mainchain         |
| 2   | H     | 22  | THR  | Mainchain         |
| 3   | I     | 75  | ALA  | Mainchain         |
| 3   | I     | 85  | GLU  | Mainchain         |
| 1   | J     | 623 | PHE  | Sidechain         |
| 1   | J     | 637 | LYS  | Mainchain         |
| 1   | J     | 649 | VAL  | Mainchain         |
| 1   | J     | 709 | LYS  | Peptide,Mainchain |
| 1   | J     | 98  | HIS  | Mainchain         |
| 2   | K     | 150 | TYR  | Sidechain         |
| 2   | K     | 155 | TYR  | Mainchain         |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | K     | 22  | THR  | Mainchain |
| 3   | L     | 75  | ALA  | Mainchain |
| 3   | L     | 85  | GLU  | Mainchain |
| 4   | V     | 62  | ARG  | Sidechain |
| 4   | W     | 62  | ARG  | Sidechain |
| 4   | X     | 62  | ARG  | Sidechain |
| 4   | Y     | 62  | ARG  | Sidechain |
| 4   | Z     | 62  | ARG  | Sidechain |

## 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     | 6797  | 0        | 6760     | 1441    | 0            |
| 1   | D     | 6797  | 0        | 6769     | 1466    | 0            |
| 1   | G     | 6797  | 0        | 6768     | 1432    | 0            |
| 1   | J     | 6797  | 0        | 6775     | 1448    | 0            |
| 2   | B     | 1127  | 0        | 1086     | 253     | 0            |
| 2   | E     | 1127  | 0        | 1087     | 325     | 0            |
| 2   | H     | 1127  | 0        | 1087     | 231     | 0            |
| 2   | K     | 1127  | 0        | 1087     | 232     | 0            |
| 3   | C     | 1123  | 0        | 1084     | 180     | 0            |
| 3   | F     | 1123  | 0        | 1082     | 143     | 0            |
| 3   | I     | 1123  | 0        | 1084     | 169     | 0            |
| 3   | L     | 1123  | 0        | 1084     | 167     | 0            |
| 4   | 0     | 2906  | 0        | 2865     | 182     | 0            |
| 4   | 1     | 2906  | 0        | 2865     | 207     | 0            |
| 4   | 2     | 2906  | 0        | 2865     | 139     | 0            |
| 4   | 3     | 2906  | 0        | 2863     | 182     | 0            |
| 4   | 4     | 2906  | 0        | 2865     | 98      | 0            |
| 4   | 5     | 2906  | 0        | 2865     | 100     | 0            |
| 4   | 7     | 2906  | 0        | 2866     | 84      | 0            |
| 4   | 8     | 2906  | 0        | 2857     | 324     | 0            |
| 4   | 9     | 2906  | 0        | 2855     | 348     | 0            |
| 4   | V     | 2906  | 0        | 2851     | 392     | 0            |
| 4   | W     | 2906  | 0        | 2851     | 389     | 0            |
| 4   | X     | 2906  | 0        | 2862     | 217     | 0            |
| 4   | Y     | 2906  | 0        | 2863     | 191     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | Z     | 2906  | 0        | 2862     | 194     | 0            |
| All | All   | 76872 | 0        | 75808    | 7895    | 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 52.

All (7895) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:797:PHE:CD1  | 3:I:149:VAL:HG11 | 1.21                     | 1.69              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CD1  | 1.22                     | 1.66              |
| 1:A:725:ARG:HE   | 1:A:733:PRO:CB   | 1.09                     | 1.64              |
| 1:D:725:ARG:HE   | 1:D:733:PRO:CB   | 1.09                     | 1.64              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:HD21 | 1.22                     | 1.64              |
| 1:D:831:TRP:HZ2  | 2:E:47:LEU:CA    | 1.09                     | 1.64              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CG1  | 1.17                     | 1.64              |
| 1:D:830:PRO:CG   | 2:E:67:MET:HE1   | 1.27                     | 1.63              |
| 4:X:291:LYS:HE3  | 4:Z:243:PRO:CB   | 1.17                     | 1.63              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HD13  | 1.22                     | 1.62              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:HD11 | 1.20                     | 1.62              |
| 1:J:510:TRP:CH2  | 1:J:768:MLY:HH11 | 1.33                     | 1.62              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CD1  | 1.22                     | 1.62              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CG1  | 1.17                     | 1.62              |
| 4:1:287:ILE:HG23 | 4:3:202:THR:CB   | 1.26                     | 1.62              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:HA2  | 1.24                     | 1.61              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HA    | 1.11                     | 1.61              |
| 1:A:206:LYS:CD   | 1:A:217:THR:HG23 | 1.28                     | 1.61              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CG1  | 1.17                     | 1.59              |
| 1:G:206:LYS:CD   | 1:G:217:THR:HG23 | 1.28                     | 1.59              |
| 1:G:831:TRP:HH2  | 2:H:47:LEU:CD2   | 1.08                     | 1.59              |
| 1:J:206:LYS:CD   | 1:J:217:THR:HG23 | 1.28                     | 1.59              |
| 1:J:538:GLU:CA   | 4:W:349:LEU:CD1  | 1.79                     | 1.59              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:CD1  | 1.27                     | 1.59              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CD1  | 1.22                     | 1.59              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CD1  | 1.22                     | 1.59              |
| 1:A:799:MET:SD   | 3:C:32:ASP:HB3   | 1.43                     | 1.58              |
| 1:G:725:ARG:HE   | 1:G:733:PRO:CB   | 1.09                     | 1.58              |
| 1:J:725:ARG:HE   | 1:J:733:PRO:CB   | 1.09                     | 1.58              |
| 1:G:93:MET:CE    | 1:G:763:THR:HB   | 1.23                     | 1.58              |
| 4:1:203:THR:H    | 4:Z:287:ILE:CG1  | 1.10                     | 1.58              |
| 1:D:538:GLU:CA   | 4:9:349:LEU:CD1  | 1.78                     | 1.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:538:GLU:CA   | 4:V:349:LEU:CD1  | 1.79                     | 1.57              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:CE    | 1.26                     | 1.57              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CG1  | 1.17                     | 1.57              |
| 1:J:84:MLY:CH1   | 1:J:715:VAL:HG13 | 1.23                     | 1.57              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:HB   | 1.23                     | 1.57              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:HD21 | 1.27                     | 1.56              |
| 1:A:836:PHE:CZ   | 2:B:160:GLY:N    | 1.69                     | 1.56              |
| 1:J:530:MET:HG2  | 4:W:354:GLN:CB   | 1.36                     | 1.56              |
| 1:D:206:LYS:CD   | 1:D:217:THR:HG23 | 1.28                     | 1.56              |
| 1:G:797:PHE:HD1  | 3:I:149:VAL:CG1  | 1.18                     | 1.55              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:CB   | 1.35                     | 1.55              |
| 4:1:202:THR:HB   | 4:Z:287:ILE:CG2  | 1.30                     | 1.55              |
| 1:A:530:MET:HG2  | 4:8:354:GLN:CB   | 1.35                     | 1.55              |
| 1:G:530:MET:HG2  | 4:V:354:GLN:CB   | 1.35                     | 1.54              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:HD22 | 1.36                     | 1.54              |
| 1:G:93:MET:HE1   | 1:G:763:THR:CB   | 1.10                     | 1.54              |
| 1:J:800:ARG:CD   | 3:L:149:VAL:CG2  | 1.81                     | 1.54              |
| 4:0:247:VAL:CG2  | 4:Y:324:THR:HG22 | 1.35                     | 1.54              |
| 1:G:831:TRP:CH2  | 2:H:47:LEU:HD22  | 1.40                     | 1.54              |
| 1:A:538:GLU:CA   | 4:8:349:LEU:CD1  | 1.78                     | 1.54              |
| 1:D:530:MET:HG2  | 4:9:354:GLN:CB   | 1.35                     | 1.53              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:CG   | 1.36                     | 1.53              |
| 1:D:834:LEU:CG   | 2:E:54:MET:HG3   | 1.37                     | 1.53              |
| 1:G:93:MET:HE1   | 1:G:763:THR:CG2  | 1.35                     | 1.53              |
| 4:1:287:ILE:CG1  | 4:3:203:THR:N    | 1.67                     | 1.53              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:CG   | 1.37                     | 1.53              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CZ    | 1.27                     | 1.53              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:CG2  | 1.70                     | 1.53              |
| 2:E:111:SER:HB2  | 2:E:148:VAL:C    | 1.23                     | 1.52              |
| 2:K:111:SER:HB2  | 2:K:148:VAL:C    | 1.23                     | 1.52              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:CB   | 1.35                     | 1.52              |
| 1:D:799:MET:SD   | 3:F:32:ASP:HB3   | 1.47                     | 1.52              |
| 4:0:243:PRO:CB   | 4:Y:291:LYS:HE3  | 1.34                     | 1.52              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CG   | 1.29                     | 1.52              |
| 2:B:111:SER:HB2  | 2:B:148:VAL:C    | 1.23                     | 1.52              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:CG   | 1.37                     | 1.52              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:CG2  | 1.40                     | 1.51              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CG   | 1.29                     | 1.51              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CZ    | 1.96                     | 1.51              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:CG   | 1.37                     | 1.51              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:CB   | 1.35                     | 1.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:757:GLN:CG   | 1:J:776:GLU:HG3  | 1.34                     | 1.51              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:CB   | 1.35                     | 1.51              |
| 1:J:538:GLU:C    | 4:W:349:LEU:CD1  | 1.84                     | 1.50              |
| 1:G:538:GLU:C    | 4:V:349:LEU:CD1  | 1.84                     | 1.50              |
| 2:H:111:SER:HB2  | 2:H:148:VAL:C    | 1.23                     | 1.50              |
| 1:J:84:MLY:CE    | 1:J:719:ASP:HB3  | 1.09                     | 1.50              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:CD   | 1.85                     | 1.50              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CG   | 1.30                     | 1.50              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:CD   | 1.84                     | 1.50              |
| 1:D:538:GLU:C    | 4:9:349:LEU:CD1  | 1.84                     | 1.50              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:CD   | 1.84                     | 1.50              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CB   | 1.41                     | 1.50              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:HD2  | 1.39                     | 1.49              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CG   | 1.30                     | 1.49              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:CG2  | 1.40                     | 1.49              |
| 4:1:287:ILE:HG12 | 4:3:202:THR:C    | 1.29                     | 1.49              |
| 1:A:538:GLU:C    | 4:8:349:LEU:CD1  | 1.84                     | 1.49              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CD2  | 1.43                     | 1.49              |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:CG2  | 1.42                     | 1.49              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CB   | 1.41                     | 1.48              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:CG2  | 1.40                     | 1.48              |
| 1:J:768:MLY:HH12 | 1:J:772:LEU:CD2  | 1.42                     | 1.48              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:HH22  | 1.27                     | 1.48              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CB   | 1.42                     | 1.48              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:HE3   | 1.41                     | 1.48              |
| 1:J:508:ILE:HD11 | 1:J:759:ALA:CB   | 1.41                     | 1.48              |
| 1:J:800:ARG:CD   | 3:L:149:VAL:HG22 | 1.40                     | 1.48              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:CG2  | 1.40                     | 1.48              |
| 1:D:831:TRP:CZ3  | 2:E:34:ILE:HG23  | 1.46                     | 1.48              |
| 1:G:84:MLY:CH1   | 1:G:715:VAL:HG13 | 1.36                     | 1.48              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:CG2  | 1.03                     | 1.48              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:NE2  | 1.76                     | 1.47              |
| 4:W:324:THR:CG2  | 4:Y:247:VAL:H    | 1.25                     | 1.47              |
| 1:D:641:LYS:CD   | 1:D:647:GLN:CD   | 1.85                     | 1.46              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CB   | 1.42                     | 1.46              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:CA   | 1.44                     | 1.46              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:NH2   | 1.22                     | 1.46              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:NE2  | 1.76                     | 1.46              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:NE2  | 1.76                     | 1.46              |
| 1:A:836:PHE:CE1  | 2:B:160:GLY:N    | 1.81                     | 1.46              |
| 1:D:768:MLY:C    | 1:D:771:LEU:HD13 | 1.31                     | 1.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:831:TRP:CH2  | 2:E:47:LEU:HA    | 1.45                     | 1.46              |
| 1:D:830:PRO:HG2  | 2:E:67:MET:CE    | 0.98                     | 1.45              |
| 4:1:202:THR:CB   | 4:Z:287:ILE:HG23 | 1.45                     | 1.45              |
| 1:D:830:PRO:CG   | 2:E:67:MET:CE    | 1.82                     | 1.45              |
| 4:1:203:THR:N    | 4:Z:287:ILE:HG12 | 1.22                     | 1.45              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CA    | 1.84                     | 1.44              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:NE2  | 1.76                     | 1.44              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:CG2  | 1.45                     | 1.44              |
| 4:3:288:ASP:CG   | 4:5:203:THR:CG2  | 1.89                     | 1.44              |
| 1:D:814:PHE:CD1  | 2:E:127:ARG:NH2  | 1.79                     | 1.44              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:CG   | 1.15                     | 1.43              |
| 1:G:567:LYS:NZ   | 4:X:92:ASN:HD22  | 1.17                     | 1.43              |
| 1:G:800:ARG:NH1  | 3:I:149:VAL:HG22 | 1.31                     | 1.43              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:CD2  | 1.95                     | 1.42              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:CB   | 1.64                     | 1.42              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:CG   | 1.15                     | 1.42              |
| 1:D:736:GLN:N    | 1:D:743:ALA:HB1  | 1.35                     | 1.42              |
| 1:G:556:ASP:CG   | 4:X:47:MET:CE    | 1.75                     | 1.42              |
| 1:G:733:PRO:O    | 1:G:737:PHE:CD1  | 1.73                     | 1.42              |
| 1:A:733:PRO:O    | 1:A:737:PHE:CD1  | 1.73                     | 1.41              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:CD   | 1.93                     | 1.41              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:CD   | 1.45                     | 1.41              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:CD1  | 1.99                     | 1.41              |
| 1:G:736:GLN:N    | 1:G:743:ALA:HB1  | 1.34                     | 1.41              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:CD1  | 1.98                     | 1.41              |
| 1:A:530:MET:CG   | 4:8:354:GLN:HB2  | 1.50                     | 1.41              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:CD   | 1.93                     | 1.41              |
| 1:J:202:SER:HA   | 1:J:207:LYS:CE   | 1.51                     | 1.41              |
| 1:D:530:MET:CG   | 4:9:354:GLN:HB2  | 1.50                     | 1.40              |
| 1:J:218:LEU:CB   | 1:J:221:GLN:HG3  | 1.51                     | 1.40              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CG   | 1.51                     | 1.40              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:HB2  | 1.52                     | 1.40              |
| 1:A:202:SER:HA   | 1:A:207:LYS:CE   | 1.51                     | 1.40              |
| 1:D:218:LEU:CB   | 1:D:221:GLN:HG3  | 1.52                     | 1.40              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:CB   | 2.00                     | 1.40              |
| 1:G:730:SER:OG   | 3:I:109:HIS:CD2  | 1.73                     | 1.40              |
| 4:1:287:ILE:HG12 | 4:3:203:THR:N    | 1.25                     | 1.40              |
| 1:A:831:TRP:NE1  | 2:B:51:PHE:CZ    | 1.89                     | 1.39              |
| 1:A:537:GLU:O    | 4:8:349:LEU:CD1  | 1.70                     | 1.39              |
| 1:J:733:PRO:O    | 1:J:737:PHE:CD1  | 1.73                     | 1.39              |
| 1:D:537:GLU:O    | 4:9:349:LEU:CD1  | 1.70                     | 1.39              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:144:VAL:CG1  | 2:E:153:ILE:CD1  | 1.99                     | 1.39              |
| 1:G:202:SER:HA   | 1:G:207:LYS:CE   | 1.51                     | 1.39              |
| 4:1:287:ILE:HG12 | 4:3:202:THR:CA   | 1.50                     | 1.39              |
| 1:D:202:SER:HA   | 1:D:207:LYS:CE   | 1.51                     | 1.39              |
| 1:D:733:PRO:O    | 1:D:737:PHE:CD1  | 1.73                     | 1.39              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:CD1  | 1.99                     | 1.39              |
| 4:2:290:ARG:CZ   | 4:4:202:THR:HG21 | 1.52                     | 1.39              |
| 1:A:149:GLN:CB   | 1:A:719:ASP:OD1  | 1.71                     | 1.39              |
| 1:G:819:ASN:CA   | 2:H:90:GLY:O     | 1.67                     | 1.39              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:CD   | 1.93                     | 1.38              |
| 1:G:795:ARG:CD   | 3:I:35:ARG:HH22  | 1.33                     | 1.38              |
| 1:J:530:MET:CG   | 4:W:354:GLN:HB2  | 1.51                     | 1.38              |
| 1:A:218:LEU:CB   | 1:A:221:GLN:HG3  | 1.52                     | 1.38              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:CD   | 1.45                     | 1.38              |
| 1:J:736:GLN:CA   | 1:J:743:ALA:CB   | 2.00                     | 1.38              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:CD   | 1.93                     | 1.38              |
| 1:J:537:GLU:O    | 4:W:349:LEU:CD1  | 1.70                     | 1.38              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:HB1  | 1.53                     | 1.38              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:CB   | 2.00                     | 1.37              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:HG22 | 1.54                     | 1.37              |
| 1:G:218:LEU:CB   | 1:G:221:GLN:HG3  | 1.51                     | 1.37              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:HG12 | 1.54                     | 1.37              |
| 1:G:534:SER:O    | 4:V:351:THR:CG2  | 1.64                     | 1.37              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:HG2  | 1.06                     | 1.37              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:HB1  | 1.53                     | 1.37              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:CG   | 1.96                     | 1.37              |
| 1:A:736:GLN:N    | 1:A:743:ALA:HB1  | 1.34                     | 1.37              |
| 1:D:642:LYS:HG3  | 4:9:23:GLY:N     | 1.40                     | 1.37              |
| 1:J:721:LYS:CG   | 1:J:736:GLN:CD   | 1.98                     | 1.37              |
| 1:J:736:GLN:CA   | 1:J:743:ALA:HB1  | 1.53                     | 1.37              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:CG1  | 2.03                     | 1.37              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:ND2  | 1.39                     | 1.36              |
| 1:G:537:GLU:O    | 4:V:349:LEU:CD1  | 1.70                     | 1.36              |
| 1:G:721:LYS:CG   | 1:G:736:GLN:CD   | 1.98                     | 1.36              |
| 1:G:831:TRP:CH2  | 2:H:47:LEU:CD2   | 2.00                     | 1.36              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:ND2  | 1.39                     | 1.36              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HG12 | 1.54                     | 1.36              |
| 1:A:649:VAL:O    | 1:A:649:VAL:CG1  | 1.73                     | 1.36              |
| 1:A:721:LYS:HG3  | 1:A:736:GLN:CG   | 1.15                     | 1.36              |
| 1:J:642:LYS:HG3  | 4:W:23:GLY:N     | 1.40                     | 1.36              |
| 4:0:287:ILE:HB   | 4:2:203:THR:CG2  | 1.54                     | 1.36              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HG12 | 1.54                     | 1.36              |
| 1:G:530:MET:CG   | 4:V:354:GLN:HB2  | 1.51                     | 1.36              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HG12 | 1.54                     | 1.36              |
| 1:G:649:VAL:O    | 1:G:649:VAL:CG1  | 1.74                     | 1.36              |
| 1:J:768:MLY:CH1  | 1:J:772:LEU:HD22 | 1.53                     | 1.36              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:CG2  | 1.56                     | 1.36              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:OD1  | 1.74                     | 1.35              |
| 4:O:287:ILE:CB   | 4:2:203:THR:HG22 | 1.56                     | 1.35              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:CD   | 1.98                     | 1.35              |
| 1:G:538:GLU:CA   | 4:V:349:LEU:HD12 | 0.88                     | 1.35              |
| 1:G:642:LYS:HG3  | 4:V:23:GLY:N     | 1.39                     | 1.35              |
| 1:J:736:GLN:N    | 1:J:743:ALA:HB1  | 1.35                     | 1.35              |
| 1:J:831:TRP:HZ3  | 2:K:34:ILE:CD1   | 1.37                     | 1.35              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:CB   | 2.00                     | 1.35              |
| 4:O:202:THR:CB   | 4:Y:286:ASP:OD1  | 1.75                     | 1.35              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:CG1  | 2.03                     | 1.35              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:CD   | 1.98                     | 1.35              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:CD   | 1.45                     | 1.35              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:ND2  | 1.39                     | 1.35              |
| 1:A:530:MET:HA   | 4:8:354:GLN:CG   | 1.56                     | 1.35              |
| 1:A:534:SER:O    | 4:8:351:THR:CG2  | 1.64                     | 1.35              |
| 1:G:553:MLY:CH1  | 4:X:45:VAL:HG11  | 1.54                     | 1.35              |
| 1:G:721:LYS:CG   | 1:G:736:GLN:CG   | 1.97                     | 1.35              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:HB1  | 1.53                     | 1.35              |
| 1:D:534:SER:O    | 4:9:351:THR:CG2  | 1.64                     | 1.34              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:CG   | 1.15                     | 1.34              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:CG1  | 2.03                     | 1.34              |
| 1:J:538:GLU:CA   | 4:W:349:LEU:HD12 | 0.88                     | 1.34              |
| 1:G:735:GLY:C    | 1:G:743:ALA:CB   | 2.01                     | 1.34              |
| 1:G:834:LEU:HD13 | 2:H:51:PHE:CE1   | 1.61                     | 1.34              |
| 1:D:735:GLY:C    | 1:D:743:ALA:CB   | 2.01                     | 1.34              |
| 1:D:831:TRP:HZ2  | 2:E:47:LEU:CB    | 1.40                     | 1.34              |
| 1:D:649:VAL:O    | 1:D:649:VAL:CG1  | 1.73                     | 1.34              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:HD22  | 1.63                     | 1.34              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:CG1  | 2.03                     | 1.34              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:OD1  | 1.74                     | 1.34              |
| 1:A:538:GLU:CA   | 4:8:349:LEU:HD12 | 0.87                     | 1.34              |
| 1:A:642:LYS:HG3  | 4:8:23:GLY:N     | 1.40                     | 1.34              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:CD   | 1.46                     | 1.34              |
| 2:H:114:LYS:CA   | 2:H:146:GLY:O    | 1.76                     | 1.34              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:OD1  | 1.74                     | 1.34              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:795:ARG:HD2  | 3:L:35:ARG:CZ    | 1.56                     | 1.34              |
| 4:O:290:ARG:HH21 | 4:2:202:THR:CG2  | 1.41                     | 1.34              |
| 4:3:288:ASP:OD2  | 4:5:203:THR:CG2  | 1.72                     | 1.34              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:OD1  | 1.74                     | 1.33              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:HB3  | 1.28                     | 1.33              |
| 1:J:537:GLU:C    | 4:W:349:LEU:HD13 | 1.52                     | 1.33              |
| 1:J:792:ALA:CB   | 3:L:40:ASN:HB3   | 1.57                     | 1.33              |
| 1:D:538:GLU:CA   | 4:9:349:LEU:HD12 | 0.87                     | 1.33              |
| 1:G:537:GLU:C    | 4:V:349:LEU:HD13 | 1.53                     | 1.33              |
| 1:J:735:GLY:C    | 1:J:743:ALA:CB   | 2.01                     | 1.33              |
| 1:D:635:GLY:CA   | 4:9:334:GLU:HG2  | 1.59                     | 1.33              |
| 1:D:799:MET:SD   | 3:F:32:ASP:CB    | 2.17                     | 1.33              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:ND2  | 1.39                     | 1.33              |
| 1:J:530:MET:HA   | 4:W:354:GLN:CG   | 1.56                     | 1.33              |
| 1:J:629:GLU:HA   | 1:J:643:GLY:O    | 1.17                     | 1.33              |
| 1:J:649:VAL:O    | 1:J:649:VAL:CG1  | 1.73                     | 1.33              |
| 1:D:530:MET:HA   | 4:9:354:GLN:CG   | 1.56                     | 1.33              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HD23  | 1.64                     | 1.33              |
| 4:1:203:THR:H    | 4:Z:287:ILE:CB   | 1.42                     | 1.33              |
| 1:A:735:GLY:C    | 1:A:743:ALA:CB   | 2.01                     | 1.33              |
| 1:J:635:GLY:CA   | 4:W:334:GLU:HG2  | 1.59                     | 1.33              |
| 1:D:629:GLU:HA   | 1:D:643:GLY:O    | 1.17                     | 1.32              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:CD2  | 2.13                     | 1.32              |
| 1:G:530:MET:HA   | 4:V:354:GLN:CG   | 1.57                     | 1.32              |
| 1:J:534:SER:O    | 4:W:351:THR:CG2  | 1.64                     | 1.32              |
| 1:J:735:GLY:O    | 1:J:743:ALA:HB2  | 1.29                     | 1.32              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:CB   | 1.87                     | 1.32              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:CG    | 1.42                     | 1.32              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:CD   | 2.07                     | 1.32              |
| 1:A:537:GLU:C    | 4:8:349:LEU:HD13 | 1.51                     | 1.32              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:HG2  | 1.43                     | 1.32              |
| 4:O:247:VAL:HG22 | 4:Y:324:THR:CG2  | 1.58                     | 1.32              |
| 4:1:287:ILE:CB   | 4:3:202:THR:HB   | 1.60                     | 1.32              |
| 1:A:725:ARG:NE   | 1:A:733:PRO:HB3  | 0.99                     | 1.32              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:CD   | 1.58                     | 1.32              |
| 2:E:114:LYS:CA   | 2:E:146:GLY:O    | 1.76                     | 1.32              |
| 4:3:288:ASP:CG   | 4:5:203:THR:HG23 | 1.47                     | 1.32              |
| 1:A:538:GLU:O    | 4:8:349:LEU:CD1  | 1.78                     | 1.31              |
| 1:A:629:GLU:HA   | 1:A:643:GLY:O    | 1.17                     | 1.31              |
| 1:D:723:ARG:O    | 1:D:782:MLY:HD3  | 1.29                     | 1.31              |
| 1:D:831:TRP:NE1  | 2:E:47:LEU:HD22  | 1.43                     | 1.31              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:114:LYS:CA   | 2:K:146:GLY:O    | 1.76                     | 1.31              |
| 2:K:121:LEU:O    | 2:K:128:PHE:CB   | 1.78                     | 1.31              |
| 2:B:114:LYS:CA   | 2:B:146:GLY:O    | 1.76                     | 1.31              |
| 1:G:629:GLU:HA   | 1:G:643:GLY:O    | 1.17                     | 1.31              |
| 1:A:831:TRP:CE2  | 2:B:51:PHE:CZ    | 2.18                     | 1.31              |
| 1:D:721:LYS:HG2  | 1:D:736:GLN:OE1  | 1.28                     | 1.31              |
| 1:G:635:GLY:CA   | 4:V:334:GLU:HG2  | 1.59                     | 1.31              |
| 1:G:800:ARG:HH11 | 3:I:149:VAL:CG2  | 1.41                     | 1.31              |
| 1:J:725:ARG:NE   | 1:J:733:PRO:HB3  | 0.99                     | 1.31              |
| 4:W:324:THR:HG21 | 4:Y:247:VAL:N    | 0.98                     | 1.31              |
| 1:D:537:GLU:C    | 4:9:349:LEU:HD13 | 1.52                     | 1.31              |
| 1:D:599:ASN:HA   | 1:D:649:VAL:CB   | 1.60                     | 1.31              |
| 1:A:635:GLY:CA   | 4:8:334:GLU:HG2  | 1.58                     | 1.30              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:CD   | 1.54                     | 1.30              |
| 1:D:725:ARG:NE   | 1:D:733:PRO:HB3  | 1.00                     | 1.30              |
| 2:E:121:LEU:O    | 2:E:128:PHE:CB   | 1.79                     | 1.30              |
| 1:G:789:ALA:HB2  | 3:I:81:GLN:NE2   | 1.44                     | 1.30              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:CD1   | 2.12                     | 1.30              |
| 4:1:202:THR:C    | 4:Z:287:ILE:HG12 | 1.56                     | 1.30              |
| 1:G:538:GLU:O    | 4:V:349:LEU:CD1  | 1.78                     | 1.30              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:CG   | 2.05                     | 1.30              |
| 1:J:599:ASN:HA   | 1:J:649:VAL:CB   | 1.60                     | 1.30              |
| 4:1:203:THR:N    | 4:Z:287:ILE:CG1  | 1.82                     | 1.30              |
| 1:G:725:ARG:NE   | 1:G:733:PRO:HB3  | 0.99                     | 1.30              |
| 1:A:735:GLY:O    | 1:A:743:ALA:HB2  | 1.29                     | 1.29              |
| 1:A:819:ASN:OD1  | 2:B:91:ALA:CA    | 1.79                     | 1.29              |
| 4:X:286:ASP:CG   | 4:Z:202:THR:HB   | 1.32                     | 1.29              |
| 1:A:599:ASN:HA   | 1:A:649:VAL:CB   | 1.60                     | 1.29              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:CB    | 1.60                     | 1.29              |
| 1:A:836:PHE:HB2  | 2:B:161:GLU:OE1  | 1.31                     | 1.29              |
| 2:B:121:LEU:O    | 2:B:128:PHE:CB   | 1.79                     | 1.29              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:CD2   | 2.13                     | 1.29              |
| 1:G:795:ARG:HD2  | 3:I:35:ARG:NH2   | 1.46                     | 1.29              |
| 1:G:599:ASN:HA   | 1:G:649:VAL:CB   | 1.60                     | 1.29              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:CD   | 1.53                     | 1.29              |
| 1:D:215:GLN:N    | 1:D:340:ILE:HG12 | 1.20                     | 1.29              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:CA   | 2.10                     | 1.29              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:CD2  | 1.57                     | 1.29              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:HB2  | 1.72                     | 1.29              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:CB   | 2.06                     | 1.29              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:CD   | 1.54                     | 1.28              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:117:LEU:CD1  | 2:K:147:ASN:CG   | 2.05                     | 1.28              |
| 4:0:166:TYR:CE2  | 4:2:64:ILE:HG21  | 1.68                     | 1.28              |
| 1:G:721:LYS:HG2  | 1:G:736:GLN:OE1  | 1.29                     | 1.28              |
| 1:J:215:GLN:N    | 1:J:340:ILE:HG12 | 1.19                     | 1.28              |
| 1:J:768:MLY:CH1  | 1:J:772:LEU:CD2  | 2.11                     | 1.28              |
| 1:J:800:ARG:CB   | 3:L:149:VAL:HG21 | 1.63                     | 1.28              |
| 1:G:836:PHE:CE1  | 2:H:159:HIS:HA   | 1.66                     | 1.28              |
| 1:J:721:LYS:HG2  | 1:J:736:GLN:OE1  | 1.29                     | 1.28              |
| 2:E:121:LEU:C    | 2:E:128:PHE:CB   | 2.07                     | 1.28              |
| 1:G:93:MET:CE    | 1:G:763:THR:CB   | 1.89                     | 1.28              |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:CB   | 1.60                     | 1.28              |
| 1:G:552:ASN:O    | 4:X:47:MET:SD    | 1.91                     | 1.28              |
| 2:H:121:LEU:O    | 2:H:128:PHE:CB   | 1.78                     | 1.28              |
| 1:J:819:ASN:HA   | 2:K:90:GLY:O     | 1.17                     | 1.28              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:CG   | 2.05                     | 1.28              |
| 1:J:557:GLU:CA   | 4:Y:47:MET:HA    | 1.08                     | 1.27              |
| 2:K:121:LEU:C    | 2:K:128:PHE:CB   | 2.07                     | 1.27              |
| 1:G:538:GLU:C    | 4:V:349:LEU:HD12 | 1.48                     | 1.27              |
| 1:G:556:ASP:CG   | 4:X:47:MET:HE3   | 1.10                     | 1.27              |
| 2:H:121:LEU:C    | 2:H:128:PHE:CB   | 2.07                     | 1.27              |
| 4:3:288:ASP:OD2  | 4:5:203:THR:HG21 | 1.14                     | 1.27              |
| 1:D:538:GLU:C    | 4:9:349:LEU:HD12 | 1.48                     | 1.27              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CG    | 1.62                     | 1.27              |
| 1:J:538:GLU:O    | 4:W:349:LEU:CD1  | 1.78                     | 1.27              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:OE1  | 1.83                     | 1.27              |
| 1:D:799:MET:SD   | 3:F:32:ASP:C     | 2.17                     | 1.27              |
| 1:G:530:MET:HE2  | 4:V:354:GLN:CG   | 1.64                     | 1.27              |
| 1:G:752:ASP:O    | 1:G:779:ARG:NH1  | 1.67                     | 1.27              |
| 1:A:534:SER:O    | 4:8:351:THR:CA   | 1.81                     | 1.26              |
| 2:B:121:LEU:C    | 2:B:128:PHE:CB   | 2.07                     | 1.26              |
| 1:D:534:SER:O    | 4:9:351:THR:CA   | 1.81                     | 1.26              |
| 1:J:534:SER:O    | 4:W:351:THR:CA   | 1.82                     | 1.26              |
| 4:1:288:ASP:OD2  | 4:3:203:THR:HG21 | 1.32                     | 1.26              |
| 1:A:797:PHE:CD1  | 3:C:149:VAL:HG11 | 1.69                     | 1.26              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:CG   | 1.98                     | 1.26              |
| 1:J:733:PRO:O    | 1:J:737:PHE:HD1  | 0.92                     | 1.26              |
| 1:A:530:MET:HE2  | 4:8:354:GLN:CG   | 1.65                     | 1.26              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CD2   | 2.18                     | 1.26              |
| 1:A:836:PHE:CB   | 2:B:161:GLU:OE1  | 1.81                     | 1.26              |
| 1:D:735:GLY:O    | 1:D:743:ALA:HB2  | 1.29                     | 1.26              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:CG   | 2.05                     | 1.26              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:CE   | 1.64                     | 1.26              |
| 1:D:538:GLU:O    | 4:9:349:LEU:CD1  | 1.78                     | 1.26              |
| 1:G:93:MET:SD    | 1:G:716:LEU:HD12 | 1.73                     | 1.26              |
| 1:A:733:PRO:O    | 1:A:737:PHE:HD1  | 0.92                     | 1.25              |
| 1:G:508:ILE:CD1  | 1:G:759:ALA:HB2  | 1.66                     | 1.25              |
| 1:G:735:GLY:O    | 1:G:743:ALA:HB2  | 1.29                     | 1.25              |
| 1:J:530:MET:HE2  | 4:W:354:GLN:CG   | 1.65                     | 1.25              |
| 4:X:291:LYS:HD2  | 4:Z:244:ASP:N    | 1.48                     | 1.25              |
| 1:A:149:GLN:HB3  | 1:A:719:ASP:OD1  | 1.12                     | 1.25              |
| 1:J:508:ILE:CD1  | 1:J:759:ALA:HB2  | 1.62                     | 1.25              |
| 1:J:792:ALA:HB1  | 3:L:40:ASN:CB    | 1.66                     | 1.25              |
| 4:1:288:ASP:CG   | 4:3:203:THR:HG21 | 1.59                     | 1.25              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:NE   | 1.47                     | 1.25              |
| 1:D:530:MET:HE2  | 4:9:354:GLN:CG   | 1.65                     | 1.25              |
| 1:J:630:ALA:O    | 4:W:25:ASP:OD2   | 1.52                     | 1.25              |
| 4:1:288:ASP:CG   | 4:3:203:THR:CG2  | 2.09                     | 1.25              |
| 4:V:324:THR:HG21 | 4:X:247:VAL:N    | 1.49                     | 1.25              |
| 1:G:534:SER:O    | 4:V:351:THR:CA   | 1.83                     | 1.24              |
| 1:J:557:GLU:HA   | 4:Y:47:MET:C     | 1.62                     | 1.24              |
| 4:9:322:PRO:CB   | 4:W:244:ASP:OD2  | 1.86                     | 1.24              |
| 1:G:790:THR:OG1  | 3:I:87:PHE:CE2   | 1.90                     | 1.24              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CB   | 1.67                     | 1.24              |
| 1:A:721:LYS:HG3  | 1:A:736:GLN:CD   | 1.53                     | 1.24              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:HD11 | 1.73                     | 1.24              |
| 1:G:733:PRO:O    | 1:G:737:PHE:HD1  | 0.93                     | 1.24              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:NH2   | 1.89                     | 1.24              |
| 4:0:243:PRO:CB   | 4:Y:291:LYS:CE   | 2.14                     | 1.24              |
| 1:A:538:GLU:C    | 4:8:349:LEU:HD11 | 1.54                     | 1.24              |
| 4:V:325:MET:SD   | 4:X:244:ASP:HB2  | 1.77                     | 1.24              |
| 1:A:538:GLU:C    | 4:8:349:LEU:HD12 | 1.48                     | 1.24              |
| 1:A:836:PHE:CZ   | 2:B:160:GLY:CA   | 2.18                     | 1.24              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:HD11 | 1.73                     | 1.24              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:HH11 | 1.60                     | 1.24              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:HD11 | 1.73                     | 1.23              |
| 1:A:721:LYS:HG2  | 1:A:736:GLN:OE1  | 1.29                     | 1.23              |
| 1:J:721:LYS:CG   | 1:J:736:GLN:OE1  | 1.83                     | 1.23              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:OD1  | 1.32                     | 1.23              |
| 4:7:322:PRO:CB   | 4:9:244:ASP:OD2  | 1.86                     | 1.23              |
| 1:G:721:LYS:CG   | 1:G:736:GLN:OE1  | 1.83                     | 1.23              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:HB2  | 1.68                     | 1.23              |
| 4:8:322:PRO:CB   | 4:V:244:ASP:OD2  | 1.86                     | 1.23              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:538:GLU:O    | 4:8:349:LEU:HD11 | 1.35                     | 1.23              |
| 1:A:630:ALA:O    | 4:8:25:ASP:OD2   | 1.53                     | 1.23              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:NH1   | 1.50                     | 1.23              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:CG    | 1.67                     | 1.23              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:OE2  | 1.67                     | 1.23              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:HD11 | 1.73                     | 1.23              |
| 4:0:290:ARG:NH2  | 4:2:202:THR:HG22 | 1.50                     | 1.23              |
| 1:A:629:GLU:CA   | 1:A:643:GLY:O    | 1.87                     | 1.23              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:OE1  | 1.82                     | 1.23              |
| 1:D:836:PHE:HB3  | 2:E:161:GLU:OE1  | 1.35                     | 1.23              |
| 4:1:202:THR:CB   | 4:Z:287:ILE:CG2  | 2.10                     | 1.23              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:CG2  | 1.68                     | 1.23              |
| 1:G:557:GLU:CB   | 4:X:46:GLY:O     | 1.86                     | 1.23              |
| 1:G:707:CYS:HB3  | 1:G:714:ARG:NH1  | 1.53                     | 1.23              |
| 1:G:783:LEU:O    | 1:G:787:ILE:N    | 1.71                     | 1.23              |
| 4:0:287:ILE:CG2  | 4:2:203:THR:HG22 | 1.69                     | 1.23              |
| 1:A:506:GLU:OE2  | 1:A:717:TYR:OH   | 1.57                     | 1.22              |
| 1:A:534:SER:O    | 4:8:351:THR:CB   | 1.87                     | 1.22              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:CB   | 1.85                     | 1.22              |
| 1:J:538:GLU:C    | 4:W:349:LEU:HD12 | 1.48                     | 1.22              |
| 1:A:215:GLN:N    | 1:A:340:ILE:CG1  | 2.02                     | 1.22              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:CG   | 2.15                     | 1.22              |
| 1:D:799:MET:SD   | 3:F:32:ASP:O     | 1.97                     | 1.22              |
| 1:J:93:MET:SD    | 1:J:716:LEU:HD12 | 1.80                     | 1.22              |
| 4:1:287:ILE:CB   | 4:3:203:THR:N    | 2.00                     | 1.22              |
| 4:W:324:THR:CG2  | 4:Y:247:VAL:N    | 1.89                     | 1.22              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:OE2  | 1.70                     | 1.22              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:CG2  | 2.18                     | 1.22              |
| 1:D:630:ALA:O    | 4:9:25:ASP:OD2   | 1.52                     | 1.22              |
| 1:D:641:LYS:CD   | 1:D:647:GLN:NE2  | 1.99                     | 1.22              |
| 1:D:733:PRO:O    | 1:D:737:PHE:HD1  | 0.93                     | 1.22              |
| 1:G:215:GLN:N    | 1:G:340:ILE:CG1  | 2.02                     | 1.22              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HD11 | 1.64                     | 1.22              |
| 1:J:215:GLN:N    | 1:J:340:ILE:CG1  | 2.02                     | 1.22              |
| 1:G:567:LYS:NZ   | 4:X:92:ASN:ND2   | 1.87                     | 1.22              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:CD2  | 2.16                     | 1.21              |
| 1:D:534:SER:O    | 4:9:351:THR:CB   | 1.87                     | 1.21              |
| 1:G:538:GLU:O    | 4:V:349:LEU:HD11 | 1.34                     | 1.21              |
| 1:J:534:SER:O    | 4:W:351:THR:CB   | 1.87                     | 1.21              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:HG3  | 1.71                     | 1.21              |
| 1:A:797:PHE:HD1  | 3:C:149:VAL:CG1  | 1.53                     | 1.21              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HD11 | 1.65                     | 1.21              |
| 1:G:629:GLU:CA   | 1:G:643:GLY:O    | 1.87                     | 1.21              |
| 4:3:287:ILE:HD13 | 4:5:203:THR:HB   | 1.22                     | 1.21              |
| 1:A:795:ARG:HB3  | 3:C:35:ARG:NH2   | 1.55                     | 1.21              |
| 1:D:215:GLN:N    | 1:D:340:ILE:CG1  | 2.02                     | 1.21              |
| 1:D:629:GLU:CA   | 1:D:643:GLY:O    | 1.87                     | 1.21              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:HD11 | 1.64                     | 1.21              |
| 1:G:556:ASP:OD1  | 4:X:47:MET:HE3   | 1.39                     | 1.21              |
| 1:J:629:GLU:CA   | 1:J:643:GLY:O    | 1.87                     | 1.21              |
| 1:J:817:GLN:CD   | 2:K:127:ARG:HD2  | 1.64                     | 1.21              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:NE2  | 1.99                     | 1.21              |
| 1:A:757:GLN:CG   | 1:A:771:LEU:HD11 | 1.71                     | 1.21              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:HG3  | 1.70                     | 1.21              |
| 4:2:322:PRO:HB3  | 4:4:244:ASP:OD2  | 1.39                     | 1.21              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:CB   | 2.19                     | 1.20              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:CA   | 1.70                     | 1.20              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:HG3  | 1.71                     | 1.20              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:CB   | 2.19                     | 1.20              |
| 1:J:538:GLU:C    | 4:W:349:LEU:HD11 | 1.54                     | 1.20              |
| 1:J:800:ARG:CD   | 3:L:149:VAL:HG23 | 1.56                     | 1.20              |
| 1:D:822:SER:OG   | 2:E:88:LEU:HD23  | 1.04                     | 1.20              |
| 1:G:215:GLN:N    | 1:G:340:ILE:HG12 | 1.19                     | 1.20              |
| 1:D:553:MLY:CE   | 4:W:45:VAL:HA    | 1.52                     | 1.20              |
| 4:0:202:THR:HB   | 4:Y:286:ASP:OD1  | 1.06                     | 1.20              |
| 1:D:538:GLU:C    | 4:9:349:LEU:HD11 | 1.54                     | 1.20              |
| 1:G:769:ALA:HB3  | 1:G:770:GLY:CA   | 1.67                     | 1.20              |
| 4:0:202:THR:HB   | 4:Y:286:ASP:CG   | 1.45                     | 1.20              |
| 4:0:244:ASP:OD2  | 4:Y:325:MET:SD   | 1.99                     | 1.20              |
| 4:0:290:ARG:NH2  | 4:2:202:THR:CG2  | 2.04                     | 1.20              |
| 4:1:287:ILE:CG1  | 4:3:202:THR:CA   | 2.19                     | 1.20              |
| 4:9:322:PRO:HB2  | 4:W:244:ASP:OD2  | 1.39                     | 1.20              |
| 1:A:538:GLU:OE2  | 4:8:355:MET:CE   | 1.91                     | 1.19              |
| 1:D:830:PRO:HB2  | 2:E:51:PHE:CZ    | 1.76                     | 1.19              |
| 2:E:111:SER:CB   | 2:E:148:VAL:C    | 1.93                     | 1.19              |
| 1:G:534:SER:O    | 4:V:351:THR:CB   | 1.88                     | 1.19              |
| 1:D:725:ARG:N    | 1:D:782:MLY:HH21 | 1.55                     | 1.19              |
| 1:G:538:GLU:OE2  | 4:V:355:MET:CE   | 1.90                     | 1.19              |
| 1:J:538:GLU:OE2  | 4:W:355:MET:CE   | 1.90                     | 1.19              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:HE1   | 1.56                     | 1.19              |
| 2:K:121:LEU:C    | 2:K:128:PHE:HB2  | 1.67                     | 1.19              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:HB   | 1.05                     | 1.19              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:291:LYS:HE3  | 4:Z:243:PRO:HB3  | 1.23                     | 1.19              |
| 1:D:538:GLU:OE2  | 4:9:355:MET:CE   | 1.90                     | 1.19              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:HD2  | 1.71                     | 1.19              |
| 4:8:322:PRO:HB2  | 4:V:244:ASP:OD2  | 1.39                     | 1.19              |
| 1:A:557:GLU:H    | 4:V:48:GLY:CA    | 1.56                     | 1.18              |
| 1:G:641:LYS:CB   | 1:G:647:GLN:NE2  | 2.07                     | 1.18              |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD21  | 1.20                     | 1.18              |
| 4:W:324:THR:HG21 | 4:Y:246:GLN:C    | 1.61                     | 1.18              |
| 1:D:557:GLU:H    | 4:W:48:GLY:CA    | 1.56                     | 1.18              |
| 1:G:510:TRP:CZ3  | 1:G:768:MLY:HH11 | 1.77                     | 1.18              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:NH2   | 2.07                     | 1.18              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:CB   | 2.19                     | 1.18              |
| 1:A:735:GLY:O    | 1:A:743:ALA:CB   | 1.91                     | 1.18              |
| 1:A:822:SER:OG   | 2:B:88:LEU:HD23  | 1.04                     | 1.18              |
| 2:B:121:LEU:C    | 2:B:128:PHE:HB2  | 1.67                     | 1.18              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:CG   | 2.15                     | 1.18              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:HG3  | 1.71                     | 1.18              |
| 1:J:641:LYS:CB   | 1:J:647:GLN:NE2  | 2.07                     | 1.18              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:HG2  | 1.25                     | 1.18              |
| 1:J:768:MLY:HD3  | 1:J:772:LEU:CB   | 1.72                     | 1.18              |
| 4:1:203:THR:HG21 | 4:Z:288:ASP:CG   | 1.68                     | 1.18              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:CA   | 1.72                     | 1.18              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:NE2  | 1.99                     | 1.18              |
| 1:G:721:LYS:HA   | 1:G:736:GLN:NE2  | 1.58                     | 1.18              |
| 1:G:819:ASN:CG   | 2:H:92:ASP:HB2   | 1.62                     | 1.18              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:CD1  | 1.55                     | 1.18              |
| 1:D:541:MET:C    | 4:9:143:TYR:OH   | 1.87                     | 1.17              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CE2   | 1.62                     | 1.17              |
| 4:0:247:VAL:CG2  | 4:Y:324:THR:CG2  | 2.16                     | 1.17              |
| 1:A:541:MET:C    | 4:8:143:TYR:OH   | 1.87                     | 1.17              |
| 1:A:831:TRP:CD1  | 2:B:51:PHE:HZ    | 1.61                     | 1.17              |
| 1:D:538:GLU:OE2  | 4:9:355:MET:HE1  | 1.44                     | 1.17              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:CB   | 2.19                     | 1.17              |
| 1:G:201:ALA:O    | 1:G:202:SER:HB3  | 1.36                     | 1.17              |
| 1:G:541:MET:C    | 4:V:143:TYR:OH   | 1.87                     | 1.17              |
| 1:A:215:GLN:N    | 1:A:340:ILE:HG12 | 1.20                     | 1.17              |
| 1:A:721:LYS:HA   | 1:A:736:GLN:NE2  | 1.58                     | 1.17              |
| 1:G:557:GLU:HA   | 4:X:48:GLY:N     | 1.13                     | 1.17              |
| 1:J:541:MET:C    | 4:W:143:TYR:OH   | 1.87                     | 1.17              |
| 1:J:800:ARG:CB   | 3:L:149:VAL:CG2  | 2.21                     | 1.17              |
| 1:J:829:TRP:CH2  | 2:K:84:PHE:CE1   | 2.33                     | 1.17              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:48:LYS:C     | 3:L:52:ASN:ND2   | 2.03                     | 1.17              |
| 4:8:290:ARG:NH2  | 4:V:202:THR:HG23 | 1.59                     | 1.17              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:CD1  | 1.55                     | 1.17              |
| 1:D:822:SER:OG   | 2:E:88:LEU:CD2   | 1.90                     | 1.17              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:HG3   | 1.74                     | 1.17              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:HB3  | 1.75                     | 1.17              |
| 1:G:735:GLY:O    | 1:G:743:ALA:CB   | 1.91                     | 1.17              |
| 4:7:322:PRO:HB2  | 4:9:244:ASP:OD2  | 1.39                     | 1.17              |
| 1:A:502:GLU:HG3  | 1:A:761:GLY:CA   | 1.75                     | 1.17              |
| 1:D:641:LYS:CB   | 1:D:647:GLN:NE2  | 2.07                     | 1.17              |
| 1:D:641:LYS:CE   | 4:9:348:SER:O    | 1.93                     | 1.17              |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:CD2  | 1.78                     | 1.17              |
| 1:G:553:MLY:CE   | 4:X:45:VAL:CB    | 2.22                     | 1.17              |
| 3:I:48:LYS:C     | 3:I:52:ASN:ND2   | 2.03                     | 1.17              |
| 1:J:641:LYS:CE   | 4:W:348:SER:O    | 1.93                     | 1.17              |
| 1:J:735:GLY:O    | 1:J:743:ALA:CB   | 1.91                     | 1.17              |
| 1:A:553:MLY:CE   | 4:V:45:VAL:HA    | 1.52                     | 1.16              |
| 1:A:641:LYS:CB   | 1:A:647:GLN:NE2  | 2.07                     | 1.16              |
| 3:C:48:LYS:C     | 3:C:52:ASN:ND2   | 2.03                     | 1.16              |
| 1:G:553:MLY:HG3  | 4:X:45:VAL:O     | 1.01                     | 1.16              |
| 1:J:510:TRP:CH2  | 1:J:768:MLY:CH1  | 2.28                     | 1.16              |
| 1:J:798:LEU:CD2  | 3:L:126:LEU:HD11 | 1.74                     | 1.16              |
| 1:J:829:TRP:HH2  | 2:K:84:PHE:CE1   | 1.61                     | 1.16              |
| 1:G:201:ALA:O    | 1:G:202:SER:CB   | 1.92                     | 1.16              |
| 1:G:788:THR:C    | 3:I:42:THR:HG22  | 1.55                     | 1.16              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:NE2  | 1.99                     | 1.16              |
| 1:J:721:LYS:CG   | 1:J:736:GLN:CG   | 1.97                     | 1.16              |
| 4:9:290:ARG:NH2  | 4:W:202:THR:HG23 | 1.59                     | 1.16              |
| 1:A:201:ALA:O    | 1:A:202:SER:HB3  | 1.35                     | 1.16              |
| 1:G:215:GLN:HA   | 1:G:340:ILE:CG2  | 1.75                     | 1.16              |
| 1:G:557:GLU:HB3  | 4:X:46:GLY:O     | 0.99                     | 1.16              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:CD   | 2.18                     | 1.16              |
| 1:D:726:VAL:HB   | 1:D:782:MLY:CH1  | 1.75                     | 1.16              |
| 3:F:48:LYS:C     | 3:F:52:ASN:ND2   | 2.03                     | 1.16              |
| 1:G:642:LYS:CG   | 4:V:23:GLY:N     | 2.08                     | 1.16              |
| 1:G:754:ASP:HB2  | 1:G:776:GLU:OE2  | 1.43                     | 1.16              |
| 1:G:819:ASN:CG   | 2:H:90:GLY:O     | 1.88                     | 1.16              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:CG   | 1.70                     | 1.16              |
| 1:J:215:GLN:HA   | 1:J:340:ILE:CG2  | 1.75                     | 1.16              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HD11 | 1.65                     | 1.16              |
| 4:7:290:ARG:NH2  | 4:9:202:THR:HG23 | 1.59                     | 1.16              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:639:GLY:CA   | 4:8:345:ILE:HA   | 1.73                     | 1.16              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:CG   | 1.70                     | 1.16              |
| 1:G:553:MLY:HE2  | 4:X:45:VAL:CB    | 1.75                     | 1.16              |
| 1:G:739:ASP:HB3  | 1:G:742:LYS:HB3  | 1.21                     | 1.16              |
| 2:H:111:SER:CB   | 2:H:148:VAL:C    | 1.93                     | 1.16              |
| 1:J:201:ALA:O    | 1:J:202:SER:CB   | 1.92                     | 1.16              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:NE2  | 1.59                     | 1.16              |
| 4:V:325:MET:SD   | 4:X:244:ASP:CB   | 2.33                     | 1.16              |
| 4:X:291:LYS:CD   | 4:Z:244:ASP:N    | 2.07                     | 1.16              |
| 1:A:553:MLY:HB3  | 4:V:46:GLY:CA    | 1.50                     | 1.15              |
| 1:A:641:LYS:CE   | 4:8:348:SER:O    | 1.93                     | 1.15              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:NE2  | 1.59                     | 1.15              |
| 1:G:538:GLU:OE2  | 4:V:355:MET:HE1  | 1.44                     | 1.15              |
| 1:G:640:LYS:HB3  | 1:G:645:SER:OG   | 1.46                     | 1.15              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:CD   | 2.18                     | 1.15              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:HB3  | 1.76                     | 1.15              |
| 4:O:290:ARG:HH21 | 4:2:202:THR:HG21 | 1.05                     | 1.15              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:CG2  | 1.76                     | 1.15              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:NE   | 2.03                     | 1.15              |
| 1:D:830:PRO:HG2  | 2:E:67:MET:HE3   | 1.17                     | 1.15              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:HD2  | 1.69                     | 1.15              |
| 2:H:111:SER:CA   | 2:H:148:VAL:O    | 1.95                     | 1.15              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:HB3  | 1.75                     | 1.15              |
| 1:J:640:LYS:HB3  | 1:J:645:SER:OG   | 1.45                     | 1.15              |
| 1:A:538:GLU:OE2  | 4:8:355:MET:HE1  | 1.44                     | 1.15              |
| 1:A:639:GLY:HA3  | 4:8:344:SER:O    | 1.46                     | 1.15              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:NE2  | 1.58                     | 1.15              |
| 1:D:834:LEU:HG   | 2:E:54:MET:HG3   | 1.22                     | 1.15              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:CG   | 1.70                     | 1.15              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:NE2  | 1.58                     | 1.15              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:CD   | 2.18                     | 1.15              |
| 1:J:635:GLY:HA2  | 4:W:334:GLU:HG2  | 1.16                     | 1.15              |
| 1:A:215:GLN:HA   | 1:A:340:ILE:CG2  | 1.76                     | 1.15              |
| 1:A:542:PHE:HA   | 4:8:143:TYR:CE1  | 1.82                     | 1.15              |
| 1:A:836:PHE:CE2  | 2:B:160:GLY:HA3  | 1.80                     | 1.15              |
| 1:D:215:GLN:HA   | 1:D:340:ILE:CG2  | 1.76                     | 1.15              |
| 1:D:542:PHE:HA   | 4:9:143:TYR:CE1  | 1.82                     | 1.15              |
| 1:D:642:LYS:CG   | 4:9:23:GLY:N     | 2.08                     | 1.15              |
| 1:D:721:LYS:HA   | 1:D:736:GLN:NE2  | 1.58                     | 1.15              |
| 1:J:510:TRP:CZ2  | 1:J:768:MLY:HH11 | 1.81                     | 1.15              |
| 1:J:542:PHE:HA   | 4:W:143:TYR:CE1  | 1.82                     | 1.15              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:642:LYS:CG   | 4:W:23:GLY:N     | 2.08                     | 1.15              |
| 1:J:721:LYS:HA   | 1:J:736:GLN:NE2  | 1.58                     | 1.15              |
| 4:1:203:THR:CG2  | 4:Z:287:ILE:HB   | 1.77                     | 1.15              |
| 4:3:322:PRO:HB3  | 4:5:244:ASP:CG   | 1.72                     | 1.15              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CD   | 2.18                     | 1.15              |
| 1:A:642:LYS:CG   | 4:8:23:GLY:N     | 2.09                     | 1.15              |
| 1:A:819:ASN:CG   | 2:B:91:ALA:HA    | 1.66                     | 1.15              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:HB3  | 1.77                     | 1.15              |
| 1:J:768:MLY:NZ   | 1:J:772:LEU:HD22 | 1.61                     | 1.15              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:HG13 | 1.60                     | 1.15              |
| 4:X:325:MET:SD   | 4:Z:244:ASP:OD2  | 2.04                     | 1.15              |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:HG22 | 1.21                     | 1.14              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:HB3  | 1.75                     | 1.14              |
| 1:D:639:GLY:CA   | 4:9:345:ILE:HA   | 1.73                     | 1.14              |
| 1:D:640:LYS:HB3  | 1:D:645:SER:OG   | 1.46                     | 1.14              |
| 1:D:839:MLY:HH13 | 2:E:159:HIS:CD2  | 1.79                     | 1.14              |
| 1:G:639:GLY:HA3  | 4:V:344:SER:O    | 1.46                     | 1.14              |
| 1:G:639:GLY:HA2  | 4:V:345:ILE:HA   | 1.26                     | 1.14              |
| 1:J:649:VAL:HA   | 1:J:649:VAL:CG2  | 1.76                     | 1.14              |
| 1:J:749:GLY:O    | 3:L:114:LEU:HD21 | 1.45                     | 1.14              |
| 4:7:287:ILE:HG21 | 4:9:205:GLU:HG2  | 1.17                     | 1.14              |
| 1:A:721:LYS:HA   | 1:A:736:GLN:CD   | 1.73                     | 1.14              |
| 2:E:111:SER:CA   | 2:E:148:VAL:O    | 1.95                     | 1.14              |
| 2:E:121:LEU:C    | 2:E:128:PHE:HB2  | 1.67                     | 1.14              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:HB3  | 1.77                     | 1.14              |
| 1:G:542:PHE:HA   | 4:V:143:TYR:CE1  | 1.82                     | 1.14              |
| 1:G:649:VAL:HA   | 1:G:649:VAL:CG2  | 1.76                     | 1.14              |
| 1:J:639:GLY:HA3  | 4:W:344:SER:O    | 1.46                     | 1.14              |
| 1:J:739:ASP:HB3  | 1:J:742:LYS:HB3  | 1.21                     | 1.14              |
| 1:A:640:LYS:HB3  | 1:A:645:SER:OG   | 1.46                     | 1.14              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:HB3  | 1.77                     | 1.14              |
| 1:D:201:ALA:O    | 1:D:202:SER:HB3  | 1.35                     | 1.14              |
| 1:D:507:GLY:O    | 1:D:761:GLY:CA   | 1.96                     | 1.14              |
| 1:D:641:LYS:NZ   | 4:9:348:SER:O    | 1.80                     | 1.14              |
| 1:D:829:TRP:NE1  | 2:E:67:MET:HG2   | 1.59                     | 1.14              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:CG    | 2.25                     | 1.14              |
| 1:G:641:LYS:CE   | 4:V:348:SER:O    | 1.93                     | 1.14              |
| 1:J:721:LYS:HA   | 1:J:736:GLN:CD   | 1.73                     | 1.14              |
| 1:J:757:GLN:HG2  | 1:J:776:GLU:CG   | 1.76                     | 1.14              |
| 2:K:111:SER:CA   | 2:K:148:VAL:O    | 1.95                     | 1.14              |
| 1:A:649:VAL:HA   | 1:A:649:VAL:CG2  | 1.76                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:831:TRP:NE1  | 2:B:51:PHE:HZ    | 1.30                     | 1.14              |
| 1:D:635:GLY:HA2  | 4:9:334:GLU:HG2  | 1.16                     | 1.14              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:HB3  | 1.83                     | 1.14              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:OD1  | 1.32                     | 1.14              |
| 2:H:121:LEU:C    | 2:H:128:PHE:HB2  | 1.67                     | 1.14              |
| 1:J:757:GLN:CG   | 1:J:776:GLU:CG   | 2.23                     | 1.14              |
| 2:K:112:ILE:O    | 2:K:147:ASN:O    | 1.65                     | 1.14              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:HB3  | 1.77                     | 1.14              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:ND1  | 1.62                     | 1.14              |
| 2:B:111:SER:CA   | 2:B:148:VAL:O    | 1.95                     | 1.14              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:OD1  | 1.32                     | 1.14              |
| 1:D:726:VAL:HG23 | 1:D:782:MLY:HH22 | 1.16                     | 1.14              |
| 1:D:736:GLN:N    | 1:D:743:ALA:CB   | 2.05                     | 1.14              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:CB   | 1.96                     | 1.14              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:HG2   | 1.63                     | 1.14              |
| 1:J:510:TRP:CZ3  | 1:J:768:MLY:HH11 | 1.81                     | 1.14              |
| 1:J:797:PHE:HD1  | 3:L:149:VAL:CG1  | 1.59                     | 1.14              |
| 4:9:287:ILE:HG21 | 4:W:205:GLU:HG2  | 1.17                     | 1.14              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:CB   | 2.34                     | 1.14              |
| 1:D:831:TRP:CZ3  | 2:E:34:ILE:CG2   | 2.31                     | 1.13              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:OD1  | 1.32                     | 1.13              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:CG   | 1.70                     | 1.13              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:OE1  | 1.97                     | 1.13              |
| 2:B:111:SER:CB   | 2:B:148:VAL:C    | 1.93                     | 1.13              |
| 1:D:639:GLY:HA3  | 4:9:344:SER:O    | 1.46                     | 1.13              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:HG3  | 1.20                     | 1.13              |
| 1:D:721:LYS:HA   | 1:D:736:GLN:CD   | 1.73                     | 1.13              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:C    | 1.70                     | 1.13              |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HG13 | 1.21                     | 1.13              |
| 2:K:121:LEU:C    | 2:K:128:PHE:HB3  | 1.71                     | 1.13              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:CB   | 1.96                     | 1.13              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:CZ   | 1.78                     | 1.13              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:CB   | 1.96                     | 1.13              |
| 1:D:726:VAL:CB   | 1:D:782:MLY:HH13 | 1.77                     | 1.13              |
| 1:D:739:ASP:HB3  | 1:D:742:LYS:HB3  | 1.21                     | 1.13              |
| 2:H:112:ILE:O    | 2:H:147:ASN:O    | 1.65                     | 1.13              |
| 1:J:538:GLU:OE2  | 4:W:355:MET:HE1  | 1.44                     | 1.13              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:CB   | 1.96                     | 1.13              |
| 4:0:243:PRO:HB3  | 4:Y:291:LYS:HE3  | 1.15                     | 1.13              |
| 1:A:149:GLN:CG   | 1:A:719:ASP:OD1  | 1.97                     | 1.13              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:OE1  | 1.97                     | 1.13              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:800:ARG:NH1  | 3:C:149:VAL:HG13 | 1.61                     | 1.13              |
| 1:A:839:MLY:HH21 | 2:B:158:THR:HG22 | 1.30                     | 1.12              |
| 1:D:201:ALA:O    | 1:D:202:SER:CB   | 1.92                     | 1.13              |
| 1:G:93:MET:SD    | 1:G:716:LEU:CD1  | 2.37                     | 1.12              |
| 1:G:639:GLY:CA   | 4:V:345:ILE:HA   | 1.73                     | 1.13              |
| 1:G:641:LYS:NZ   | 4:V:348:SER:O    | 1.80                     | 1.12              |
| 1:J:557:GLU:HA   | 4:Y:47:MET:CA    | 1.47                     | 1.12              |
| 1:A:641:LYS:NZ   | 4:8:348:SER:O    | 1.79                     | 1.12              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:HD13 | 1.32                     | 1.12              |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:HB3  | 1.00                     | 1.12              |
| 1:A:814:PHE:CD1  | 2:B:127:ARG:NH2  | 2.15                     | 1.12              |
| 2:B:121:LEU:C    | 2:B:128:PHE:HB3  | 1.72                     | 1.12              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:OE1  | 1.97                     | 1.12              |
| 2:E:121:LEU:C    | 2:E:128:PHE:HB3  | 1.72                     | 1.12              |
| 1:G:84:MLY:HH11  | 1:G:715:VAL:CG1  | 1.77                     | 1.12              |
| 1:A:201:ALA:O    | 1:A:202:SER:CB   | 1.92                     | 1.12              |
| 2:B:112:ILE:O    | 2:B:147:ASN:O    | 1.65                     | 1.12              |
| 1:D:538:GLU:O    | 4:9:349:LEU:HD11 | 1.35                     | 1.12              |
| 1:G:557:GLU:CA   | 4:X:48:GLY:N     | 1.99                     | 1.12              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:OE1  | 1.97                     | 1.12              |
| 1:G:721:LYS:HA   | 1:G:736:GLN:CD   | 1.73                     | 1.12              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:CD   | 1.70                     | 1.12              |
| 2:K:111:SER:HB3  | 2:K:148:VAL:O    | 1.50                     | 1.12              |
| 2:B:121:LEU:O    | 2:B:128:PHE:HB2  | 0.94                     | 1.12              |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:HD21 | 1.27                     | 1.12              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:CB   | 2.33                     | 1.12              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:HH12 | 1.12                     | 1.12              |
| 1:D:799:MET:SD   | 3:F:32:ASP:CA    | 2.37                     | 1.12              |
| 2:E:112:ILE:O    | 2:E:147:ASN:O    | 1.65                     | 1.12              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:CD2  | 1.80                     | 1.12              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:CE1   | 2.30                     | 1.12              |
| 4:1:287:ILE:HG23 | 4:3:202:THR:OG1  | 1.48                     | 1.12              |
| 4:X:324:THR:CG2  | 4:Z:247:VAL:CG2  | 2.26                     | 1.12              |
| 1:J:641:LYS:NZ   | 4:W:348:SER:O    | 1.80                     | 1.11              |
| 2:K:111:SER:CB   | 2:K:148:VAL:C    | 1.93                     | 1.11              |
| 1:D:735:GLY:O    | 1:D:743:ALA:CB   | 1.91                     | 1.11              |
| 1:D:822:SER:CB   | 2:E:88:LEU:HD23  | 1.80                     | 1.11              |
| 1:G:538:GLU:C    | 4:V:349:LEU:HD11 | 1.54                     | 1.11              |
| 1:G:649:VAL:O    | 1:G:649:VAL:HG12 | 0.94                     | 1.11              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD21 | 1.29                     | 1.11              |
| 3:C:24:LYS:CB    | 3:C:63:ILE:O     | 1.99                     | 1.11              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:768:MLY:HD3  | 1:G:772:LEU:HD22 | 1.20                     | 1.11              |
| 1:J:795:ARG:NH2  | 3:L:116:GLU:OE2  | 1.83                     | 1.11              |
| 1:J:829:TRP:CH2  | 2:K:84:PHE:CZ    | 2.39                     | 1.11              |
| 1:J:831:TRP:HZ2  | 2:K:47:LEU:HD22  | 1.08                     | 1.11              |
| 3:L:24:LYS:CB    | 3:L:63:ILE:O     | 1.99                     | 1.11              |
| 4:O:244:ASP:N    | 4:Y:291:LYS:HD2  | 1.66                     | 1.11              |
| 4:9:290:ARG:CZ   | 4:W:202:THR:HG21 | 1.81                     | 1.11              |
| 1:A:623:PHE:CB   | 1:A:623:PHE:CG   | 2.33                     | 1.11              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:NH1  | 1.64                     | 1.11              |
| 1:D:623:PHE:CB   | 1:D:623:PHE:CG   | 2.33                     | 1.11              |
| 1:G:798:LEU:HD13 | 3:I:126:LEU:CD2  | 1.68                     | 1.11              |
| 1:J:92:ALA:O     | 1:J:714:ARG:HD2  | 1.50                     | 1.11              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:CG   | 2.14                     | 1.11              |
| 4:1:202:THR:CA   | 4:Z:287:ILE:HG12 | 1.81                     | 1.11              |
| 1:A:649:VAL:O    | 1:A:649:VAL:HG12 | 0.94                     | 1.11              |
| 1:A:800:ARG:NH1  | 3:C:149:VAL:C    | 2.08                     | 1.11              |
| 1:D:530:MET:CE   | 4:9:354:GLN:HG2  | 1.80                     | 1.11              |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:CD   | 1.58                     | 1.11              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:CG   | 2.16                     | 1.11              |
| 1:J:800:ARG:NE   | 3:L:149:VAL:HG22 | 1.64                     | 1.11              |
| 1:G:557:GLU:HB3  | 4:X:46:GLY:C     | 1.76                     | 1.10              |
| 1:G:623:PHE:CB   | 1:G:623:PHE:CG   | 2.33                     | 1.10              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:HG3  | 1.21                     | 1.10              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:CA   | 1.98                     | 1.10              |
| 1:J:798:LEU:HD22 | 3:L:126:LEU:CD1  | 1.80                     | 1.10              |
| 4:2:322:PRO:HB3  | 4:4:244:ASP:CG   | 1.75                     | 1.10              |
| 2:E:121:LEU:O    | 2:E:128:PHE:HB2  | 0.94                     | 1.10              |
| 1:G:791:GLN:OE1  | 3:I:116:GLU:HB2  | 1.51                     | 1.10              |
| 1:J:530:MET:CE   | 4:W:354:GLN:HG2  | 1.80                     | 1.10              |
| 1:J:538:GLU:O    | 4:W:349:LEU:HD11 | 1.35                     | 1.10              |
| 1:A:799:MET:SD   | 3:C:32:ASP:CB    | 2.37                     | 1.10              |
| 1:A:822:SER:OG   | 2:B:88:LEU:CD2   | 2.00                     | 1.10              |
| 1:D:649:VAL:HG22 | 1:D:649:VAL:HG13 | 1.21                     | 1.10              |
| 1:A:202:SER:CA   | 1:A:207:LYS:HE2  | 1.82                     | 1.10              |
| 2:H:121:LEU:O    | 2:H:128:PHE:HB2  | 0.94                     | 1.10              |
| 1:J:218:LEU:HB2  | 1:J:221:GLN:HG3  | 1.17                     | 1.10              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CD   | 1.77                     | 1.10              |
| 1:J:797:PHE:CD1  | 3:L:149:VAL:CG1  | 2.34                     | 1.10              |
| 4:7:290:ARG:CZ   | 4:9:202:THR:HG21 | 1.81                     | 1.10              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:OE1  | 1.50                     | 1.10              |
| 1:A:739:ASP:HB3  | 1:A:742:LYS:HB3  | 1.21                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:734:GLU:O    | 1:D:738:MET:HG2  | 1.51                     | 1.10              |
| 1:G:93:MET:HE3   | 1:G:763:THR:HB   | 1.31                     | 1.10              |
| 1:G:202:SER:CA   | 1:G:207:LYS:HE2  | 1.82                     | 1.10              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:OE1  | 1.50                     | 1.10              |
| 4:2:288:ASP:H    | 4:4:203:THR:HG22 | 1.17                     | 1.10              |
| 1:A:218:LEU:HB2  | 1:A:221:GLN:HG3  | 1.17                     | 1.09              |
| 1:A:530:MET:CE   | 4:8:354:GLN:HG2  | 1.80                     | 1.09              |
| 1:D:817:GLN:HE21 | 2:E:127:ARG:HG2  | 1.12                     | 1.09              |
| 1:D:831:TRP:CH2  | 2:E:34:ILE:HG23  | 1.86                     | 1.09              |
| 1:G:707:CYS:CB   | 1:G:714:ARG:HH12 | 1.64                     | 1.09              |
| 3:I:24:LYS:CB    | 3:I:63:ILE:O     | 1.99                     | 1.09              |
| 1:J:538:GLU:CD   | 4:W:355:MET:HE1  | 1.77                     | 1.09              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:CA   | 2.30                     | 1.09              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:CD1  | 1.54                     | 1.09              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CD   | 1.77                     | 1.09              |
| 1:D:538:GLU:CD   | 4:9:355:MET:HE1  | 1.77                     | 1.09              |
| 1:D:639:GLY:HA2  | 4:9:345:ILE:HA   | 1.26                     | 1.09              |
| 3:F:24:LYS:CB    | 3:F:63:ILE:O     | 1.99                     | 1.09              |
| 1:G:530:MET:CE   | 4:V:354:GLN:HG2  | 1.80                     | 1.09              |
| 1:J:84:MLY:HH11  | 1:J:715:VAL:CG1  | 1.70                     | 1.09              |
| 1:J:571:ALA:O    | 1:J:572:LYS:HG3  | 1.52                     | 1.09              |
| 4:8:290:ARG:CZ   | 4:V:202:THR:HG21 | 1.81                     | 1.09              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:C    | 1.60                     | 1.09              |
| 1:D:218:LEU:HB2  | 1:D:221:GLN:HG3  | 1.17                     | 1.09              |
| 1:D:571:ALA:O    | 1:D:572:LYS:HG3  | 1.52                     | 1.09              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CD   | 1.77                     | 1.09              |
| 1:D:768:MLY:O    | 1:D:771:LEU:HD11 | 1.27                     | 1.09              |
| 1:J:201:ALA:O    | 1:J:202:SER:HB3  | 1.35                     | 1.09              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:HG3  | 1.21                     | 1.09              |
| 1:J:649:VAL:O    | 1:J:649:VAL:HG12 | 0.94                     | 1.09              |
| 1:J:734:GLU:O    | 1:J:738:MET:HG2  | 1.51                     | 1.09              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:CG   | 1.97                     | 1.09              |
| 1:D:202:SER:CA   | 1:D:207:LYS:HE2  | 1.82                     | 1.09              |
| 1:D:649:VAL:O    | 1:D:649:VAL:HG12 | 0.94                     | 1.09              |
| 1:D:809:ARG:NH1  | 2:E:124:GLY:HA2  | 1.68                     | 1.09              |
| 1:G:84:MLY:HH12  | 1:G:715:VAL:HG13 | 1.33                     | 1.09              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CD   | 1.77                     | 1.09              |
| 1:J:93:MET:O     | 1:J:714:ARG:O    | 1.71                     | 1.09              |
| 2:K:121:LEU:O    | 2:K:128:PHE:HB2  | 0.93                     | 1.09              |
| 4:2:324:THR:CB   | 4:4:243:PRO:O    | 2.01                     | 1.09              |
| 1:A:734:GLU:O    | 1:A:738:MET:HG2  | 1.51                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:641:LYS:HE3  | 1:D:647:GLN:OE1  | 1.50                     | 1.09              |
| 1:G:218:LEU:HB2  | 1:G:221:GLN:HG3  | 1.17                     | 1.09              |
| 1:G:557:GLU:CB   | 4:X:46:GLY:C     | 2.26                     | 1.09              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:HG2   | 0.92                     | 1.09              |
| 2:H:111:SER:OG   | 2:H:148:VAL:O    | 1.71                     | 1.09              |
| 1:J:643:GLY:O    | 1:J:644:SER:OG   | 1.70                     | 1.09              |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:HG13 | 1.21                     | 1.09              |
| 4:2:290:ARG:CZ   | 4:4:202:THR:CG2  | 2.20                     | 1.09              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:HG2  | 1.25                     | 1.08              |
| 1:G:84:MLY:HH13  | 1:G:715:VAL:HG13 | 1.18                     | 1.08              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:CD1  | 1.55                     | 1.08              |
| 2:K:111:SER:OG   | 2:K:148:VAL:O    | 1.71                     | 1.08              |
| 1:D:800:ARG:CB   | 3:F:149:VAL:HG22 | 1.83                     | 1.08              |
| 1:G:538:GLU:CD   | 4:V:355:MET:HE1  | 1.77                     | 1.08              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:CG    | 2.13                     | 1.08              |
| 1:J:567:LYS:NZ   | 4:Y:92:ASN:HD22  | 1.50                     | 1.08              |
| 1:J:639:GLY:HA3  | 4:W:344:SER:C    | 1.78                     | 1.08              |
| 1:J:639:GLY:CA   | 4:W:345:ILE:HA   | 1.73                     | 1.08              |
| 1:A:635:GLY:HA2  | 4:8:334:GLU:HG2  | 1.16                     | 1.08              |
| 1:A:639:GLY:HA2  | 4:8:345:ILE:HA   | 1.26                     | 1.08              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:HD21 | 1.08                     | 1.08              |
| 1:G:553:MLY:HE2  | 4:X:45:VAL:HB    | 1.09                     | 1.08              |
| 1:G:734:GLU:O    | 1:G:738:MET:HG2  | 1.51                     | 1.08              |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:CG   | 1.63                     | 1.08              |
| 1:J:202:SER:CA   | 1:J:207:LYS:HE2  | 1.82                     | 1.08              |
| 1:J:797:PHE:CD1  | 3:L:149:VAL:HG11 | 1.88                     | 1.08              |
| 1:J:831:TRP:CZ2  | 2:K:47:LEU:HD22  | 1.87                     | 1.08              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:HB   | 1.10                     | 1.08              |
| 4:8:287:ILE:HG21 | 4:V:205:GLU:HG2  | 1.17                     | 1.08              |
| 1:A:538:GLU:CD   | 4:8:355:MET:HE1  | 1.78                     | 1.08              |
| 2:E:111:SER:HB3  | 2:E:148:VAL:O    | 1.50                     | 1.08              |
| 1:G:93:MET:CE    | 1:G:763:THR:CG2  | 2.23                     | 1.08              |
| 1:G:639:GLY:HA3  | 4:V:344:SER:C    | 1.78                     | 1.08              |
| 1:J:639:GLY:HA2  | 4:W:345:ILE:HA   | 1.26                     | 1.08              |
| 1:A:639:GLY:HA3  | 4:8:344:SER:C    | 1.78                     | 1.08              |
| 2:B:111:SER:CB   | 2:B:148:VAL:O    | 0.78                     | 1.08              |
| 1:D:834:LEU:CG   | 2:E:54:MET:CG    | 2.32                     | 1.08              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:HG3   | 1.82                     | 1.08              |
| 2:E:111:SER:OG   | 2:E:148:VAL:O    | 1.71                     | 1.08              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:OE1  | 1.50                     | 1.08              |
| 1:G:643:GLY:O    | 1:G:644:SER:OG   | 1.69                     | 1.08              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:730:SER:OG   | 3:I:109:HIS:CG   | 2.07                     | 1.08              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB3  | 1.35                     | 1.08              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD2  | 1.79                     | 1.07              |
| 1:D:638:GLY:CA   | 4:9:341:ILE:O    | 2.01                     | 1.07              |
| 1:D:643:GLY:O    | 1:D:644:SER:OG   | 1.69                     | 1.07              |
| 2:E:111:SER:CB   | 2:E:148:VAL:O    | 0.78                     | 1.07              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:HG2  | 1.25                     | 1.07              |
| 2:H:111:SER:CB   | 2:H:148:VAL:O    | 0.78                     | 1.07              |
| 1:J:768:MLY:HD3  | 1:J:772:LEU:HB3  | 1.31                     | 1.07              |
| 4:3:3:ASP:HA     | 4:3:6:THR:HB     | 1.36                     | 1.07              |
| 1:D:529:PRO:HB3  | 4:9:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:C    | 1.78                     | 1.07              |
| 1:J:95:THR:OG1   | 1:J:713:SER:HB3  | 1.51                     | 1.07              |
| 1:A:409:GLY:N    | 1:A:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:A:641:LYS:HB2  | 1:A:647:GLN:NE2  | 1.68                     | 1.07              |
| 1:D:409:GLY:N    | 1:D:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:D:541:MET:SD   | 4:9:345:ILE:O    | 2.12                     | 1.07              |
| 1:D:829:TRP:HE1  | 2:E:67:MET:HG2   | 0.91                     | 1.07              |
| 1:G:72:VAL:HG13  | 1:G:76:GLN:HB3   | 1.36                     | 1.07              |
| 1:G:529:PRO:C    | 4:V:354:GLN:HB3  | 1.79                     | 1.07              |
| 1:G:529:PRO:HB3  | 4:V:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:CG   | 2.16                     | 1.07              |
| 1:G:641:LYS:HB2  | 1:G:647:GLN:NE2  | 1.68                     | 1.07              |
| 1:J:529:PRO:HB3  | 4:W:353:GLN:OE1  | 1.53                     | 1.07              |
| 2:K:111:SER:CB   | 2:K:148:VAL:O    | 0.78                     | 1.07              |
| 4:0:246:GLN:HA   | 4:Y:324:THR:CB   | 1.83                     | 1.07              |
| 4:3:288:ASP:CG   | 4:5:203:THR:HG21 | 1.63                     | 1.07              |
| 1:A:501:GLU:O    | 1:A:762:HIS:NE2  | 1.87                     | 1.07              |
| 1:A:529:PRO:HB3  | 4:8:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:G:553:MLY:CE   | 4:X:45:VAL:HG12  | 1.68                     | 1.07              |
| 1:G:638:GLY:CA   | 4:V:341:ILE:O    | 2.02                     | 1.07              |
| 1:J:510:TRP:CZ3  | 1:J:768:MLY:CH1  | 2.38                     | 1.07              |
| 1:J:529:PRO:C    | 4:W:354:GLN:HB3  | 1.77                     | 1.07              |
| 1:J:541:MET:SD   | 4:W:345:ILE:O    | 2.13                     | 1.07              |
| 1:J:638:GLY:CA   | 4:W:341:ILE:O    | 2.01                     | 1.07              |
| 1:J:793:ARG:HE   | 3:L:147:MET:HA   | 0.93                     | 1.07              |
| 4:5:3:ASP:HA     | 4:5:6:THR:HB     | 1.36                     | 1.07              |
| 4:X:3:ASP:HA     | 4:X:6:THR:HB     | 1.36                     | 1.07              |
| 4:X:324:THR:CG2  | 4:Z:247:VAL:HG22 | 1.82                     | 1.07              |
| 1:A:638:GLY:CA   | 4:8:341:ILE:O    | 2.01                     | 1.07              |
| 1:A:839:MLY:HD2  | 2:B:159:HIS:CG   | 1.88                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:639:GLY:HA3  | 4:9:344:SER:C    | 1.78                     | 1.07              |
| 1:G:409:GLY:N    | 1:G:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:G:797:PHE:CD1  | 3:I:149:VAL:CG1  | 2.04                     | 1.07              |
| 1:J:409:GLY:N    | 1:J:636:LYS:HG3  | 1.69                     | 1.07              |
| 4:1:203:THR:HB   | 4:Z:287:ILE:HD13 | 1.08                     | 1.07              |
| 1:A:541:MET:SD   | 4:8:345:ILE:O    | 2.12                     | 1.06              |
| 1:G:635:GLY:HA2  | 4:V:334:GLU:HG2  | 1.16                     | 1.06              |
| 1:J:84:MLY:HH13  | 1:J:715:VAL:HG13 | 1.30                     | 1.06              |
| 1:J:768:MLY:HH22 | 1:J:772:LEU:HB2  | 1.37                     | 1.06              |
| 1:J:819:ASN:CA   | 2:K:90:GLY:O     | 2.02                     | 1.06              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:HG23 | 1.41                     | 1.06              |
| 1:A:502:GLU:HG3  | 1:A:761:GLY:HA3  | 1.34                     | 1.06              |
| 1:A:571:ALA:O    | 1:A:572:LYS:HG3  | 1.52                     | 1.06              |
| 1:A:643:GLY:O    | 1:A:644:SER:OG   | 1.69                     | 1.06              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:HD13 | 1.31                     | 1.06              |
| 1:D:829:TRP:HE1  | 2:E:67:MET:CG    | 1.66                     | 1.06              |
| 1:D:831:TRP:CD1  | 2:E:67:MET:SD    | 2.48                     | 1.06              |
| 1:G:541:MET:SD   | 4:V:345:ILE:O    | 2.13                     | 1.06              |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:HG11  | 1.37                     | 1.06              |
| 4:1:287:ILE:HB   | 4:3:203:THR:HG22 | 1.32                     | 1.06              |
| 1:D:576:GLU:HG2  | 1:D:577:ALA:N    | 1.66                     | 1.06              |
| 1:G:537:GLU:C    | 4:V:349:LEU:CD1  | 2.21                     | 1.06              |
| 1:J:793:ARG:NE   | 3:L:147:MET:HA   | 1.70                     | 1.06              |
| 2:K:114:LYS:HA   | 2:K:146:GLY:O    | 0.89                     | 1.06              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:OG1  | 2.03                     | 1.06              |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:N    | 1.69                     | 1.06              |
| 1:A:72:VAL:HG13  | 1:A:76:GLN:HB3   | 1.36                     | 1.06              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:CD   | 1.70                     | 1.06              |
| 1:D:542:PHE:CG   | 4:9:143:TYR:HE1  | 1.73                     | 1.06              |
| 2:E:114:LYS:HA   | 2:E:146:GLY:O    | 0.89                     | 1.06              |
| 2:H:111:SER:HB3  | 2:H:148:VAL:O    | 1.49                     | 1.06              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:CD2  | 2.11                     | 1.06              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:HA2  | 1.86                     | 1.06              |
| 1:J:795:ARG:HD3  | 3:L:35:ARG:HH22  | 1.13                     | 1.06              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:HB3  | 1.35                     | 1.06              |
| 1:A:797:PHE:CD1  | 3:C:149:VAL:CG1  | 2.32                     | 1.06              |
| 1:A:819:ASN:OD1  | 2:B:91:ALA:HA    | 0.88                     | 1.06              |
| 2:B:111:SER:OG   | 2:B:148:VAL:O    | 1.71                     | 1.06              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:HB3  | 1.35                     | 1.06              |
| 1:G:571:ALA:O    | 1:G:572:LYS:HG3  | 1.52                     | 1.06              |
| 1:G:831:TRP:HH2  | 2:H:47:LEU:HD21  | 1.14                     | 1.06              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:795:ARG:HE  | 3:L:118:MET:HE1  | 0.92                     | 1.06              |
| 1:A:795:ARG:CD  | 3:C:35:ARG:HH22  | 1.68                     | 1.05              |
| 2:B:114:LYS:HA  | 2:B:146:GLY:O    | 0.89                     | 1.05              |
| 1:D:641:LYS:HE3 | 4:9:348:SER:O    | 1.56                     | 1.05              |
| 1:D:641:LYS:HB2 | 1:D:647:GLN:NE2  | 1.68                     | 1.05              |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:CB    | 2.27                     | 1.05              |
| 2:E:140:PHE:O   | 2:E:141:PRO:O    | 1.74                     | 1.05              |
| 1:G:635:GLY:HA3 | 4:V:341:ILE:HD13 | 1.36                     | 1.05              |
| 1:J:530:MET:CA  | 4:W:354:GLN:HG3  | 1.86                     | 1.05              |
| 1:J:800:ARG:CZ  | 3:L:149:VAL:HG22 | 1.85                     | 1.05              |
| 2:K:140:PHE:O   | 2:K:141:PRO:O    | 1.75                     | 1.05              |
| 1:A:721:LYS:HG3 | 1:A:736:GLN:HG2  | 1.25                     | 1.05              |
| 1:G:641:LYS:HD2 | 1:G:647:GLN:CD   | 1.69                     | 1.05              |
| 1:J:638:GLY:HA2 | 4:W:341:ILE:O    | 1.57                     | 1.05              |
| 1:J:757:GLN:OE1 | 1:J:772:LEU:C    | 1.99                     | 1.05              |
| 4:2:322:PRO:HB2 | 4:4:244:ASP:CB   | 1.85                     | 1.05              |
| 1:A:505:MLY:CB  | 1:A:762:HIS:H    | 1.67                     | 1.05              |
| 1:A:530:MET:CA  | 4:8:354:GLN:HG3  | 1.86                     | 1.05              |
| 1:A:542:PHE:CG  | 4:8:143:TYR:HE1  | 1.73                     | 1.05              |
| 1:D:72:VAL:HG13 | 1:D:76:GLN:HB3   | 1.36                     | 1.05              |
| 1:D:830:PRO:CB  | 2:E:67:MET:HE1   | 1.85                     | 1.05              |
| 1:G:819:ASN:HA  | 2:H:90:GLY:O     | 0.88                     | 1.05              |
| 1:G:829:TRP:CH2 | 2:H:87:LYS:HE2   | 1.90                     | 1.05              |
| 1:J:641:LYS:HB2 | 1:J:647:GLN:NE2  | 1.68                     | 1.05              |
| 1:J:795:ARG:NH1 | 3:L:35:ARG:HH12  | 1.55                     | 1.05              |
| 4:1:3:ASP:HA    | 4:1:6:THR:HB     | 1.36                     | 1.05              |
| 4:W:325:MET:CE  | 4:Y:244:ASP:OD2  | 2.04                     | 1.05              |
| 1:A:529:PRO:C   | 4:8:354:GLN:HB3  | 1.78                     | 1.05              |
| 1:G:542:PHE:CG  | 4:V:143:TYR:HE1  | 1.74                     | 1.05              |
| 1:G:817:GLN:HB3 | 2:H:127:ARG:CD   | 1.86                     | 1.05              |
| 1:J:72:VAL:HG13 | 1:J:76:GLN:HB3   | 1.36                     | 1.05              |
| 1:J:534:SER:C   | 4:W:351:THR:HA   | 1.81                     | 1.05              |
| 1:J:641:LYS:HE3 | 4:W:348:SER:O    | 1.55                     | 1.05              |
| 1:D:529:PRO:C   | 4:9:354:GLN:HB3  | 1.77                     | 1.05              |
| 1:D:530:MET:HE2 | 4:9:354:GLN:HG2  | 1.06                     | 1.05              |
| 1:A:635:GLY:HA3 | 4:8:341:ILE:HD13 | 1.37                     | 1.04              |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:HB3  | 1.69                     | 1.04              |
| 1:D:530:MET:CA  | 4:9:354:GLN:HG3  | 1.87                     | 1.04              |
| 1:G:534:SER:C   | 4:V:351:THR:HA   | 1.82                     | 1.04              |
| 1:G:553:MLY:CE  | 4:X:45:VAL:HG11  | 1.53                     | 1.04              |
| 1:J:576:GLU:HG2 | 1:J:577:ALA:N    | 1.66                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:599:ASN:HA   | 1:A:649:VAL:HB   | 1.05                     | 1.04              |
| 1:A:793:ARG:NE   | 3:C:147:MET:HG2  | 1.71                     | 1.04              |
| 1:A:836:PHE:CE2  | 2:B:160:GLY:CA   | 2.38                     | 1.04              |
| 3:C:49:ILE:CA    | 3:C:52:ASN:HD22  | 1.70                     | 1.04              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:CG   | 1.93                     | 1.04              |
| 1:D:638:GLY:HA2  | 4:9:341:ILE:O    | 1.57                     | 1.04              |
| 2:H:114:LYS:HA   | 2:H:146:GLY:O    | 0.88                     | 1.04              |
| 1:J:542:PHE:CG   | 4:W:143:TYR:HE1  | 1.73                     | 1.04              |
| 1:J:736:GLN:N    | 1:J:743:ALA:CB   | 2.05                     | 1.04              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:NH1   | 1.72                     | 1.04              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:HH12  | 0.89                     | 1.04              |
| 2:B:111:SER:HB3  | 2:B:148:VAL:O    | 1.49                     | 1.04              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:CG   | 2.03                     | 1.04              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:HG21 | 1.36                     | 1.04              |
| 4:Z:3:ASP:HA     | 4:Z:6:THR:HB     | 1.36                     | 1.04              |
| 1:A:534:SER:C    | 4:8:351:THR:HA   | 1.81                     | 1.04              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:C    | 1.82                     | 1.04              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:HG22 | 1.84                     | 1.04              |
| 1:D:534:SER:C    | 4:9:351:THR:HA   | 1.81                     | 1.04              |
| 1:G:552:ASN:O    | 4:X:47:MET:CE    | 2.04                     | 1.04              |
| 1:J:797:PHE:HD1  | 3:L:149:VAL:HG12 | 1.21                     | 1.04              |
| 1:D:202:SER:CA   | 1:D:207:LYS:CE   | 2.36                     | 1.04              |
| 1:D:830:PRO:HD2  | 2:E:67:MET:HE2   | 1.35                     | 1.04              |
| 1:G:93:MET:O     | 1:G:714:ARG:O    | 1.76                     | 1.04              |
| 1:G:530:MET:HE2  | 4:V:354:GLN:HG2  | 1.06                     | 1.04              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:N    | 1.91                     | 1.04              |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CB   | 1.71                     | 1.03              |
| 1:G:639:GLY:N    | 4:V:345:ILE:N    | 1.94                     | 1.03              |
| 1:G:789:ALA:CB   | 3:I:81:GLN:HE21  | 1.69                     | 1.03              |
| 1:J:56:GLU:HB2   | 1:J:59:MLY:HB3   | 1.40                     | 1.03              |
| 4:0:287:ILE:HB   | 4:2:203:THR:HG22 | 1.08                     | 1.03              |
| 4:8:3:ASP:HA     | 4:8:6:THR:HB     | 1.36                     | 1.03              |
| 1:A:834:LEU:CD1  | 2:B:54:MET:HG3   | 1.86                     | 1.03              |
| 1:G:56:GLU:HB2   | 1:G:59:MLY:HB3   | 1.40                     | 1.03              |
| 1:G:599:ASN:HA   | 1:G:649:VAL:HB   | 1.05                     | 1.03              |
| 1:G:769:ALA:HB1  | 1:G:770:GLY:HA2  | 1.38                     | 1.03              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:HD2  | 1.88                     | 1.03              |
| 3:L:49:ILE:CA    | 3:L:52:ASN:HD22  | 1.71                     | 1.03              |
| 4:1:203:THR:HG22 | 4:Z:287:ILE:CB   | 1.87                     | 1.03              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:HB3   | 1.31                     | 1.03              |
| 1:A:836:PHE:HB3  | 2:B:161:GLU:CD   | 1.83                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:112:ILE:O    | 2:B:147:ASN:C    | 2.01                     | 1.03              |
| 2:B:140:PHE:O    | 2:B:141:PRO:O    | 1.74                     | 1.03              |
| 2:E:112:ILE:O    | 2:E:147:ASN:C    | 2.01                     | 1.03              |
| 3:F:49:ILE:CA    | 3:F:52:ASN:HD22  | 1.70                     | 1.03              |
| 1:G:93:MET:HE1   | 1:G:763:THR:HG22 | 1.40                     | 1.03              |
| 1:G:836:PHE:CE2  | 2:H:160:GLY:N    | 2.25                     | 1.03              |
| 1:J:202:SER:CA   | 1:J:207:LYS:CE   | 2.36                     | 1.03              |
| 4:0:287:ILE:HG12 | 4:2:203:THR:H    | 1.17                     | 1.03              |
| 4:7:3:ASP:HA     | 4:7:6:THR:HB     | 1.36                     | 1.03              |
| 1:A:502:GLU:OE1  | 1:A:763:THR:N    | 1.90                     | 1.03              |
| 1:A:642:LYS:HG3  | 4:8:23:GLY:H     | 0.87                     | 1.03              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:CG   | 2.32                     | 1.03              |
| 1:D:553:MLY:CB   | 4:W:46:GLY:CA    | 2.32                     | 1.03              |
| 1:D:724:TYR:C    | 1:D:782:MLY:HH21 | 1.83                     | 1.03              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:N    | 1.91                     | 1.03              |
| 4:0:3:ASP:HA     | 4:0:6:THR:HB     | 1.36                     | 1.03              |
| 1:A:202:SER:CA   | 1:A:207:LYS:CE   | 2.36                     | 1.03              |
| 1:A:638:GLY:HA2  | 4:8:341:ILE:O    | 1.56                     | 1.03              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:HD21 | 1.24                     | 1.03              |
| 2:H:112:ILE:O    | 2:H:147:ASN:C    | 2.01                     | 1.03              |
| 2:H:121:LEU:C    | 2:H:128:PHE:HB3  | 1.71                     | 1.03              |
| 3:I:49:ILE:CA    | 3:I:52:ASN:HD22  | 1.70                     | 1.03              |
| 1:J:541:MET:HB3  | 4:W:143:TYR:OH   | 1.59                     | 1.03              |
| 2:K:112:ILE:O    | 2:K:147:ASN:C    | 2.02                     | 1.03              |
| 4:8:290:ARG:CZ   | 4:V:202:THR:CG2  | 2.36                     | 1.03              |
| 4:V:324:THR:HG21 | 4:X:246:GLN:C    | 1.70                     | 1.03              |
| 1:A:541:MET:HB3  | 4:8:143:TYR:OH   | 1.59                     | 1.02              |
| 1:A:641:LYS:HE3  | 4:8:348:SER:O    | 1.56                     | 1.02              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:HG21 | 1.06                     | 1.02              |
| 1:D:839:MLY:HH13 | 2:E:159:HIS:CG   | 1.94                     | 1.02              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:HD11 | 1.21                     | 1.02              |
| 1:G:530:MET:CA   | 4:V:354:GLN:HG3  | 1.88                     | 1.02              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:CG   | 2.32                     | 1.02              |
| 2:H:140:PHE:O    | 2:H:141:PRO:O    | 1.75                     | 1.02              |
| 1:J:530:MET:HE2  | 4:W:354:GLN:HG2  | 1.06                     | 1.02              |
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:HE3  | 1.06                     | 1.02              |
| 4:1:203:THR:N    | 4:Z:287:ILE:CB   | 2.13                     | 1.02              |
| 4:2:3:ASP:HA     | 4:2:6:THR:HB     | 1.36                     | 1.02              |
| 4:V:3:ASP:HA     | 4:V:6:THR:HB     | 1.36                     | 1.02              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:HG3  | 1.21                     | 1.02              |
| 1:A:813:ILE:HG23 | 2:B:127:ARG:HD2  | 1.06                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:149:ASP:OD2  | 2:B:150:TYR:N    | 1.91                     | 1.02              |
| 2:E:150:TYR:C    | 2:E:151:LYS:HG3  | 1.83                     | 1.02              |
| 2:E:150:TYR:O    | 2:E:151:LYS:CB   | 2.06                     | 1.02              |
| 1:G:638:GLY:HA2  | 4:V:341:ILE:O    | 1.58                     | 1.02              |
| 1:G:642:LYS:HG3  | 4:V:23:GLY:H     | 0.85                     | 1.02              |
| 1:G:751:GLY:HA2  | 3:I:114:LEU:HD13 | 1.38                     | 1.02              |
| 1:J:754:ASP:HB2  | 1:J:776:GLU:HB3  | 1.38                     | 1.02              |
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:CD   | 1.87                     | 1.02              |
| 4:7:290:ARG:CZ   | 4:9:202:THR:CG2  | 2.36                     | 1.02              |
| 4:9:290:ARG:CZ   | 4:W:202:THR:CG2  | 2.36                     | 1.02              |
| 1:A:502:GLU:O    | 1:A:761:GLY:HA2  | 1.59                     | 1.02              |
| 2:B:150:TYR:C    | 2:B:151:LYS:HG3  | 1.83                     | 1.02              |
| 1:D:830:PRO:CD   | 2:E:67:MET:HE2   | 1.90                     | 1.02              |
| 3:F:24:LYS:HG2   | 3:F:63:ILE:O     | 1.59                     | 1.02              |
| 1:J:599:ASN:CA   | 1:J:649:VAL:HB   | 1.89                     | 1.02              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:HD11 | 1.21                     | 1.02              |
| 2:K:144:VAL:HG11 | 2:K:153:ILE:HG12 | 1.37                     | 1.02              |
| 3:L:24:LYS:CG    | 3:L:63:ILE:O     | 2.08                     | 1.02              |
| 4:W:3:ASP:HA     | 4:W:6:THR:HB     | 1.36                     | 1.02              |
| 1:A:501:GLU:O    | 1:A:762:HIS:CD2  | 2.13                     | 1.02              |
| 1:A:502:GLU:C    | 1:A:761:GLY:HA3  | 1.84                     | 1.02              |
| 1:D:642:LYS:HG3  | 4:9:23:GLY:H     | 0.86                     | 1.02              |
| 1:D:768:MLY:O    | 1:D:771:LEU:CD1  | 0.72                     | 1.02              |
| 4:4:3:ASP:HA     | 4:4:6:THR:HB     | 1.36                     | 1.02              |
| 1:A:642:LYS:HD3  | 4:8:340:TRP:CZ3  | 1.95                     | 1.02              |
| 2:B:121:LEU:HG   | 2:B:128:PHE:CA   | 1.59                     | 1.02              |
| 1:D:557:GLU:N    | 4:W:48:GLY:CA    | 2.12                     | 1.02              |
| 1:J:98:HIS:HB3   | 1:J:100:PRO:HD2  | 1.42                     | 1.02              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:C    | 2.03                     | 1.02              |
| 1:J:757:GLN:CD   | 1:J:776:GLU:CG   | 2.33                     | 1.02              |
| 1:J:800:ARG:HB2  | 3:L:149:VAL:HG21 | 1.36                     | 1.02              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:CG   | 2.32                     | 1.02              |
| 4:1:322:PRO:HB3  | 4:3:244:ASP:CB   | 1.90                     | 1.02              |
| 4:W:291:LYS:HD2  | 4:Y:243:PRO:HB2  | 1.41                     | 1.02              |
| 4:W:325:MET:HE2  | 4:Y:244:ASP:OD2  | 1.59                     | 1.02              |
| 4:Y:3:ASP:HA     | 4:Y:6:THR:HB     | 1.36                     | 1.02              |
| 1:A:530:MET:HE2  | 4:8:354:GLN:HG2  | 1.06                     | 1.01              |
| 1:A:642:LYS:HD3  | 4:8:340:TRP:CH2  | 1.95                     | 1.01              |
| 1:D:599:ASN:CA   | 1:D:649:VAL:HB   | 1.89                     | 1.01              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:HG2  | 1.75                     | 1.01              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:CG   | 2.32                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:163:ALA:O    | 2:K:22:THR:N     | 1.93                     | 1.01              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB3  | 1.35                     | 1.01              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HD11 | 1.21                     | 1.01              |
| 1:J:707:CYS:SG   | 1:J:714:ARG:NH1  | 2.30                     | 1.01              |
| 4:7:290:ARG:NH2  | 4:9:202:THR:CG2  | 2.23                     | 1.01              |
| 4:X:287:ILE:C    | 4:Z:205:GLU:CD   | 2.27                     | 1.01              |
| 3:C:24:LYS:HG2   | 3:C:63:ILE:O     | 1.59                     | 1.01              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:N    | 1.91                     | 1.01              |
| 1:G:576:GLU:HG2  | 1:G:577:ALA:H    | 0.85                     | 1.01              |
| 1:G:819:ASN:HA   | 2:H:90:GLY:C     | 1.85                     | 1.01              |
| 3:I:24:LYS:CG    | 3:I:63:ILE:O     | 2.08                     | 1.01              |
| 3:I:49:ILE:HA    | 3:I:52:ASN:HD22  | 1.23                     | 1.01              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:NZ   | 1.72                     | 1.01              |
| 1:J:635:GLY:HA3  | 4:W:341:ILE:HD13 | 1.36                     | 1.01              |
| 2:K:150:TYR:C    | 2:K:151:LYS:HG3  | 1.83                     | 1.01              |
| 4:9:290:ARG:NH2  | 4:W:202:THR:CG2  | 2.23                     | 1.01              |
| 1:A:599:ASN:CA   | 1:A:649:VAL:HB   | 1.89                     | 1.01              |
| 1:A:639:GLY:N    | 4:8:345:ILE:N    | 1.94                     | 1.01              |
| 2:B:144:VAL:HG11 | 2:B:153:ILE:HG12 | 1.38                     | 1.01              |
| 2:B:150:TYR:O    | 2:B:151:LYS:CB   | 2.06                     | 1.01              |
| 1:D:541:MET:HB3  | 4:9:143:TYR:OH   | 1.59                     | 1.01              |
| 1:D:553:MLY:HG2  | 4:W:44:MET:O     | 1.59                     | 1.01              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:HG22 | 1.38                     | 1.01              |
| 1:D:830:PRO:CD   | 2:E:67:MET:CE    | 2.37                     | 1.01              |
| 2:E:144:VAL:HG11 | 2:E:153:ILE:HG12 | 1.38                     | 1.01              |
| 1:G:202:SER:CA   | 1:G:207:LYS:CE   | 2.36                     | 1.01              |
| 1:G:797:PHE:CG   | 3:I:149:VAL:HG11 | 1.95                     | 1.01              |
| 2:H:150:TYR:C    | 2:H:151:LYS:HG3  | 1.83                     | 1.01              |
| 1:D:635:GLY:HA3  | 4:9:341:ILE:HD13 | 1.37                     | 1.01              |
| 1:D:814:PHE:CE1  | 2:E:127:ARG:NH2  | 2.27                     | 1.01              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CB    | 1.90                     | 1.01              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:HB2  | 1.42                     | 1.01              |
| 1:J:599:ASN:HA   | 1:J:649:VAL:HB   | 1.05                     | 1.01              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:HB2  | 1.42                     | 1.01              |
| 2:K:121:LEU:CB   | 2:K:128:PHE:HB3  | 1.69                     | 1.01              |
| 4:8:290:ARG:NH2  | 4:V:202:THR:CG2  | 2.23                     | 1.01              |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:HG23 | 1.38                     | 1.01              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:CD   | 2.34                     | 1.01              |
| 1:A:800:ARG:CG   | 3:C:149:VAL:HG22 | 1.90                     | 1.01              |
| 1:A:822:SER:CB   | 2:B:88:LEU:HD23  | 1.91                     | 1.01              |
| 3:C:48:LYS:O     | 3:C:52:ASN:ND2   | 1.94                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:769:ALA:HA   | 1:D:771:LEU:HA   | 1.41                     | 1.01              |
| 1:G:599:ASN:CA   | 1:G:649:VAL:HB   | 1.89                     | 1.01              |
| 2:H:144:VAL:HG11 | 2:H:153:ILE:HG12 | 1.38                     | 1.01              |
| 3:I:48:LYS:O     | 3:I:52:ASN:ND2   | 1.94                     | 1.01              |
| 1:J:90:ASP:CB    | 1:J:764:MLY:HH21 | 1.89                     | 1.01              |
| 1:J:642:LYS:HG3  | 4:W:23:GLY:H     | 0.86                     | 1.01              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:HD21 | 1.24                     | 1.01              |
| 3:L:48:LYS:O     | 3:L:52:ASN:ND2   | 1.94                     | 1.01              |
| 4:9:3:ASP:HA     | 4:9:6:THR:HB     | 1.36                     | 1.01              |
| 1:A:502:GLU:CA   | 1:A:761:GLY:HA3  | 1.91                     | 1.00              |
| 1:A:793:ARG:HE   | 3:C:147:MET:HG2  | 1.25                     | 1.00              |
| 1:D:206:LYS:HD2  | 1:D:217:THR:HG23 | 1.41                     | 1.00              |
| 1:D:553:MLY:HB3  | 4:W:46:GLY:CA    | 1.51                     | 1.00              |
| 1:D:599:ASN:HA   | 1:D:649:VAL:HB   | 1.05                     | 1.00              |
| 1:D:792:ALA:C    | 3:F:40:ASN:HB3   | 1.85                     | 1.00              |
| 1:G:735:GLY:C    | 1:G:743:ALA:CA   | 2.34                     | 1.00              |
| 3:I:24:LYS:HG2   | 3:I:63:ILE:O     | 1.60                     | 1.00              |
| 4:9:287:ILE:HB   | 4:W:204:ALA:H    | 1.25                     | 1.00              |
| 1:A:206:LYS:HD2  | 1:A:217:THR:HG23 | 1.41                     | 1.00              |
| 1:A:534:SER:O    | 4:8:351:THR:HA   | 1.60                     | 1.00              |
| 1:D:174:SER:HB3  | 1:D:667:THR:HG21 | 1.44                     | 1.00              |
| 1:D:735:GLY:C    | 1:D:743:ALA:CA   | 2.34                     | 1.00              |
| 3:F:24:LYS:CG    | 3:F:63:ILE:O     | 2.08                     | 1.00              |
| 1:G:215:GLN:CA   | 1:G:340:ILE:HG23 | 1.92                     | 1.00              |
| 1:G:642:LYS:HD3  | 4:V:340:TRP:CH2  | 1.96                     | 1.00              |
| 1:G:646:PHE:HE2  | 1:G:652:LEU:HD21 | 1.24                     | 1.00              |
| 1:J:642:LYS:HD3  | 4:W:340:TRP:CH2  | 1.96                     | 1.00              |
| 1:J:795:ARG:NE   | 3:L:118:MET:HE1  | 1.76                     | 1.00              |
| 3:L:24:LYS:HG2   | 3:L:63:ILE:O     | 1.59                     | 1.00              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:C    | 2.34                     | 1.00              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CB   | 1.91                     | 1.00              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CD   | 2.19                     | 1.00              |
| 1:A:797:PHE:HD1  | 3:C:149:VAL:HG12 | 1.27                     | 1.00              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:HB2  | 1.42                     | 1.00              |
| 3:F:49:ILE:HA    | 3:F:52:ASN:HD22  | 1.22                     | 1.00              |
| 1:G:534:SER:O    | 4:V:351:THR:HA   | 1.60                     | 1.00              |
| 1:G:576:GLU:CG   | 1:G:577:ALA:H    | 1.74                     | 1.00              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CB   | 1.91                     | 1.00              |
| 1:G:642:LYS:HD3  | 4:V:340:TRP:CZ3  | 1.96                     | 1.00              |
| 1:J:174:SER:HB3  | 1:J:667:THR:HG21 | 1.44                     | 1.00              |
| 1:J:642:LYS:HD3  | 4:W:340:TRP:CZ3  | 1.96                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:735:GLY:C    | 1:J:743:ALA:CA   | 2.34                     | 1.00              |
| 1:J:757:GLN:NE2  | 1:J:776:GLU:HG2  | 1.76                     | 1.00              |
| 4:V:324:THR:CG2  | 4:X:247:VAL:N    | 2.24                     | 1.00              |
| 1:A:501:GLU:O    | 1:A:762:HIS:CE1  | 2.14                     | 1.00              |
| 1:A:735:GLY:C    | 1:A:743:ALA:CA   | 2.34                     | 1.00              |
| 1:A:736:GLN:N    | 1:A:743:ALA:CB   | 2.05                     | 1.00              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:HG3  | 1.90                     | 1.00              |
| 1:D:534:SER:O    | 4:9:351:THR:HA   | 1.59                     | 1.00              |
| 1:G:541:MET:HB3  | 4:V:143:TYR:OH   | 1.59                     | 1.00              |
| 2:H:150:TYR:O    | 2:H:151:LYS:CB   | 2.06                     | 1.00              |
| 1:A:56:GLU:HB2   | 1:A:59:MLY:HB3   | 1.40                     | 1.00              |
| 1:A:576:GLU:HG2  | 1:A:577:ALA:H    | 0.85                     | 1.00              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:HB2  | 1.42                     | 1.00              |
| 3:C:24:LYS:CG    | 3:C:63:ILE:O     | 2.08                     | 1.00              |
| 1:D:642:LYS:HD3  | 4:9:340:TRP:CZ3  | 1.96                     | 1.00              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:CD   | 2.34                     | 1.00              |
| 1:D:788:THR:HG23 | 3:F:42:THR:HG21  | 1.43                     | 1.00              |
| 1:G:552:ASN:O    | 4:X:47:MET:HE1   | 1.61                     | 1.00              |
| 4:X:291:LYS:HE2  | 4:Z:243:PRO:C    | 1.85                     | 1.00              |
| 1:A:576:GLU:CG   | 1:A:577:ALA:H    | 1.75                     | 1.00              |
| 1:G:84:MLY:HH12  | 1:G:715:VAL:CG1  | 1.83                     | 1.00              |
| 1:G:98:HIS:HB3   | 1:G:100:PRO:HD2  | 1.42                     | 1.00              |
| 1:G:736:GLN:N    | 1:G:743:ALA:CB   | 2.04                     | 1.00              |
| 4:0:245:GLY:HA3  | 4:Y:324:THR:O    | 1.58                     | 1.00              |
| 4:1:203:THR:HG22 | 4:Z:287:ILE:HB   | 1.00                     | 1.00              |
| 1:G:206:LYS:HD2  | 1:G:217:THR:HG23 | 1.41                     | 1.00              |
| 1:J:800:ARG:CG   | 3:L:149:VAL:CG2  | 2.39                     | 1.00              |
| 4:1:288:ASP:CG   | 4:3:203:THR:HG23 | 1.86                     | 1.00              |
| 1:D:98:HIS:HB3   | 1:D:100:PRO:HD2  | 1.42                     | 0.99              |
| 1:D:642:LYS:HD3  | 4:9:340:TRP:CH2  | 1.96                     | 0.99              |
| 2:E:163:ALA:C    | 2:K:22:THR:H     | 1.68                     | 0.99              |
| 3:F:48:LYS:O     | 3:F:52:ASN:ND2   | 1.93                     | 0.99              |
| 4:1:244:ASP:CB   | 4:Z:322:PRO:HB3  | 1.92                     | 0.99              |
| 4:V:286:ASP:CG   | 4:X:203:THR:HG22 | 1.87                     | 0.99              |
| 1:A:576:GLU:HG2  | 1:A:577:ALA:N    | 1.66                     | 0.99              |
| 1:A:795:ARG:HH22 | 3:C:116:GLU:CD   | 1.70                     | 0.99              |
| 2:B:139:ALA:O    | 2:B:141:PRO:HD3  | 1.62                     | 0.99              |
| 1:D:537:GLU:C    | 4:9:349:LEU:CD1  | 2.20                     | 0.99              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:CD   | 2.34                     | 0.99              |
| 1:G:800:ARG:HD2  | 3:I:149:VAL:CG2  | 1.91                     | 0.99              |
| 1:J:206:LYS:HD2  | 1:J:217:THR:HG23 | 1.41                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:836:PHE:CE1  | 2:B:159:HIS:C    | 2.40                     | 0.99              |
| 1:D:56:GLU:HB2   | 1:D:59:MLY:HB3   | 1.40                     | 0.99              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:J:831:TRP:CZ2  | 2:K:47:LEU:CD2   | 2.46                     | 0.99              |
| 2:K:141:PRO:HB2  | 2:K:142:PRO:HD2  | 1.44                     | 0.99              |
| 4:3:288:ASP:N    | 4:5:203:THR:HG22 | 1.75                     | 0.99              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:CA   | 1.75                     | 0.99              |
| 2:E:139:ALA:O    | 2:E:141:PRO:HD3  | 1.62                     | 0.99              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:HG22 | 1.92                     | 0.99              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:HB2  | 1.40                     | 0.99              |
| 1:G:831:TRP:CZ2  | 2:H:67:MET:SD    | 2.56                     | 0.99              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CB   | 1.91                     | 0.99              |
| 4:8:286:ASP:OD1  | 4:V:203:THR:HG22 | 1.62                     | 0.99              |
| 1:A:149:GLN:HG2  | 1:A:719:ASP:OD1  | 1.58                     | 0.99              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:CD   | 2.34                     | 0.99              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:O    | 1.80                     | 0.99              |
| 4:8:322:PRO:HB3  | 4:V:244:ASP:OD2  | 1.62                     | 0.99              |
| 1:A:502:GLU:CG   | 1:A:761:GLY:HA3  | 1.92                     | 0.99              |
| 1:A:553:MLY:HG2  | 4:V:44:MET:O     | 1.59                     | 0.99              |
| 1:D:809:ARG:NH1  | 2:E:124:GLY:CA   | 2.24                     | 0.99              |
| 1:D:809:ARG:HH12 | 2:E:124:GLY:HA2  | 1.28                     | 0.99              |
| 1:A:215:GLN:CA   | 1:A:340:ILE:HG23 | 1.92                     | 0.99              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:HG3  | 1.90                     | 0.99              |
| 1:A:709:LYS:C    | 1:A:710:GLY:HA3  | 1.88                     | 0.99              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:CA   | 1.75                     | 0.99              |
| 1:D:800:ARG:CB   | 3:F:149:VAL:CG2  | 2.38                     | 0.99              |
| 2:H:121:LEU:HG   | 2:H:128:PHE:CA   | 1.60                     | 0.99              |
| 1:J:508:ILE:CD1  | 1:J:759:ALA:CB   | 2.30                     | 0.99              |
| 4:9:286:ASP:OD1  | 4:W:203:THR:HG22 | 1.62                     | 0.99              |
| 4:X:287:ILE:CG1  | 4:Z:201:VAL:HG23 | 1.91                     | 0.99              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:O    | 1.80                     | 0.99              |
| 2:B:149:ASP:OD2  | 2:B:150:TYR:O    | 1.80                     | 0.99              |
| 1:J:84:MLY:HH12  | 1:J:715:VAL:HG13 | 1.02                     | 0.99              |
| 1:A:502:GLU:CD   | 1:A:764:MLY:N    | 2.21                     | 0.99              |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:HD2  | 1.15                     | 0.99              |
| 1:J:215:GLN:CA   | 1:J:340:ILE:HG23 | 1.92                     | 0.99              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:CG1  | 2.17                     | 0.99              |
| 2:K:121:LEU:HG   | 2:K:128:PHE:CA   | 1.59                     | 0.99              |
| 4:7:287:ILE:HB   | 4:9:204:ALA:H    | 1.25                     | 0.99              |
| 1:A:98:HIS:HB3   | 1:A:100:PRO:HD2  | 1.42                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:501:GLU:CG   | 1:A:762:HIS:HD1  | 1.75                     | 0.98              |
| 1:A:639:GLY:CA   | 4:8:345:ILE:CA   | 2.41                     | 0.98              |
| 1:D:576:GLU:HG2  | 1:D:577:ALA:H    | 0.85                     | 0.98              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:HG22 | 1.92                     | 0.98              |
| 1:J:553:MLY:HE3  | 4:Y:45:VAL:CG1   | 1.92                     | 0.98              |
| 4:1:203:THR:HG21 | 4:Z:288:ASP:OD2  | 1.61                     | 0.98              |
| 4:2:287:ILE:HD13 | 4:4:203:THR:HB   | 1.42                     | 0.98              |
| 1:A:530:MET:CE   | 4:8:354:GLN:CG   | 2.40                     | 0.98              |
| 1:A:795:ARG:HE   | 3:C:118:MET:HE1  | 1.27                     | 0.98              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:CB   | 1.93                     | 0.98              |
| 4:3:322:PRO:CB   | 4:5:244:ASP:CB   | 2.40                     | 0.98              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:HG22 | 1.92                     | 0.98              |
| 1:A:819:ASN:H    | 2:B:90:GLY:HA3   | 1.28                     | 0.98              |
| 2:B:141:PRO:HB2  | 2:B:142:PRO:HD2  | 1.44                     | 0.98              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CB   | 1.91                     | 0.98              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:CA   | 1.75                     | 0.98              |
| 1:G:707:CYS:C    | 1:G:714:ARG:HH22 | 1.69                     | 0.98              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:HG22 | 1.92                     | 0.98              |
| 1:A:795:ARG:HD3  | 3:C:35:ARG:HH22  | 1.26                     | 0.98              |
| 1:D:215:GLN:CA   | 1:D:340:ILE:HG23 | 1.92                     | 0.98              |
| 1:D:530:MET:CE   | 4:9:354:GLN:CG   | 2.40                     | 0.98              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:NE    | 1.35                     | 0.98              |
| 1:G:530:MET:CE   | 4:V:354:GLN:CG   | 2.39                     | 0.98              |
| 1:G:639:GLY:CA   | 4:V:345:ILE:CA   | 2.40                     | 0.98              |
| 1:G:641:LYS:HE3  | 4:V:348:SER:O    | 1.56                     | 0.98              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:NE2  | 1.58                     | 0.98              |
| 2:K:150:TYR:O    | 2:K:151:LYS:CB   | 2.06                     | 0.98              |
| 1:A:505:MLY:HB2  | 1:A:762:HIS:N    | 1.76                     | 0.98              |
| 2:E:130:PRO:O    | 2:E:133:ILE:N    | 1.96                     | 0.98              |
| 1:J:797:PHE:CB   | 3:L:149:VAL:HG11 | 1.93                     | 0.98              |
| 3:C:49:ILE:HA    | 3:C:52:ASN:HD22  | 1.22                     | 0.98              |
| 1:D:576:GLU:CG   | 1:D:577:ALA:H    | 1.75                     | 0.98              |
| 1:D:642:LYS:HD2  | 4:9:24:ASP:O     | 1.64                     | 0.98              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:HD21 | 1.24                     | 0.98              |
| 3:L:52:ASN:HB2   | 3:L:53:PRO:HD3   | 1.45                     | 0.98              |
| 3:C:52:ASN:HB2   | 3:C:53:PRO:HD3   | 1.46                     | 0.98              |
| 1:D:792:ALA:HB1  | 3:F:40:ASN:CB    | 1.93                     | 0.98              |
| 1:G:576:GLU:HG2  | 1:G:577:ALA:N    | 1.66                     | 0.98              |
| 1:G:829:TRP:CZ3  | 2:H:87:LYS:NZ    | 2.29                     | 0.98              |
| 2:H:141:PRO:HB2  | 2:H:142:PRO:HD2  | 1.44                     | 0.98              |
| 1:J:534:SER:O    | 4:W:351:THR:HA   | 1.59                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:537:GLU:C    | 4:W:349:LEU:CD1  | 2.20                     | 0.98              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:CD2  | 2.46                     | 0.98              |
| 1:A:797:PHE:HE2  | 3:C:126:LEU:HD23 | 1.27                     | 0.98              |
| 1:D:768:MLY:C    | 1:D:771:LEU:HD12 | 1.59                     | 0.98              |
| 2:E:141:PRO:HB2  | 2:E:142:PRO:HD2  | 1.44                     | 0.98              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:CA   | 1.75                     | 0.98              |
| 1:J:798:LEU:CD2  | 3:L:126:LEU:CD1  | 2.37                     | 0.98              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:CA   | 2.12                     | 0.98              |
| 4:8:287:ILE:HB   | 4:V:204:ALA:H    | 1.25                     | 0.98              |
| 2:E:121:LEU:HG   | 2:E:128:PHE:CA   | 1.59                     | 0.98              |
| 4:1:204:ALA:H    | 4:Z:287:ILE:HG21 | 1.28                     | 0.98              |
| 4:2:324:THR:HG21 | 4:4:244:ASP:O    | 1.59                     | 0.98              |
| 2:K:139:ALA:O    | 2:K:141:PRO:HD3  | 1.62                     | 0.98              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:CG   | 2.37                     | 0.98              |
| 4:7:322:PRO:HB3  | 4:9:244:ASP:OD2  | 1.62                     | 0.98              |
| 4:V:325:MET:CE   | 4:X:244:ASP:CG   | 2.37                     | 0.98              |
| 3:F:46:ILE:O     | 3:F:50:LEU:HG    | 1.64                     | 0.97              |
| 1:A:174:SER:HB3  | 1:A:667:THR:HG21 | 1.44                     | 0.97              |
| 1:A:831:TRP:HH2  | 2:B:50:THR:HB    | 1.24                     | 0.97              |
| 2:B:130:PRO:O    | 2:B:133:ILE:N    | 1.96                     | 0.97              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:CG   | 2.42                     | 0.97              |
| 1:G:798:LEU:HD23 | 3:I:122:GLU:HB3  | 1.46                     | 0.97              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:O    | 1.80                     | 0.97              |
| 1:J:576:GLU:HG2  | 1:J:577:ALA:H    | 0.85                     | 0.97              |
| 3:L:49:ILE:HA    | 3:L:52:ASN:HD22  | 1.23                     | 0.97              |
| 4:0:201:VAL:N    | 4:Y:287:ILE:HG12 | 1.78                     | 0.97              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:C    | 2.37                     | 0.97              |
| 1:J:817:GLN:CG   | 2:K:127:ARG:HD2  | 1.93                     | 0.97              |
| 4:7:286:ASP:OD1  | 4:9:203:THR:HG22 | 1.62                     | 0.97              |
| 1:A:215:GLN:H    | 1:A:340:ILE:CG1  | 1.73                     | 0.97              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:CG   | 2.42                     | 0.97              |
| 1:A:542:PHE:CG   | 4:8:143:TYR:CE1  | 2.52                     | 0.97              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:HG3   | 1.37                     | 0.97              |
| 1:D:724:TYR:HE1  | 1:D:778:MET:HB3  | 1.22                     | 0.97              |
| 1:G:553:MLY:CE   | 4:X:45:VAL:HB    | 1.91                     | 0.97              |
| 2:H:139:ALA:O    | 2:H:141:PRO:HD3  | 1.62                     | 0.97              |
| 4:0:287:ILE:HG12 | 4:2:203:THR:N    | 1.79                     | 0.97              |
| 1:D:549:SER:C    | 4:W:46:GLY:HA3   | 1.89                     | 0.97              |
| 1:G:788:THR:O    | 3:I:42:THR:HG22  | 1.63                     | 0.97              |
| 1:J:639:GLY:N    | 4:W:345:ILE:N    | 1.94                     | 0.97              |
| 1:A:505:MLY:NZ   | 1:A:762:HIS:C    | 2.16                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:642:LYS:HG2  | 4:8:21:PHE:O     | 1.65                     | 0.97              |
| 1:G:174:SER:HB3  | 1:G:667:THR:HG21 | 1.44                     | 0.97              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:HB2  | 1.95                     | 0.97              |
| 1:G:784:ALA:O    | 1:G:788:THR:N    | 1.96                     | 0.97              |
| 2:H:121:LEU:HG   | 2:H:128:PHE:HA   | 1.46                     | 0.97              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:CH1  | 2.37                     | 0.97              |
| 1:J:213:LYS:HA   | 1:J:220:ASP:CG   | 1.90                     | 0.97              |
| 1:J:642:LYS:HG2  | 4:W:21:PHE:O     | 1.65                     | 0.97              |
| 2:K:130:PRO:O    | 2:K:133:ILE:N    | 1.96                     | 0.97              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:CG   | 2.42                     | 0.97              |
| 4:1:202:THR:HB   | 4:Z:287:ILE:CB   | 1.94                     | 0.97              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:HD1  | 0.84                     | 0.97              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:CG   | 2.42                     | 0.97              |
| 1:J:793:ARG:HE   | 3:L:147:MET:CA   | 1.77                     | 0.97              |
| 4:3:287:ILE:HD13 | 4:5:203:THR:CB   | 1.92                     | 0.97              |
| 2:E:121:LEU:HG   | 2:E:128:PHE:HA   | 1.46                     | 0.97              |
| 1:J:576:GLU:CG   | 1:J:577:ALA:H    | 1.75                     | 0.97              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:CA   | 2.42                     | 0.97              |
| 4:0:287:ILE:HG21 | 4:2:203:THR:N    | 1.78                     | 0.97              |
| 2:H:130:PRO:O    | 2:H:133:ILE:N    | 1.96                     | 0.97              |
| 4:W:286:ASP:OD2  | 4:Y:203:THR:HG22 | 1.62                     | 0.97              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:CG   | 1.90                     | 0.96              |
| 1:D:542:PHE:CG   | 4:9:143:TYR:CE1  | 2.52                     | 0.96              |
| 1:D:553:MLY:HB3  | 4:W:46:GLY:HA2   | 1.47                     | 0.96              |
| 2:E:163:ALA:C    | 2:K:22:THR:N     | 2.23                     | 0.96              |
| 1:G:642:LYS:HG2  | 4:V:21:PHE:O     | 1.65                     | 0.96              |
| 1:J:642:LYS:HD2  | 4:W:24:ASP:O     | 1.64                     | 0.96              |
| 3:L:46:ILE:O     | 3:L:50:LEU:HG    | 1.64                     | 0.96              |
| 4:3:322:PRO:HB2  | 4:5:244:ASP:CB   | 1.94                     | 0.96              |
| 4:3:324:THR:HG23 | 4:5:244:ASP:C    | 1.86                     | 0.96              |
| 1:D:724:TYR:HA   | 1:D:782:MLY:NZ   | 1.80                     | 0.96              |
| 1:A:534:SER:O    | 4:8:351:THR:HG23 | 1.13                     | 0.96              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:HD11 | 1.22                     | 0.96              |
| 1:D:649:VAL:CG2  | 1:D:649:VAL:CA   | 2.42                     | 0.96              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:HB2  | 1.95                     | 0.96              |
| 1:G:637:LYS:NZ   | 4:V:141:SER:O    | 1.99                     | 0.96              |
| 1:J:553:MLY:HE3  | 4:Y:45:VAL:HG11  | 1.47                     | 0.96              |
| 4:3:288:ASP:H    | 4:5:203:THR:HG22 | 1.29                     | 0.96              |
| 1:A:502:GLU:O    | 1:A:761:GLY:CA   | 2.13                     | 0.96              |
| 1:A:642:LYS:HD2  | 4:8:24:ASP:O     | 1.64                     | 0.96              |
| 1:D:215:GLN:H    | 1:D:340:ILE:CG1  | 1.73                     | 0.96              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:831:TRP:HD1  | 2:E:67:MET:SD   | 1.85                     | 0.96              |
| 1:G:649:VAL:CG2  | 1:G:649:VAL:CA  | 2.42                     | 0.96              |
| 1:J:557:GLU:HA   | 4:Y:47:MET:HA   | 1.04                     | 0.96              |
| 4:1:287:ILE:CG2  | 4:3:204:ALA:H   | 1.78                     | 0.96              |
| 4:1:287:ILE:CG1  | 4:3:202:THR:HA  | 1.92                     | 0.96              |
| 1:A:538:GLU:N    | 4:8:349:LEU:CD1 | 2.28                     | 0.96              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HA  | 1.90                     | 0.96              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:HH12 | 1.78                     | 0.96              |
| 1:G:635:GLY:HA3  | 4:V:334:GLU:HG2 | 1.47                     | 0.96              |
| 1:G:642:LYS:HD2  | 4:V:24:ASP:O    | 1.64                     | 0.96              |
| 2:H:117:LEU:HD13 | 2:H:147:ASN:OD1 | 1.64                     | 0.96              |
| 1:J:543:PRO:CG   | 4:W:143:TYR:O   | 2.14                     | 0.96              |
| 1:J:639:GLY:CA   | 4:W:345:ILE:CA  | 2.40                     | 0.96              |
| 1:A:549:SER:C    | 4:V:46:GLY:HA3  | 1.89                     | 0.96              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:CG2 | 2.43                     | 0.96              |
| 1:A:649:VAL:CG2  | 1:A:649:VAL:CA  | 2.42                     | 0.96              |
| 1:J:795:ARG:NH1  | 3:L:35:ARG:NH1  | 2.14                     | 0.96              |
| 4:9:322:PRO:HB3  | 4:W:244:ASP:OD2 | 1.62                     | 0.96              |
| 4:V:325:MET:HE2  | 4:X:244:ASP:OD2 | 1.64                     | 0.96              |
| 4:W:325:MET:CE   | 4:Y:244:ASP:CG  | 2.37                     | 0.96              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:C   | 2.38                     | 0.96              |
| 1:A:836:PHE:HB3  | 2:B:161:GLU:OE1 | 1.61                     | 0.96              |
| 2:B:150:TYR:O    | 2:B:151:LYS:HG3 | 1.65                     | 0.96              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:HA  | 1.47                     | 0.96              |
| 1:D:642:LYS:HG2  | 4:9:21:PHE:O    | 1.65                     | 0.96              |
| 2:K:121:LEU:HG   | 2:K:128:PHE:HA  | 1.47                     | 0.96              |
| 2:B:121:LEU:HG   | 2:B:128:PHE:HA  | 1.46                     | 0.96              |
| 1:D:206:LYS:CD   | 1:D:217:THR:CG2 | 2.16                     | 0.96              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:NE2 | 1.58                     | 0.96              |
| 4:8:288:ASP:HA   | 4:V:204:ALA:HB2 | 1.48                     | 0.96              |
| 3:C:46:ILE:O     | 3:C:50:LEU:HG   | 1.64                     | 0.96              |
| 3:I:46:ILE:O     | 3:I:50:LEU:HG   | 1.64                     | 0.96              |
| 1:J:542:PHE:CG   | 4:W:143:TYR:CE1 | 2.53                     | 0.96              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:CG  | 2.37                     | 0.96              |
| 1:D:639:GLY:CA   | 4:9:345:ILE:CA  | 2.40                     | 0.96              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:C   | 2.38                     | 0.96              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HA  | 1.91                     | 0.96              |
| 1:G:206:LYS:CD   | 1:G:217:THR:CG2 | 2.16                     | 0.96              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HA  | 1.90                     | 0.96              |
| 4:1:288:ASP:OD2  | 4:3:203:THR:CG2 | 2.06                     | 0.96              |
| 1:G:410:ASN:OD1  | 4:V:334:GLU:C   | 2.09                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:649:VAL:CG1  | 1:J:649:VAL:CG2  | 2.43                     | 0.95              |
| 4:7:288:ASP:HA   | 4:9:204:ALA:HB2  | 1.48                     | 0.95              |
| 4:9:288:ASP:HA   | 4:W:204:ALA:HB2  | 1.48                     | 0.95              |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:HG22 | 1.00                     | 0.95              |
| 1:A:537:GLU:C    | 4:8:349:LEU:CD1  | 2.20                     | 0.95              |
| 2:B:149:ASP:CG   | 2:B:150:TYR:H    | 1.73                     | 0.95              |
| 1:D:538:GLU:N    | 4:9:349:LEU:CD1  | 2.28                     | 0.95              |
| 1:A:635:GLY:HA3  | 4:8:334:GLU:HG2  | 1.47                     | 0.95              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:CG2  | 2.43                     | 0.95              |
| 1:G:538:GLU:HG3  | 4:V:352:PHE:N    | 1.81                     | 0.95              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:CG2  | 2.43                     | 0.95              |
| 1:J:736:GLN:CA   | 1:J:743:ALA:HB2  | 1.95                     | 0.95              |
| 4:2:288:ASP:N    | 4:4:203:THR:HG22 | 1.80                     | 0.95              |
| 4:W:325:MET:HE1  | 4:Y:244:ASP:CG   | 1.91                     | 0.95              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:CD1  | 2.05                     | 0.95              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:C    | 2.38                     | 0.95              |
| 1:J:84:MLY:HE2   | 1:J:719:ASP:HB3  | 0.98                     | 0.95              |
| 4:0:246:GLN:HA   | 4:Y:324:THR:HB   | 1.45                     | 0.95              |
| 1:A:637:LYS:NZ   | 4:8:141:SER:O    | 1.99                     | 0.95              |
| 1:A:834:LEU:CD1  | 2:B:54:MET:CB    | 2.45                     | 0.95              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:CG   | 1.90                     | 0.95              |
| 1:G:542:PHE:CG   | 4:V:143:TYR:CE1  | 2.53                     | 0.95              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:CG   | 1.90                     | 0.95              |
| 1:D:818:TYR:HB2  | 2:E:90:GLY:N     | 1.80                     | 0.95              |
| 1:G:93:MET:CB    | 1:G:764:MLY:NZ   | 2.29                     | 0.95              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:HA   | 1.47                     | 0.95              |
| 1:G:530:MET:HA   | 4:V:354:GLN:HG3  | 0.97                     | 0.95              |
| 1:G:538:GLU:N    | 4:V:349:LEU:CD1  | 2.29                     | 0.95              |
| 1:G:546:THR:HG22 | 1:G:548:THR:H    | 1.32                     | 0.95              |
| 2:H:149:ASP:CG   | 2:H:150:TYR:H    | 1.73                     | 0.95              |
| 2:H:150:TYR:O    | 2:H:151:LYS:HG3  | 1.65                     | 0.95              |
| 2:K:150:TYR:O    | 2:K:151:LYS:HG3  | 1.65                     | 0.95              |
| 1:A:206:LYS:CD   | 1:A:217:THR:CG2  | 2.16                     | 0.95              |
| 1:A:541:MET:N    | 4:8:349:LEU:HD21 | 1.80                     | 0.95              |
| 2:B:117:LEU:HD13 | 2:B:147:ASN:OD1  | 1.64                     | 0.95              |
| 1:D:543:PRO:CG   | 4:9:143:TYR:O    | 2.14                     | 0.95              |
| 1:J:538:GLU:N    | 4:W:349:LEU:CD1  | 2.28                     | 0.95              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:C    | 2.38                     | 0.95              |
| 1:J:768:MLY:HH12 | 1:J:772:LEU:HD23 | 1.46                     | 0.95              |
| 4:1:244:ASP:HB3  | 4:Z:322:PRO:HB3  | 1.48                     | 0.95              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:NZ   | 1.81                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:150:TYR:O    | 2:E:151:LYS:CG   | 2.15                     | 0.95              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HA   | 1.90                     | 0.95              |
| 2:H:150:TYR:O    | 2:H:151:LYS:HB2  | 1.67                     | 0.95              |
| 1:J:637:LYS:NZ   | 4:W:141:SER:O    | 1.98                     | 0.95              |
| 1:J:795:ARG:HH11 | 3:L:35:ARG:NH1   | 1.65                     | 0.95              |
| 2:K:117:LEU:HD13 | 2:K:147:ASN:OD1  | 1.64                     | 0.95              |
| 1:A:538:GLU:HG3  | 4:8:352:PHE:N    | 1.82                     | 0.95              |
| 1:A:543:PRO:CG   | 4:8:143:TYR:O    | 2.14                     | 0.95              |
| 2:B:121:LEU:CB   | 2:B:128:PHE:HB3  | 1.69                     | 0.95              |
| 1:J:797:PHE:CA   | 3:L:149:VAL:HG11 | 1.97                     | 0.95              |
| 4:1:322:PRO:CB   | 4:3:244:ASP:CB   | 2.44                     | 0.95              |
| 1:A:530:MET:HA   | 4:8:354:GLN:HG3  | 0.96                     | 0.95              |
| 1:A:819:ASN:N    | 2:B:90:GLY:HA3   | 1.81                     | 0.95              |
| 1:D:215:GLN:HA   | 1:D:340:ILE:HG23 | 0.95                     | 0.95              |
| 1:D:635:GLY:HA3  | 4:9:334:GLU:HG2  | 1.47                     | 0.95              |
| 1:D:726:VAL:CG2  | 1:D:782:MLY:HH22 | 1.97                     | 0.95              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:HD23  | 1.93                     | 0.95              |
| 2:H:121:LEU:CB   | 2:H:128:PHE:HB3  | 1.69                     | 0.95              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:HA   | 1.47                     | 0.95              |
| 1:J:783:LEU:O    | 1:J:787:ILE:N    | 1.99                     | 0.95              |
| 1:D:637:LYS:NZ   | 4:9:141:SER:O    | 1.99                     | 0.94              |
| 3:F:52:ASN:HB2   | 3:F:53:PRO:HD3   | 1.45                     | 0.94              |
| 1:J:635:GLY:HA3  | 4:W:334:GLU:HG2  | 1.47                     | 0.94              |
| 1:J:757:GLN:CD   | 1:J:776:GLU:HG2  | 1.91                     | 0.94              |
| 1:J:786:ILE:HG12 | 3:L:86:ASP:HB3   | 1.49                     | 0.94              |
| 1:J:821:ARG:HH21 | 2:K:127:ARG:HG2  | 1.20                     | 0.94              |
| 1:D:541:MET:N    | 4:9:349:LEU:HD21 | 1.80                     | 0.94              |
| 1:J:538:GLU:HG3  | 4:W:352:PHE:N    | 1.81                     | 0.94              |
| 2:K:150:TYR:O    | 2:K:151:LYS:CG   | 2.15                     | 0.94              |
| 1:A:410:ASN:OD1  | 4:8:334:GLU:C    | 2.10                     | 0.94              |
| 1:A:530:MET:CA   | 4:8:354:GLN:CG   | 2.44                     | 0.94              |
| 2:B:150:TYR:O    | 2:B:151:LYS:HB2  | 1.67                     | 0.94              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:CD   | 1.70                     | 0.94              |
| 1:G:754:ASP:CB   | 1:G:776:GLU:OE2  | 2.15                     | 0.94              |
| 2:H:150:TYR:O    | 2:H:151:LYS:CG   | 2.15                     | 0.94              |
| 1:J:410:ASN:OD1  | 4:W:334:GLU:C    | 2.10                     | 0.94              |
| 4:1:203:THR:HB   | 4:Z:287:ILE:CD1  | 1.96                     | 0.94              |
| 4:1:204:ALA:H    | 4:Z:287:ILE:CG2  | 1.80                     | 0.94              |
| 1:D:538:GLU:HG3  | 4:9:352:PHE:N    | 1.81                     | 0.94              |
| 2:E:150:TYR:O    | 2:E:151:LYS:HB2  | 1.67                     | 0.94              |
| 1:G:642:LYS:CG   | 4:V:23:GLY:H     | 1.76                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HG12 | 1.14                     | 0.94              |
| 4:X:324:THR:HB   | 4:Z:246:GLN:HA   | 1.50                     | 0.94              |
| 1:J:798:LEU:HD22 | 3:L:126:LEU:HD11 | 0.94                     | 0.94              |
| 4:3:322:PRO:HB2  | 4:5:244:ASP:HB3  | 1.49                     | 0.94              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:HG13 | 1.21                     | 0.94              |
| 1:A:819:ASN:ND2  | 2:B:91:ALA:C     | 2.22                     | 0.94              |
| 2:E:150:TYR:O    | 2:E:151:LYS:HG3  | 1.65                     | 0.94              |
| 1:G:218:LEU:CB   | 1:G:221:GLN:CG   | 2.46                     | 0.94              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:SD    | 2.60                     | 0.94              |
| 4:2:324:THR:CG2  | 4:4:244:ASP:O    | 1.97                     | 0.94              |
| 1:A:553:MLY:HB3  | 4:V:46:GLY:HA2   | 1.47                     | 0.94              |
| 1:A:642:LYS:CG   | 4:8:23:GLY:H     | 1.77                     | 0.94              |
| 1:D:530:MET:HA   | 4:9:354:GLN:HG3  | 0.96                     | 0.94              |
| 1:D:546:THR:HG22 | 1:D:548:THR:H    | 1.31                     | 0.94              |
| 2:E:163:ALA:C    | 2:K:22:THR:OG1   | 2.10                     | 0.94              |
| 1:A:218:LEU:CB   | 1:A:221:GLN:CG   | 2.46                     | 0.94              |
| 1:A:502:GLU:CG   | 1:A:761:GLY:CA   | 2.45                     | 0.94              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:HA3  | 1.83                     | 0.94              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:HB2  | 1.95                     | 0.94              |
| 1:A:768:MLY:C    | 1:A:771:LEU:HB2  | 1.97                     | 0.94              |
| 1:A:831:TRP:CE2  | 2:B:51:PHE:CE1   | 2.55                     | 0.94              |
| 1:D:630:ALA:O    | 4:9:25:ASP:CG    | 2.09                     | 0.94              |
| 1:D:817:GLN:HG3  | 2:E:127:ARG:HD3  | 1.49                     | 0.94              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:HB2   | 1.98                     | 0.94              |
| 3:I:52:ASN:HB2   | 3:I:53:PRO:HD3   | 1.46                     | 0.94              |
| 1:J:84:MLY:HE2   | 1:J:719:ASP:CG   | 1.93                     | 0.94              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:CA   | 2.31                     | 0.94              |
| 1:J:749:GLY:O    | 3:L:114:LEU:CD2  | 2.15                     | 0.94              |
| 1:J:768:MLY:HD3  | 1:J:772:LEU:HB2  | 1.48                     | 0.94              |
| 4:2:324:THR:HB   | 4:4:243:PRO:O    | 1.14                     | 0.94              |
| 1:D:410:ASN:OD1  | 4:9:334:GLU:C    | 2.10                     | 0.94              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:HG2   | 1.50                     | 0.94              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:CB   | 1.97                     | 0.94              |
| 1:D:218:LEU:CB   | 1:D:221:GLN:CG   | 2.46                     | 0.94              |
| 1:D:507:GLY:O    | 1:D:761:GLY:HA3  | 1.68                     | 0.94              |
| 1:G:790:THR:OG1  | 3:I:87:PHE:CD2   | 2.20                     | 0.94              |
| 1:J:508:ILE:HD11 | 1:J:759:ALA:HB1  | 1.48                     | 0.94              |
| 1:J:530:MET:HA   | 4:W:354:GLN:HG3  | 0.96                     | 0.94              |
| 4:X:291:LYS:HD2  | 4:Z:244:ASP:H    | 1.23                     | 0.94              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:CB    | 2.46                     | 0.93              |
| 1:D:839:MLY:NZ   | 2:E:159:HIS:HB3  | 1.83                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:541:MET:N    | 4:V:349:LEU:HD21 | 1.80                     | 0.93              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:HA3  | 1.83                     | 0.93              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE1   | 1.47                     | 0.93              |
| 1:J:630:ALA:O    | 4:W:25:ASP:CG    | 2.09                     | 0.93              |
| 1:G:543:PRO:CG   | 4:V:143:TYR:O    | 2.14                     | 0.93              |
| 1:G:789:ALA:HB2  | 3:I:81:GLN:HE21  | 0.78                     | 0.93              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:HA3  | 1.83                     | 0.93              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:HA   | 1.47                     | 0.93              |
| 2:B:150:TYR:O    | 2:B:151:LYS:CG   | 2.15                     | 0.93              |
| 1:D:768:MLY:O    | 1:D:771:LEU:CG   | 2.17                     | 0.93              |
| 2:E:117:LEU:HD13 | 2:E:147:ASN:OD1  | 1.64                     | 0.93              |
| 1:G:834:LEU:HD13 | 2:H:51:PHE:HE1   | 0.79                     | 0.93              |
| 4:1:322:PRO:HB3  | 4:3:244:ASP:CG   | 1.93                     | 0.93              |
| 1:A:630:ALA:O    | 4:8:25:ASP:CG    | 2.10                     | 0.93              |
| 1:J:93:MET:CG    | 1:J:764:MLY:NZ   | 2.24                     | 0.93              |
| 4:1:288:ASP:N    | 4:3:203:THR:HG22 | 1.82                     | 0.93              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:HB2  | 1.47                     | 0.93              |
| 1:D:798:LEU:CD1  | 3:F:126:LEU:HD21 | 1.97                     | 0.93              |
| 1:J:530:MET:CA   | 4:W:354:GLN:CG   | 2.44                     | 0.93              |
| 4:0:244:ASP:N    | 4:Y:291:LYS:CD   | 2.31                     | 0.93              |
| 1:A:557:GLU:N    | 4:V:48:GLY:CA    | 2.12                     | 0.93              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:NE   | 2.27                     | 0.93              |
| 1:A:836:PHE:CZ   | 2:B:160:GLY:HA3  | 1.94                     | 0.93              |
| 1:G:84:MLY:CH2   | 1:G:716:LEU:O    | 2.16                     | 0.93              |
| 1:G:93:MET:HE3   | 1:G:764:MLY:HE3  | 1.50                     | 0.93              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG21  | 1.46                     | 0.93              |
| 1:D:790:THR:HA   | 3:F:87:PHE:CE2   | 2.03                     | 0.93              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:CA   | 2.31                     | 0.93              |
| 1:J:739:ASP:HB3  | 1:J:742:LYS:CB   | 1.98                     | 0.93              |
| 4:X:291:LYS:CG   | 4:Z:244:ASP:N    | 2.24                     | 0.93              |
| 1:A:629:GLU:CB   | 1:A:643:GLY:O    | 2.17                     | 0.93              |
| 1:A:648:THR:HG21 | 1:A:651:ALA:HB2  | 1.50                     | 0.93              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:CA   | 2.31                     | 0.93              |
| 1:D:639:GLY:N    | 4:9:345:ILE:N    | 1.94                     | 0.93              |
| 1:D:769:ALA:C    | 1:D:770:GLY:O    | 2.12                     | 0.93              |
| 1:G:93:MET:HE2   | 1:G:763:THR:C    | 1.94                     | 0.93              |
| 1:J:206:LYS:CD   | 1:J:217:THR:CG2  | 2.16                     | 0.93              |
| 1:J:823:PHE:CE1  | 2:K:156:VAL:O    | 2.22                     | 0.93              |
| 1:J:215:GLN:HA   | 1:J:340:ILE:HG23 | 0.95                     | 0.93              |
| 1:G:642:LYS:CB   | 4:V:21:PHE:O     | 2.17                     | 0.92              |
| 1:J:538:GLU:N    | 4:W:351:THR:H    | 1.67                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:541:MET:N    | 4:W:349:LEU:HD21 | 1.80                     | 0.92              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:CA   | 2.31                     | 0.92              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CG   | 2.00                     | 0.92              |
| 1:G:530:MET:CA   | 4:V:354:GLN:CG   | 2.45                     | 0.92              |
| 1:G:819:ASN:CB   | 2:H:90:GLY:O     | 2.17                     | 0.92              |
| 1:G:821:ARG:HH21 | 2:H:127:ARG:HG2  | 1.33                     | 0.92              |
| 4:1:287:ILE:CD1  | 4:3:203:THR:HB   | 1.98                     | 0.92              |
| 4:V:286:ASP:OD2  | 4:X:203:THR:HG22 | 1.69                     | 0.92              |
| 1:G:215:GLN:HA   | 1:G:340:ILE:HG23 | 0.95                     | 0.92              |
| 1:G:795:ARG:CG   | 3:I:35:ARG:HH22  | 1.81                     | 0.92              |
| 1:J:648:THR:HG21 | 1:J:651:ALA:HB2  | 1.50                     | 0.92              |
| 1:J:768:MLY:HH12 | 1:J:772:LEU:HD21 | 1.49                     | 0.92              |
| 1:J:818:TYR:HB3  | 2:K:90:GLY:HA3   | 1.51                     | 0.92              |
| 4:X:324:THR:CG2  | 4:Z:247:VAL:HG23 | 1.93                     | 0.92              |
| 1:A:215:GLN:HA   | 1:A:340:ILE:HG23 | 0.95                     | 0.92              |
| 1:A:502:GLU:HG3  | 1:A:761:GLY:N    | 1.85                     | 0.92              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CD1  | 1.98                     | 0.92              |
| 1:D:557:GLU:H    | 4:W:48:GLY:HA2   | 1.32                     | 0.92              |
| 1:D:629:GLU:CB   | 1:D:643:GLY:O    | 2.17                     | 0.92              |
| 1:J:636:LYS:HD2  | 4:W:332:PRO:HB3  | 1.52                     | 0.92              |
| 4:O:246:GLN:HA   | 4:Y:324:THR:OG1  | 1.70                     | 0.92              |
| 4:W:286:ASP:OD1  | 4:Y:202:THR:HB   | 1.69                     | 0.92              |
| 1:A:642:LYS:CB   | 4:8:21:PHE:O     | 2.17                     | 0.92              |
| 1:A:739:ASP:HB3  | 1:A:742:LYS:CB   | 1.98                     | 0.92              |
| 1:D:530:MET:CA   | 4:9:354:GLN:CG   | 2.45                     | 0.92              |
| 1:G:648:THR:HG21 | 1:G:651:ALA:HB2  | 1.50                     | 0.92              |
| 1:J:546:THR:HG22 | 1:J:548:THR:H    | 1.32                     | 0.92              |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:H    | 1.29                     | 0.92              |
| 1:D:278:GLN:HG2  | 1:D:317:GLU:HB2  | 1.52                     | 0.92              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:HA3  | 1.83                     | 0.92              |
| 1:D:790:THR:CA   | 3:F:87:PHE:CE2   | 2.47                     | 0.92              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HB2  | 1.82                     | 0.92              |
| 1:J:797:PHE:CG   | 3:L:149:VAL:HG11 | 2.04                     | 0.92              |
| 1:D:550:PHE:HA   | 4:W:46:GLY:CA    | 2.00                     | 0.92              |
| 1:G:629:GLU:CB   | 1:G:643:GLY:O    | 2.17                     | 0.92              |
| 1:G:783:LEU:O    | 1:G:787:ILE:HB   | 1.70                     | 0.92              |
| 1:J:530:MET:CE   | 4:W:354:GLN:CG   | 2.40                     | 0.92              |
| 1:J:629:GLU:CB   | 1:J:643:GLY:O    | 2.17                     | 0.92              |
| 4:8:322:PRO:HB2  | 4:V:244:ASP:CG   | 1.94                     | 0.92              |
| 1:A:546:THR:HG22 | 1:A:548:THR:H    | 1.32                     | 0.92              |
| 1:A:636:LYS:HD2  | 4:8:332:PRO:HB3  | 1.51                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:836:PHE:HB3  | 2:B:161:GLU:CG   | 2.00                     | 0.92              |
| 2:K:149:ASP:CG   | 2:K:150:TYR:H    | 1.73                     | 0.92              |
| 4:9:322:PRO:HB2  | 4:W:244:ASP:CG   | 1.94                     | 0.92              |
| 1:D:537:GLU:O    | 4:9:349:LEU:HD13 | 0.74                     | 0.92              |
| 1:D:790:THR:N    | 3:F:87:PHE:HE2   | 1.67                     | 0.92              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CG   | 2.00                     | 0.92              |
| 4:1:287:ILE:CG1  | 4:3:202:THR:HB   | 2.00                     | 0.92              |
| 4:X:291:LYS:CD   | 4:Z:243:PRO:C    | 2.41                     | 0.92              |
| 1:D:636:LYS:HD2  | 4:9:332:PRO:HB3  | 1.52                     | 0.92              |
| 1:D:648:THR:HG21 | 1:D:651:ALA:HB2  | 1.50                     | 0.92              |
| 1:D:739:ASP:HB3  | 1:D:742:LYS:CB   | 1.98                     | 0.92              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:CD   | 2.20                     | 0.92              |
| 1:J:642:LYS:CB   | 4:W:21:PHE:O     | 2.17                     | 0.92              |
| 1:A:769:ALA:C    | 1:A:772:LEU:H    | 1.78                     | 0.91              |
| 1:D:642:LYS:CB   | 4:9:21:PHE:O     | 2.17                     | 0.91              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:HB3  | 1.99                     | 0.91              |
| 1:G:754:ASP:OD2  | 1:G:776:GLU:OE2  | 1.87                     | 0.91              |
| 1:J:537:GLU:O    | 4:W:349:LEU:HD13 | 0.73                     | 0.91              |
| 4:3:288:ASP:OD1  | 4:5:203:THR:HG23 | 1.70                     | 0.91              |
| 4:7:322:PRO:HB2  | 4:9:244:ASP:CG   | 1.94                     | 0.91              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:CZ    | 1.99                     | 0.91              |
| 1:D:796:GLY:HA3  | 3:F:40:ASN:OD1   | 1.70                     | 0.91              |
| 1:J:278:GLN:HG2  | 1:J:317:GLU:HB2  | 1.52                     | 0.91              |
| 1:J:538:GLU:N    | 4:W:349:LEU:HD12 | 1.86                     | 0.91              |
| 1:J:636:LYS:H    | 4:W:334:GLU:CD   | 1.78                     | 0.91              |
| 4:1:287:ILE:HG12 | 4:3:202:THR:HA   | 1.48                     | 0.91              |
| 4:1:287:ILE:HB   | 4:3:203:THR:N    | 1.82                     | 0.91              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:CG   | 2.01                     | 0.91              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:HG21 | 1.90                     | 0.91              |
| 1:G:636:LYS:H    | 4:V:334:GLU:CD   | 1.78                     | 0.91              |
| 1:J:218:LEU:CB   | 1:J:221:GLN:CG   | 2.45                     | 0.91              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CG   | 2.00                     | 0.91              |
| 4:1:287:ILE:CG1  | 4:3:202:THR:CB   | 2.48                     | 0.91              |
| 1:A:544:LYS:HD2  | 4:8:147:ARG:HB3  | 1.52                     | 0.91              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HB2  | 1.82                     | 0.91              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HB3  | 1.34                     | 0.91              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:CG   | 2.01                     | 0.91              |
| 1:G:537:GLU:O    | 4:V:349:LEU:HD13 | 0.74                     | 0.91              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:HD23 | 1.51                     | 0.91              |
| 1:J:798:LEU:HD21 | 3:L:126:LEU:HG   | 1.50                     | 0.91              |
| 4:W:286:ASP:CG   | 4:Y:203:THR:HG22 | 1.96                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:291:LYS:CD   | 4:Z:243:PRO:HB2  | 1.99                     | 0.91              |
| 1:A:753:VAL:HA   | 1:A:778:MET:SD   | 2.11                     | 0.91              |
| 1:D:538:GLU:N    | 4:9:351:THR:H    | 1.68                     | 0.91              |
| 2:E:149:ASP:CG   | 2:E:150:TYR:H    | 1.72                     | 0.91              |
| 1:G:544:LYS:HD2  | 4:V:147:ARG:HB3  | 1.53                     | 0.91              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:HH21  | 1.33                     | 0.91              |
| 1:A:636:LYS:H    | 4:8:334:GLU:CD   | 1.77                     | 0.91              |
| 1:G:567:LYS:HZ2  | 4:X:92:ASN:HD22  | 1.00                     | 0.91              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB2  | 1.51                     | 0.91              |
| 1:A:557:GLU:H    | 4:V:48:GLY:HA2   | 1.32                     | 0.91              |
| 1:A:757:GLN:CG   | 1:A:771:LEU:CD1  | 2.43                     | 0.91              |
| 3:C:62:ALA:O     | 3:C:63:ILE:CG1   | 2.19                     | 0.91              |
| 1:D:799:MET:CE   | 3:F:32:ASP:HB3   | 2.01                     | 0.91              |
| 3:F:62:ALA:O     | 3:F:63:ILE:CG1   | 2.19                     | 0.91              |
| 1:G:538:GLU:N    | 4:V:351:THR:H    | 1.68                     | 0.91              |
| 1:G:638:GLY:HA3  | 4:V:341:ILE:O    | 1.70                     | 0.91              |
| 1:G:739:ASP:HB3  | 1:G:742:LYS:CB   | 1.98                     | 0.91              |
| 1:J:92:ALA:O     | 1:J:714:ARG:CD   | 2.18                     | 0.91              |
| 1:D:735:GLY:O    | 1:D:743:ALA:CA   | 2.19                     | 0.91              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:NH2   | 1.83                     | 0.91              |
| 4:0:287:ILE:HG23 | 4:2:202:THR:HB   | 1.53                     | 0.91              |
| 1:A:537:GLU:O    | 4:8:349:LEU:HD13 | 0.73                     | 0.91              |
| 1:A:550:PHE:HA   | 4:V:46:GLY:CA    | 2.00                     | 0.91              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:CG   | 2.44                     | 0.91              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:HG   | 1.71                     | 0.91              |
| 1:G:831:TRP:CH2  | 2:H:47:LEU:HD21  | 1.94                     | 0.91              |
| 3:I:62:ALA:O     | 3:I:63:ILE:HG12  | 1.71                     | 0.91              |
| 1:A:538:GLU:N    | 4:8:349:LEU:HD12 | 1.86                     | 0.90              |
| 1:A:538:GLU:N    | 4:8:351:THR:H    | 1.67                     | 0.90              |
| 1:A:649:VAL:CB   | 1:A:649:VAL:CG2  | 2.49                     | 0.90              |
| 1:D:553:MLY:HE2  | 4:W:45:VAL:HA    | 1.53                     | 0.90              |
| 1:D:636:LYS:H    | 4:9:334:GLU:CD   | 1.78                     | 0.90              |
| 1:D:836:PHE:CB   | 2:E:161:GLU:OE1  | 2.19                     | 0.90              |
| 1:J:561:LYS:HE3  | 4:Y:48:GLY:HA3   | 1.50                     | 0.90              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:HG2  | 1.33                     | 0.90              |
| 1:A:638:GLY:HA3  | 4:8:341:ILE:O    | 1.70                     | 0.90              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:CG   | 2.54                     | 0.90              |
| 1:D:649:VAL:CG2  | 1:D:649:VAL:HG13 | 2.02                     | 0.90              |
| 3:F:62:ALA:O     | 3:F:63:ILE:HG12  | 1.71                     | 0.90              |
| 1:G:278:GLN:HG2  | 1:G:317:GLU:HB2  | 1.52                     | 0.90              |
| 1:G:636:LYS:HD2  | 4:V:332:PRO:HB3  | 1.52                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:649:VAL:CB   | 1:G:649:VAL:CG2  | 2.49                     | 0.90              |
| 1:J:544:LYS:HD2  | 4:W:147:ARG:HB3  | 1.53                     | 0.90              |
| 4:V:324:THR:CG2  | 4:X:247:VAL:H    | 1.83                     | 0.90              |
| 1:A:505:MLY:CH2  | 1:A:762:HIS:O    | 2.19                     | 0.90              |
| 1:D:538:GLU:O    | 4:9:349:LEU:CG   | 2.20                     | 0.90              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CG   | 2.00                     | 0.90              |
| 1:G:553:MLY:HG3  | 4:X:45:VAL:C     | 1.95                     | 0.90              |
| 1:G:567:LYS:HZ1  | 4:X:92:ASN:ND2   | 1.65                     | 0.90              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:CG   | 2.44                     | 0.90              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:CG   | 2.50                     | 0.90              |
| 1:G:107:MLY:HB3  | 1:G:686:MET:HE2  | 1.54                     | 0.90              |
| 1:G:538:GLU:N    | 4:V:349:LEU:HD12 | 1.87                     | 0.90              |
| 1:G:721:LYS:CB   | 1:G:736:GLN:OE1  | 2.20                     | 0.90              |
| 1:J:735:GLY:O    | 1:J:743:ALA:CA   | 2.19                     | 0.90              |
| 1:A:795:ARG:NE   | 3:C:118:MET:HE1  | 1.87                     | 0.90              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:CG   | 2.01                     | 0.90              |
| 1:D:544:LYS:HD2  | 4:9:147:ARG:HB3  | 1.53                     | 0.90              |
| 2:E:121:LEU:CB   | 2:E:128:PHE:HB3  | 1.68                     | 0.90              |
| 3:I:62:ALA:O     | 3:I:63:ILE:CG1   | 2.19                     | 0.90              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:HG13 | 2.02                     | 0.90              |
| 2:K:150:TYR:O    | 2:K:151:LYS:HB2  | 1.67                     | 0.90              |
| 4:1:287:ILE:CD1  | 4:3:203:THR:N    | 2.34                     | 0.90              |
| 1:D:534:SER:O    | 4:9:351:THR:HG23 | 1.13                     | 0.90              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:SD   | 2.65                     | 0.90              |
| 1:D:769:ALA:CB   | 1:D:770:GLY:C    | 2.44                     | 0.90              |
| 2:H:137:TRP:HA   | 2:H:145:ALA:HB2  | 1.53                     | 0.90              |
| 1:A:278:GLN:HG2  | 1:A:317:GLU:HB2  | 1.52                     | 0.90              |
| 1:G:768:MLY:HH23 | 1:G:772:LEU:HD22 | 1.53                     | 0.90              |
| 1:J:630:ALA:C    | 4:W:25:ASP:OD2   | 2.15                     | 0.90              |
| 1:J:818:TYR:HB3  | 2:K:90:GLY:CA    | 2.00                     | 0.90              |
| 1:A:817:GLN:HB2  | 2:B:127:ARG:CZ   | 2.02                     | 0.90              |
| 1:D:550:PHE:CA   | 4:W:46:GLY:HA3   | 2.02                     | 0.90              |
| 2:E:137:TRP:HA   | 2:E:145:ALA:HB2  | 1.53                     | 0.90              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:CG   | 2.44                     | 0.90              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:CG   | 2.00                     | 0.90              |
| 1:J:530:MET:N    | 4:W:354:GLN:HB3  | 1.87                     | 0.90              |
| 4:1:287:ILE:HG21 | 4:3:202:THR:CB   | 2.02                     | 0.90              |
| 1:D:538:GLU:N    | 4:9:349:LEU:HD12 | 1.86                     | 0.90              |
| 1:G:215:GLN:H    | 1:G:340:ILE:CG1  | 1.72                     | 0.90              |
| 1:G:629:GLU:HG2  | 1:G:643:GLY:O    | 1.72                     | 0.90              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:CD   | 2.35                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:629:GLU:HG2  | 1:A:643:GLY:O    | 1.72                     | 0.90              |
| 1:A:735:GLY:O    | 1:A:743:ALA:CA   | 2.19                     | 0.90              |
| 1:D:630:ALA:C    | 4:9:25:ASP:OD2   | 2.15                     | 0.90              |
| 1:D:638:GLY:HA3  | 4:9:341:ILE:O    | 1.70                     | 0.90              |
| 1:D:790:THR:N    | 3:F:87:PHE:CE2   | 2.40                     | 0.90              |
| 1:J:538:GLU:O    | 4:W:349:LEU:CG   | 2.20                     | 0.90              |
| 1:J:635:GLY:CA   | 4:W:341:ILE:HD13 | 2.02                     | 0.90              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:CG2  | 1.95                     | 0.90              |
| 1:A:107:MLY:HB3  | 1:A:686:MET:HE2  | 1.54                     | 0.89              |
| 1:A:630:ALA:C    | 4:8:25:ASP:OD2   | 2.15                     | 0.89              |
| 3:C:24:LYS:HB3   | 3:C:63:ILE:O     | 1.72                     | 0.89              |
| 1:G:735:GLY:O    | 1:G:743:ALA:CA   | 2.19                     | 0.89              |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:CD2   | 2.02                     | 0.89              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:CE    | 2.02                     | 0.89              |
| 1:D:553:MLY:CG   | 4:W:44:MET:O     | 2.20                     | 0.89              |
| 1:D:649:VAL:CB   | 1:D:649:VAL:CG2  | 2.49                     | 0.89              |
| 1:D:795:ARG:CB   | 3:F:35:ARG:NE    | 2.25                     | 0.89              |
| 1:G:553:MLY:NZ   | 4:X:45:VAL:HG11  | 1.87                     | 0.89              |
| 1:J:107:MLY:HB3  | 1:J:686:MET:HE2  | 1.54                     | 0.89              |
| 1:J:757:GLN:CD   | 1:J:776:GLU:HG3  | 1.95                     | 0.89              |
| 1:A:640:LYS:C    | 4:8:23:GLY:O     | 2.15                     | 0.89              |
| 3:C:62:ALA:O     | 3:C:63:ILE:HG12  | 1.71                     | 0.89              |
| 1:J:503:TYR:OH   | 1:J:711:PHE:HD2  | 1.55                     | 0.89              |
| 3:L:62:ALA:O     | 3:L:63:ILE:CG1   | 2.19                     | 0.89              |
| 4:O:246:GLN:CA   | 4:Y:324:THR:HB   | 2.01                     | 0.89              |
| 1:A:530:MET:N    | 4:8:354:GLN:HB3  | 1.87                     | 0.89              |
| 1:D:721:LYS:CB   | 1:D:736:GLN:OE1  | 2.20                     | 0.89              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:HB   | 1.72                     | 0.89              |
| 1:J:534:SER:HA   | 4:W:350:SER:O    | 1.71                     | 0.89              |
| 1:J:721:LYS:CB   | 1:J:736:GLN:OE1  | 2.20                     | 0.89              |
| 1:D:635:GLY:CA   | 4:9:341:ILE:HD13 | 2.02                     | 0.89              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HB2  | 1.82                     | 0.89              |
| 1:J:649:VAL:CB   | 1:J:649:VAL:CG2  | 2.49                     | 0.89              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:CG   | 2.44                     | 0.89              |
| 1:A:93:MET:HE2   | 1:A:715:VAL:HA   | 1.52                     | 0.89              |
| 1:G:538:GLU:O    | 4:V:349:LEU:CG   | 2.20                     | 0.89              |
| 1:G:795:ARG:CG   | 3:I:35:ARG:NH2   | 2.34                     | 0.89              |
| 1:J:640:LYS:C    | 4:W:23:GLY:O     | 2.15                     | 0.89              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HB1  | 1.84                     | 0.89              |
| 1:A:553:MLY:CG   | 4:V:44:MET:O     | 2.20                     | 0.89              |
| 1:A:721:LYS:CB   | 1:A:736:GLN:OE1  | 2.20                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:107:MLY:HB3  | 1:D:686:MET:HE2  | 1.54                     | 0.89              |
| 1:D:641:LYS:HD2  | 4:9:348:SER:CB   | 2.02                     | 0.89              |
| 1:J:215:GLN:H    | 1:J:340:ILE:CG1  | 1.72                     | 0.89              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:HZ    | 1.85                     | 0.89              |
| 2:K:137:TRP:HA   | 2:K:145:ALA:HB2  | 1.53                     | 0.89              |
| 4:1:203:THR:CB   | 4:Z:287:ILE:HD13 | 2.01                     | 0.89              |
| 1:D:530:MET:N    | 4:9:354:GLN:HB3  | 1.87                     | 0.89              |
| 1:D:534:SER:HA   | 4:9:350:SER:O    | 1.71                     | 0.89              |
| 1:D:629:GLU:HG2  | 1:D:643:GLY:O    | 1.72                     | 0.89              |
| 1:D:649:VAL:HG12 | 1:D:649:VAL:C    | 1.98                     | 0.89              |
| 1:D:815:CYS:O    | 2:E:90:GLY:O     | 1.89                     | 0.89              |
| 1:G:707:CYS:O    | 1:G:714:ARG:NH2  | 2.05                     | 0.89              |
| 1:A:534:SER:HA   | 4:8:350:SER:O    | 1.70                     | 0.89              |
| 1:A:795:ARG:CZ   | 3:C:116:GLU:OE2  | 2.20                     | 0.89              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HH11 | 1.38                     | 0.89              |
| 1:J:649:VAL:HG12 | 1:J:649:VAL:C    | 1.98                     | 0.89              |
| 4:0:247:VAL:HG23 | 4:Y:324:THR:CG2  | 1.99                     | 0.89              |
| 1:A:538:GLU:O    | 4:8:349:LEU:CG   | 2.20                     | 0.89              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:HG22 | 1.53                     | 0.89              |
| 4:X:324:THR:CB   | 4:Z:246:GLN:HA   | 2.03                     | 0.89              |
| 1:A:836:PHE:HE1  | 2:B:159:HIS:HA   | 1.36                     | 0.88              |
| 1:D:541:MET:CB   | 4:9:143:TYR:OH   | 2.20                     | 0.88              |
| 1:G:534:SER:HA   | 4:V:350:SER:O    | 1.71                     | 0.88              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:CB   | 2.46                     | 0.88              |
| 1:J:92:ALA:O     | 1:J:714:ARG:HG3  | 1.73                     | 0.88              |
| 1:J:641:LYS:HD2  | 4:W:348:SER:CB   | 2.02                     | 0.88              |
| 3:L:62:ALA:O     | 3:L:63:ILE:HG12  | 1.71                     | 0.88              |
| 1:A:550:PHE:CA   | 4:V:46:GLY:HA3   | 2.02                     | 0.88              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:HB2  | 2.02                     | 0.88              |
| 1:A:819:ASN:CG   | 2:B:91:ALA:CA    | 2.13                     | 0.88              |
| 1:D:640:LYS:C    | 4:9:23:GLY:O     | 2.15                     | 0.88              |
| 1:G:530:MET:N    | 4:V:354:GLN:HB3  | 1.88                     | 0.88              |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:CB   | 2.02                     | 0.88              |
| 1:J:638:GLY:HA3  | 4:W:341:ILE:O    | 1.70                     | 0.88              |
| 1:J:757:GLN:OE1  | 1:J:772:LEU:O    | 1.91                     | 0.88              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:HA2  | 0.89                     | 0.88              |
| 1:D:215:GLN:H    | 1:D:340:ILE:HG12 | 1.06                     | 0.88              |
| 1:D:507:GLY:O    | 1:D:761:GLY:HA2  | 1.72                     | 0.88              |
| 1:G:541:MET:CB   | 4:V:143:TYR:OH   | 2.21                     | 0.88              |
| 1:A:642:LYS:HG2  | 4:8:22:ALA:CA    | 2.04                     | 0.88              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:NH2   | 2.37                     | 0.88              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:641:LYS:CD  | 1:D:647:GLN:OE1  | 2.17                     | 0.88              |
| 2:E:137:TRP:HA  | 2:E:145:ALA:CB   | 2.03                     | 0.88              |
| 1:G:510:TRP:CZ3 | 1:G:768:MLY:CH1  | 2.57                     | 0.88              |
| 1:G:640:LYS:C   | 4:V:23:GLY:O     | 2.16                     | 0.88              |
| 1:J:642:LYS:HG2 | 4:W:22:ALA:CA    | 2.03                     | 0.88              |
| 4:0:167:GLU:OE1 | 4:2:43:VAL:O     | 1.91                     | 0.88              |
| 1:A:541:MET:CB  | 4:8:143:TYR:OH   | 2.20                     | 0.88              |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:HB   | 1.73                     | 0.88              |
| 1:D:792:ALA:HB1 | 3:F:40:ASN:O     | 1.73                     | 0.88              |
| 1:G:641:LYS:CD  | 1:G:647:GLN:OE1  | 2.17                     | 0.88              |
| 1:G:642:LYS:HG2 | 4:V:22:ALA:CA    | 2.03                     | 0.88              |
| 1:G:817:GLN:OE1 | 2:H:127:ARG:HD2  | 1.72                     | 0.88              |
| 1:J:818:TYR:CE1 | 2:K:127:ARG:NH2  | 2.42                     | 0.88              |
| 1:A:505:MLY:HG3 | 1:A:741:LYS:HZ2  | 1.38                     | 0.88              |
| 1:G:817:GLN:CG  | 2:H:127:ARG:CD   | 2.51                     | 0.88              |
| 1:J:84:MLY:HH12 | 1:J:715:VAL:CG1  | 1.75                     | 0.88              |
| 1:J:629:GLU:HG2 | 1:J:643:GLY:O    | 1.72                     | 0.88              |
| 3:L:24:LYS:HB3  | 3:L:63:ILE:O     | 1.72                     | 0.88              |
| 1:G:819:ASN:CG  | 2:H:92:ASP:CB    | 2.47                     | 0.88              |
| 1:J:215:GLN:H   | 1:J:340:ILE:HG12 | 1.05                     | 0.88              |
| 1:A:553:MLY:HE2 | 4:V:45:VAL:HA    | 1.53                     | 0.88              |
| 1:D:635:GLY:HA2 | 4:9:334:GLU:CG   | 2.03                     | 0.88              |
| 1:J:642:LYS:CG  | 4:W:21:PHE:O     | 2.22                     | 0.88              |
| 1:J:831:TRP:HZ2 | 2:K:47:LEU:CD2   | 1.82                     | 0.88              |
| 1:A:641:LYS:HD2 | 4:8:348:SER:CB   | 2.02                     | 0.88              |
| 3:C:139:TYR:HA  | 3:C:142:PHE:HB3  | 1.56                     | 0.88              |
| 3:F:139:TYR:HA  | 3:F:142:PHE:HB3  | 1.56                     | 0.88              |
| 1:G:642:LYS:CG  | 4:V:21:PHE:O     | 2.22                     | 0.88              |
| 1:G:649:VAL:CG2 | 1:G:649:VAL:HG13 | 2.02                     | 0.88              |
| 1:J:541:MET:CB  | 4:W:143:TYR:OH   | 2.20                     | 0.88              |
| 2:B:137:TRP:HA  | 2:B:145:ALA:HB2  | 1.54                     | 0.88              |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:CD1  | 2.58                     | 0.87              |
| 1:G:542:PHE:HA  | 4:V:143:TYR:HE1  | 1.34                     | 0.87              |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:CD1  | 2.58                     | 0.87              |
| 1:A:91:MET:HE3  | 1:A:119:SER:HB2  | 1.56                     | 0.87              |
| 1:A:707:CYS:SG  | 1:A:714:ARG:NH1  | 2.48                     | 0.87              |
| 1:A:795:ARG:HB3 | 3:C:35:ARG:CZ    | 2.04                     | 0.87              |
| 1:D:769:ALA:HA  | 1:D:771:LEU:CB   | 2.04                     | 0.87              |
| 1:G:557:GLU:HB2 | 4:X:46:GLY:C     | 2.00                     | 0.87              |
| 3:I:24:LYS:HB3  | 3:I:63:ILE:O     | 1.72                     | 0.87              |
| 3:L:139:TYR:HA  | 3:L:142:PHE:HB3  | 1.56                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:72:VAL:CG1   | 1:A:76:GLN:HB3   | 2.05                     | 0.87              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:NE2  | 1.58                     | 0.87              |
| 1:A:789:ALA:HB1  | 3:C:87:PHE:HE2   | 1.39                     | 0.87              |
| 1:D:642:LYS:CG   | 4:9:21:PHE:O     | 2.22                     | 0.87              |
| 1:G:635:GLY:CA   | 4:V:341:ILE:HD13 | 2.02                     | 0.87              |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:HB1  | 1.56                     | 0.87              |
| 1:J:567:LYS:HZ3  | 4:Y:92:ASN:HD22  | 1.19                     | 0.87              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:HG22 | 1.82                     | 0.87              |
| 4:3:287:ILE:CG2  | 4:5:204:ALA:H    | 1.87                     | 0.87              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:CD1  | 2.57                     | 0.87              |
| 1:A:635:GLY:CA   | 4:8:341:ILE:HD13 | 2.02                     | 0.87              |
| 1:A:642:LYS:CG   | 4:8:21:PHE:O     | 2.22                     | 0.87              |
| 2:B:137:TRP:HA   | 2:B:145:ALA:CB   | 2.04                     | 0.87              |
| 1:D:642:LYS:HG2  | 4:9:22:ALA:CA    | 2.03                     | 0.87              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:CA   | 2.53                     | 0.87              |
| 1:G:788:THR:C    | 3:I:42:THR:CG2   | 2.34                     | 0.87              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:CA   | 2.53                     | 0.87              |
| 2:B:111:SER:OG   | 2:B:148:VAL:C    | 2.15                     | 0.87              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:CA   | 2.53                     | 0.87              |
| 4:1:324:THR:CG2  | 4:3:244:ASP:HA   | 2.05                     | 0.87              |
| 4:X:288:ASP:N    | 4:Z:202:THR:OG1  | 2.03                     | 0.87              |
| 1:A:215:GLN:H    | 1:A:340:ILE:HG12 | 1.06                     | 0.87              |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:CG2  | 2.02                     | 0.87              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HB2  | 1.82                     | 0.87              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:HB    | 2.08                     | 0.87              |
| 1:D:724:TYR:HE1  | 1:D:778:MET:CB   | 1.88                     | 0.87              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:HG21 | 1.57                     | 0.87              |
| 1:J:84:MLY:HE2   | 1:J:719:ASP:OD2  | 1.74                     | 0.87              |
| 1:J:635:GLY:HA2  | 4:W:334:GLU:CG   | 2.03                     | 0.87              |
| 1:A:839:MLY:NZ   | 2:B:159:HIS:HB3  | 1.90                     | 0.87              |
| 2:E:163:ALA:HA   | 2:K:21:GLU:HB3   | 1.54                     | 0.87              |
| 1:G:641:LYS:HD2  | 4:V:348:SER:CB   | 2.03                     | 0.87              |
| 2:H:111:SER:OG   | 2:H:148:VAL:C    | 2.15                     | 0.87              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:CG   | 2.46                     | 0.87              |
| 4:1:202:THR:CA   | 4:Z:287:ILE:CG1  | 2.52                     | 0.87              |
| 4:1:324:THR:HG23 | 4:3:244:ASP:HA   | 1.55                     | 0.87              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:CD    | 2.05                     | 0.87              |
| 1:G:72:VAL:CG1   | 1:G:76:GLN:HB3   | 2.05                     | 0.87              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:CA   | 2.05                     | 0.87              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HD3  | 1.56                     | 0.87              |
| 1:J:639:GLY:CA   | 4:W:344:SER:C    | 2.48                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:649:VAL:CG1  | 1:J:649:VAL:CA   | 2.53                     | 0.87              |
| 4:1:322:PRO:CB   | 4:3:244:ASP:HB3  | 2.04                     | 0.87              |
| 1:A:530:MET:HG2  | 4:8:354:GLN:CG   | 2.05                     | 0.86              |
| 1:D:91:MET:HE3   | 1:D:119:SER:HB2  | 1.56                     | 0.86              |
| 1:G:639:GLY:CA   | 4:V:344:SER:C    | 2.48                     | 0.86              |
| 2:H:137:TRP:HA   | 2:H:145:ALA:CB   | 2.04                     | 0.86              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:CA   | 2.05                     | 0.86              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:OE1  | 2.17                     | 0.86              |
| 4:0:112:PRO:HG3  | 4:1:195:GLU:O    | 1.73                     | 0.86              |
| 4:V:286:ASP:OD1  | 4:X:203:THR:HG22 | 1.74                     | 0.86              |
| 1:A:542:PHE:HA   | 4:8:143:TYR:HE1  | 1.34                     | 0.86              |
| 1:A:639:GLY:CA   | 4:8:344:SER:C    | 2.48                     | 0.86              |
| 1:D:530:MET:HG2  | 4:9:354:GLN:CG   | 2.05                     | 0.86              |
| 1:D:755:HIS:HA   | 1:D:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:G:646:PHE:CD2  | 1:G:652:LEU:HD11 | 2.09                     | 0.86              |
| 1:A:798:LEU:CD2  | 3:C:122:GLU:HB3  | 2.06                     | 0.86              |
| 1:A:817:GLN:OE1  | 2:B:127:ARG:NH2  | 1.80                     | 0.86              |
| 1:J:557:GLU:HA   | 4:Y:48:GLY:N     | 1.90                     | 0.86              |
| 1:D:310:TYR:CZ   | 1:D:320:ILE:HD11 | 2.11                     | 0.86              |
| 1:D:639:GLY:CA   | 4:9:344:SER:C    | 2.48                     | 0.86              |
| 1:D:646:PHE:CD2  | 1:D:652:LEU:HD11 | 2.09                     | 0.86              |
| 1:G:795:ARG:HD2  | 3:I:35:ARG:HH22  | 0.71                     | 0.86              |
| 1:J:72:VAL:CG1   | 1:J:76:GLN:HB3   | 2.05                     | 0.86              |
| 1:J:530:MET:HG2  | 4:W:354:GLN:CG   | 2.05                     | 0.86              |
| 2:K:137:TRP:HA   | 2:K:145:ALA:CB   | 2.04                     | 0.86              |
| 4:1:287:ILE:HB   | 4:3:203:THR:CG2  | 2.04                     | 0.86              |
| 4:8:287:ILE:CG2  | 4:V:205:GLU:HG2  | 2.05                     | 0.86              |
| 4:X:287:ILE:CG2  | 4:Z:201:VAL:HG23 | 2.06                     | 0.86              |
| 1:G:93:MET:CE    | 1:G:763:THR:C    | 2.48                     | 0.86              |
| 1:G:530:MET:HG2  | 4:V:354:GLN:CG   | 2.05                     | 0.86              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HB1  | 1.84                     | 0.86              |
| 1:J:310:TYR:CZ   | 1:J:320:ILE:HD11 | 2.11                     | 0.86              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:HB   | 1.73                     | 0.86              |
| 1:J:797:PHE:CD1  | 3:L:149:VAL:HG12 | 2.07                     | 0.86              |
| 3:F:24:LYS:HB3   | 3:F:63:ILE:O     | 1.72                     | 0.86              |
| 1:J:508:ILE:HD11 | 1:J:759:ALA:HB2  | 0.87                     | 0.86              |
| 4:0:287:ILE:CG1  | 4:2:203:THR:H    | 1.88                     | 0.86              |
| 1:D:72:VAL:CG1   | 1:D:76:GLN:HB3   | 2.05                     | 0.86              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:CB   | 2.06                     | 0.86              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:CA   | 2.05                     | 0.86              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:CB   | 2.06                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:755:HIS:HA   | 1:G:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:J:797:PHE:CB   | 3:L:149:VAL:CG1  | 2.53                     | 0.86              |
| 1:A:549:SER:O    | 4:V:46:GLY:C     | 2.19                     | 0.86              |
| 1:A:793:ARG:HG3  | 3:C:146:ILE:HG22 | 1.58                     | 0.86              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:O    | 1.92                     | 0.86              |
| 1:A:538:GLU:N    | 4:8:351:THR:N    | 2.24                     | 0.86              |
| 1:D:549:SER:O    | 4:W:46:GLY:C     | 2.18                     | 0.86              |
| 1:G:823:PHE:CE1  | 2:H:156:VAL:O    | 2.29                     | 0.86              |
| 1:J:755:HIS:HA   | 1:J:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:CB    | 1.88                     | 0.86              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:CH1  | 2.05                     | 0.86              |
| 1:J:646:PHE:CD2  | 1:J:652:LEU:HD11 | 2.09                     | 0.86              |
| 1:J:797:PHE:HA   | 3:L:149:VAL:HG11 | 1.58                     | 0.86              |
| 4:O:205:GLU:CD   | 4:Y:287:ILE:C    | 2.44                     | 0.86              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:CA   | 2.05                     | 0.85              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:OE1  | 2.17                     | 0.85              |
| 1:A:755:HIS:HA   | 1:A:758:TYR:CE1  | 2.10                     | 0.85              |
| 1:D:814:PHE:HD1  | 2:E:127:ARG:NH2  | 1.70                     | 0.85              |
| 1:G:91:MET:HE3   | 1:G:119:SER:HB2  | 1.56                     | 0.85              |
| 1:G:215:GLN:H    | 1:G:340:ILE:HG12 | 1.06                     | 0.85              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:CB   | 2.06                     | 0.85              |
| 1:J:410:ASN:OD1  | 4:W:334:GLU:CA   | 2.24                     | 0.85              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:HA   | 1.76                     | 0.85              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:CA   | 2.25                     | 0.85              |
| 1:G:204:GLU:H    | 1:G:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:A:502:GLU:HA   | 1:A:762:HIS:N    | 1.91                     | 0.85              |
| 3:I:139:TYR:HA   | 3:I:142:PHE:HB3  | 1.56                     | 0.85              |
| 1:J:817:GLN:HB3  | 2:K:127:ARG:HH11 | 1.41                     | 0.85              |
| 4:O:243:PRO:C    | 4:Y:291:LYS:CD   | 2.49                     | 0.85              |
| 4:1:244:ASP:HB3  | 4:Z:322:PRO:CB   | 2.05                     | 0.85              |
| 4:1:322:PRO:HB2  | 4:3:244:ASP:HB3  | 1.57                     | 0.85              |
| 1:A:95:THR:OG1   | 1:A:769:ALA:HA   | 1.75                     | 0.85              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CB   | 2.35                     | 0.85              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HB2  | 1.57                     | 0.85              |
| 1:G:707:CYS:HB3  | 1:G:714:ARG:HH12 | 0.74                     | 0.85              |
| 1:G:725:ARG:CZ   | 1:G:733:PRO:HB3  | 2.05                     | 0.85              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:CA   | 2.25                     | 0.85              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:CB   | 2.06                     | 0.85              |
| 1:A:410:ASN:OD1  | 4:8:334:GLU:CA   | 2.24                     | 0.85              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:HD23 | 2.08                     | 0.85              |
| 1:A:831:TRP:CD1  | 2:B:51:PHE:CZ    | 2.48                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:752:ASP:OD2  | 1:G:783:LEU:CB   | 2.24                     | 0.85              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:CE    | 2.21                     | 0.85              |
| 1:A:204:GLU:H    | 1:A:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:A:836:PHE:HB3  | 2:B:161:GLU:HG2  | 1.56                     | 0.85              |
| 1:G:84:MLY:CH1   | 1:G:715:VAL:HG12 | 2.05                     | 0.85              |
| 1:G:202:SER:HA   | 1:G:207:LYS:HE2  | 0.85                     | 0.85              |
| 4:2:287:ILE:HD13 | 4:4:203:THR:CB   | 1.97                     | 0.85              |
| 1:D:204:GLU:H    | 1:D:207:LYS:HE3  | 1.41                     | 0.85              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:CA   | 2.25                     | 0.85              |
| 1:G:310:TYR:CZ   | 1:G:320:ILE:HD11 | 2.11                     | 0.85              |
| 1:G:410:ASN:OD1  | 4:V:334:GLU:CA   | 2.24                     | 0.85              |
| 1:G:410:ASN:CG   | 4:V:334:GLU:CA   | 2.47                     | 0.85              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG11  | 1.58                     | 0.85              |
| 1:G:730:SER:OG   | 3:I:109:HIS:NE2  | 2.09                     | 0.85              |
| 1:J:529:PRO:C    | 4:W:354:GLN:CB   | 2.48                     | 0.85              |
| 1:J:640:LYS:CB   | 1:J:645:SER:OG   | 2.25                     | 0.85              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE1   | 1.59                     | 0.85              |
| 1:A:725:ARG:CD   | 1:A:733:PRO:HB3  | 2.07                     | 0.85              |
| 1:D:410:ASN:OD1  | 4:9:334:GLU:CA   | 2.24                     | 0.85              |
| 1:J:410:ASN:ND2  | 4:W:336:LYS:HG2  | 1.92                     | 0.85              |
| 1:A:202:SER:HA   | 1:A:207:LYS:HE2  | 0.85                     | 0.85              |
| 1:A:646:PHE:CD2  | 1:A:652:LEU:HD11 | 2.09                     | 0.85              |
| 1:D:418:THR:HB   | 1:D:421:GLU:HG3  | 1.59                     | 0.85              |
| 1:G:538:GLU:HG3  | 4:V:351:THR:C    | 2.02                     | 0.85              |
| 1:G:728:ASN:HD21 | 3:I:110:VAL:HA   | 1.41                     | 0.85              |
| 1:J:725:ARG:CZ   | 1:J:733:PRO:HB3  | 2.06                     | 0.85              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:CB   | 2.46                     | 0.85              |
| 4:9:287:ILE:CG2  | 4:W:205:GLU:HG2  | 2.05                     | 0.85              |
| 4:V:325:MET:HE1  | 4:X:244:ASP:CG   | 2.00                     | 0.85              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:CB   | 2.60                     | 0.84              |
| 1:G:538:GLU:N    | 4:V:351:THR:N    | 2.24                     | 0.84              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HB2  | 1.57                     | 0.84              |
| 1:G:769:ALA:HB3  | 1:G:770:GLY:HA2  | 0.85                     | 0.84              |
| 1:J:529:PRO:CB   | 4:W:353:GLN:OE1  | 2.25                     | 0.84              |
| 1:J:543:PRO:HG3  | 4:W:143:TYR:O    | 1.77                     | 0.84              |
| 1:G:725:ARG:CD   | 1:G:733:PRO:HB3  | 2.07                     | 0.84              |
| 4:0:112:PRO:CG   | 4:1:195:GLU:O    | 2.25                     | 0.84              |
| 1:D:202:SER:HA   | 1:D:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:HG3  | 1.57                     | 0.84              |
| 1:G:410:ASN:ND2  | 4:V:336:LYS:HG2  | 1.92                     | 0.84              |
| 1:J:418:THR:HB   | 1:J:421:GLU:HG3  | 1.60                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CB   | 1.84                     | 0.84              |
| 4:0:201:VAL:HG23 | 4:Y:287:ILE:CG1  | 2.07                     | 0.84              |
| 4:7:287:ILE:CG2  | 4:9:205:GLU:HG2  | 2.05                     | 0.84              |
| 1:A:97:LEU:HD22  | 1:A:712:PRO:HB3  | 1.59                     | 0.84              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HB2  | 1.57                     | 0.84              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:CB   | 2.46                     | 0.84              |
| 1:D:410:ASN:CG   | 4:9:334:GLU:CA   | 2.47                     | 0.84              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HB2  | 1.57                     | 0.84              |
| 1:J:795:ARG:CZ   | 3:L:35:ARG:HH12  | 1.91                     | 0.84              |
| 4:W:291:LYS:HD2  | 4:Y:243:PRO:CB   | 2.07                     | 0.84              |
| 1:A:310:TYR:CZ   | 1:A:320:ILE:HD11 | 2.11                     | 0.84              |
| 1:A:635:GLY:HA2  | 4:8:334:GLU:CG   | 2.03                     | 0.84              |
| 1:A:797:PHE:CD2  | 3:C:126:LEU:CD2  | 2.60                     | 0.84              |
| 1:G:791:GLN:OE1  | 3:I:116:GLU:CB   | 2.26                     | 0.84              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:HA   | 1.76                     | 0.84              |
| 4:9:237:GLU:HA   | 4:9:251:GLY:HA2  | 1.60                     | 0.84              |
| 1:D:529:PRO:CB   | 4:9:353:GLN:OE1  | 2.25                     | 0.84              |
| 1:D:557:GLU:H    | 4:W:48:GLY:HA3   | 1.28                     | 0.84              |
| 1:G:649:VAL:HG12 | 1:G:649:VAL:C    | 1.98                     | 0.84              |
| 1:J:202:SER:HA   | 1:J:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:A:410:ASN:ND2  | 4:8:336:LYS:HG2  | 1.92                     | 0.84              |
| 1:A:542:PHE:CA   | 4:8:143:TYR:CE1  | 2.61                     | 0.84              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:CD2  | 1.94                     | 0.84              |
| 1:A:800:ARG:NH1  | 3:C:149:VAL:O    | 2.10                     | 0.84              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:CG1  | 1.91                     | 0.84              |
| 1:A:814:PHE:HD1  | 2:B:127:ARG:HH22 | 1.12                     | 0.84              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:CG   | 2.40                     | 0.84              |
| 2:E:111:SER:OG   | 2:E:148:VAL:C    | 2.15                     | 0.84              |
| 1:G:648:THR:CG2  | 1:G:651:ALA:HB2  | 2.08                     | 0.84              |
| 1:G:752:ASP:OD2  | 1:G:783:LEU:HB2  | 1.78                     | 0.84              |
| 4:0:237:GLU:HA   | 4:0:251:GLY:HA2  | 1.60                     | 0.84              |
| 4:7:237:GLU:HA   | 4:7:251:GLY:HA2  | 1.60                     | 0.84              |
| 1:A:795:ARG:CG   | 3:C:118:MET:HE1  | 2.06                     | 0.84              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:NE2  | 1.59                     | 0.84              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD13 | 0.91                     | 0.84              |
| 2:H:141:PRO:CB   | 2:H:142:PRO:CD   | 2.56                     | 0.84              |
| 1:A:538:GLU:HG3  | 4:8:351:THR:C    | 2.03                     | 0.84              |
| 1:D:725:ARG:CD   | 1:D:733:PRO:HB3  | 2.07                     | 0.84              |
| 1:J:629:GLU:CG   | 1:J:643:GLY:O    | 2.26                     | 0.84              |
| 4:0:287:ILE:HG21 | 4:2:203:THR:H    | 1.43                     | 0.84              |
| 4:W:237:GLU:HA   | 4:W:251:GLY:HA2  | 1.60                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:538:GLU:N    | 4:9:351:THR:N    | 2.25                     | 0.84              |
| 1:D:640:LYS:CB   | 1:D:645:SER:OG   | 2.25                     | 0.84              |
| 1:D:792:ALA:HB1  | 3:F:40:ASN:HB2   | 1.56                     | 0.84              |
| 1:G:635:GLY:HA2  | 4:V:334:GLU:CG   | 2.03                     | 0.84              |
| 1:A:543:PRO:HG3  | 4:8:143:TYR:O    | 1.77                     | 0.83              |
| 1:A:836:PHE:HE1  | 2:B:159:HIS:CA   | 1.91                     | 0.83              |
| 1:D:410:ASN:ND2  | 4:9:336:LYS:HG2  | 1.92                     | 0.83              |
| 1:D:629:GLU:CG   | 1:D:643:GLY:O    | 2.26                     | 0.83              |
| 1:D:648:THR:CG2  | 1:D:651:ALA:HB2  | 2.08                     | 0.83              |
| 1:D:730:SER:O    | 1:D:734:GLU:HG3  | 1.78                     | 0.83              |
| 1:G:795:ARG:HB2  | 3:I:35:ARG:NH2   | 1.90                     | 0.83              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:CG   | 2.08                     | 0.83              |
| 1:J:204:GLU:H    | 1:J:207:LYS:HE3  | 1.42                     | 0.83              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:CA   | 2.25                     | 0.83              |
| 1:J:783:LEU:O    | 1:J:787:ILE:HB   | 1.78                     | 0.83              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:CD   | 1.90                     | 0.83              |
| 2:K:141:PRO:CB   | 2:K:142:PRO:CD   | 2.56                     | 0.83              |
| 4:2:237:GLU:HA   | 4:2:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:A:648:THR:CG2  | 1:A:651:ALA:HB2  | 2.08                     | 0.83              |
| 3:I:50:LEU:C     | 3:I:53:PRO:HD2   | 2.03                     | 0.83              |
| 3:L:50:LEU:C     | 3:L:53:PRO:HD2   | 2.03                     | 0.83              |
| 4:7:286:ASP:OD1  | 4:9:203:THR:CG2  | 2.26                     | 0.83              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:OG1  | 1.95                     | 0.83              |
| 1:G:93:MET:HE1   | 1:G:763:THR:CA   | 2.07                     | 0.83              |
| 1:J:91:MET:HE3   | 1:J:119:SER:HB2  | 1.56                     | 0.83              |
| 1:J:410:ASN:CG   | 4:W:334:GLU:CA   | 2.47                     | 0.83              |
| 1:J:534:SER:O    | 4:W:351:THR:HG23 | 1.13                     | 0.83              |
| 1:J:542:PHE:CA   | 4:W:143:TYR:CE1  | 2.61                     | 0.83              |
| 1:J:561:LYS:CE   | 4:Y:48:GLY:HA3   | 2.07                     | 0.83              |
| 1:A:822:SER:OG   | 2:B:88:LEU:HA    | 1.78                     | 0.83              |
| 3:F:50:LEU:C     | 3:F:53:PRO:HD2   | 2.03                     | 0.83              |
| 1:G:529:PRO:CB   | 4:V:353:GLN:OE1  | 2.25                     | 0.83              |
| 1:G:752:ASP:C    | 1:G:779:ARG:NH1  | 2.35                     | 0.83              |
| 1:G:754:ASP:HB2  | 1:G:776:GLU:CD   | 2.03                     | 0.83              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:HG23 | 0.84                     | 0.83              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:CB   | 2.55                     | 0.83              |
| 4:3:322:PRO:HB3  | 4:5:244:ASP:OD2  | 1.78                     | 0.83              |
| 4:W:286:ASP:OD1  | 4:Y:203:THR:N    | 2.11                     | 0.83              |
| 4:Y:237:GLU:HA   | 4:Y:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:A:549:SER:O    | 4:V:46:GLY:HA3   | 1.77                     | 0.83              |
| 1:A:553:MLY:HG2  | 4:V:47:MET:H     | 1.44                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:599:ASN:OD1  | 1:A:649:VAL:HB   | 1.72                     | 0.83              |
| 1:A:814:PHE:HA   | 2:B:127:ARG:NH2  | 1.93                     | 0.83              |
| 1:G:640:LYS:CB   | 1:G:645:SER:OG   | 2.25                     | 0.83              |
| 1:J:218:LEU:HB3  | 1:J:221:GLN:HG3  | 1.60                     | 0.83              |
| 1:J:730:SER:O    | 1:J:734:GLU:HG3  | 1.78                     | 0.83              |
| 1:A:649:VAL:HG12 | 1:A:649:VAL:C    | 1.98                     | 0.83              |
| 1:D:549:SER:O    | 4:W:46:GLY:HA3   | 1.77                     | 0.83              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:HD13 | 1.34                     | 0.83              |
| 1:G:542:PHE:CA   | 4:V:143:TYR:CE1  | 2.61                     | 0.83              |
| 1:G:553:MLY:CH1  | 4:X:45:VAL:CG1   | 2.49                     | 0.83              |
| 1:G:768:MLY:CD   | 1:G:772:LEU:HD22 | 2.08                     | 0.83              |
| 1:J:538:GLU:HG3  | 4:W:351:THR:C    | 2.03                     | 0.83              |
| 1:J:753:VAL:HA   | 1:J:780:ASP:OD2  | 1.78                     | 0.83              |
| 4:3:287:ILE:CD1  | 4:5:203:THR:HB   | 2.06                     | 0.83              |
| 4:5:237:GLU:HA   | 4:5:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:A:529:PRO:CB   | 4:8:353:GLN:OE1  | 2.25                     | 0.83              |
| 1:A:629:GLU:CG   | 1:A:643:GLY:O    | 2.26                     | 0.83              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CD1  | 2.58                     | 0.83              |
| 2:B:141:PRO:CB   | 2:B:142:PRO:CD   | 2.56                     | 0.83              |
| 1:D:725:ARG:CZ   | 1:D:733:PRO:HB3  | 2.05                     | 0.83              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:HE   | 1.76                     | 0.83              |
| 1:G:418:THR:HB   | 1:G:421:GLU:HG3  | 1.59                     | 0.83              |
| 1:G:530:MET:HE2  | 4:V:354:GLN:HG3  | 1.60                     | 0.83              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB2  | 1.51                     | 0.83              |
| 1:D:768:MLY:CA   | 1:D:771:LEU:HD13 | 2.08                     | 0.83              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:CB   | 2.46                     | 0.83              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:CD   | 2.56                     | 0.83              |
| 4:4:237:GLU:HA   | 4:4:251:GLY:HA2  | 1.60                     | 0.83              |
| 4:9:286:ASP:OD1  | 4:W:203:THR:CG2  | 2.26                     | 0.83              |
| 1:A:410:ASN:CG   | 4:8:334:GLU:CA   | 2.48                     | 0.83              |
| 1:A:506:GLU:H    | 1:A:761:GLY:HA2  | 1.43                     | 0.83              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:HD13 | 1.34                     | 0.83              |
| 3:C:50:LEU:C     | 3:C:53:PRO:HD2   | 2.03                     | 0.83              |
| 1:D:279:LEU:HB2  | 1:D:282:GLU:HG3  | 1.60                     | 0.83              |
| 1:D:800:ARG:CD   | 3:F:149:VAL:C    | 2.52                     | 0.83              |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:CD1  | 2.09                     | 0.83              |
| 1:J:279:LEU:HB2  | 1:J:282:GLU:HG3  | 1.60                     | 0.83              |
| 1:J:538:GLU:N    | 4:W:351:THR:N    | 2.24                     | 0.83              |
| 4:0:201:VAL:H    | 4:Y:287:ILE:HG12 | 1.42                     | 0.83              |
| 4:3:237:GLU:HA   | 4:3:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:A:831:TRP:HZ3  | 2:B:50:THR:HG21  | 1.44                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:538:GLU:HG3  | 4:9:351:THR:C    | 2.03                     | 0.82              |
| 1:D:553:MLY:HG2  | 4:W:47:MET:H     | 1.44                     | 0.82              |
| 1:D:641:LYS:HG2  | 1:D:647:GLN:HG3  | 1.61                     | 0.82              |
| 1:G:543:PRO:HG3  | 4:V:143:TYR:O    | 1.78                     | 0.82              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:CH1  | 2.26                     | 0.82              |
| 1:J:757:GLN:NE2  | 1:J:776:GLU:CG   | 2.41                     | 0.82              |
| 1:A:418:THR:HB   | 1:A:421:GLU:HG3  | 1.59                     | 0.82              |
| 1:D:724:TYR:C    | 1:D:782:MLY:HH11 | 2.04                     | 0.82              |
| 1:J:641:LYS:HG2  | 1:J:647:GLN:HG3  | 1.61                     | 0.82              |
| 4:0:166:TYR:HE2  | 4:2:64:ILE:HG21  | 1.42                     | 0.82              |
| 1:A:557:GLU:H    | 4:V:48:GLY:HA3   | 1.28                     | 0.82              |
| 1:A:578:HIS:HB3  | 1:A:592:ILE:HD12 | 1.61                     | 0.82              |
| 1:A:769:ALA:C    | 1:A:772:LEU:N    | 2.35                     | 0.82              |
| 1:D:542:PHE:CA   | 4:9:143:TYR:CE1  | 2.61                     | 0.82              |
| 1:D:817:GLN:OE1  | 2:E:127:ARG:CZ   | 2.27                     | 0.82              |
| 1:J:95:THR:OG1   | 1:J:713:SER:CB   | 2.26                     | 0.82              |
| 1:J:831:TRP:CH2  | 2:K:34:ILE:HG21  | 2.14                     | 0.82              |
| 4:8:290:ARG:NH1  | 4:V:202:THR:HG21 | 1.94                     | 0.82              |
| 1:A:834:LEU:CD1  | 2:B:54:MET:HB3   | 2.07                     | 0.82              |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:HD2  | 1.44                     | 0.82              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:HG2  | 1.61                     | 0.82              |
| 1:J:542:PHE:CA   | 4:W:143:TYR:HE1  | 1.92                     | 0.82              |
| 1:J:648:THR:CG2  | 1:J:651:ALA:HB2  | 2.08                     | 0.82              |
| 4:0:244:ASP:N    | 4:Y:291:LYS:CG   | 2.43                     | 0.82              |
| 4:1:287:ILE:HG21 | 4:3:204:ALA:H    | 1.42                     | 0.82              |
| 1:A:279:LEU:HB2  | 1:A:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:NE   | 2.27                     | 0.82              |
| 1:G:629:GLU:CG   | 1:G:643:GLY:O    | 2.26                     | 0.82              |
| 4:7:290:ARG:NH1  | 4:9:202:THR:HG21 | 1.94                     | 0.82              |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:HD2  | 1.44                     | 0.82              |
| 1:A:530:MET:HE2  | 4:8:354:GLN:HG3  | 1.62                     | 0.82              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:CE1  | 2.15                     | 0.82              |
| 1:D:543:PRO:HG3  | 4:9:143:TYR:O    | 1.77                     | 0.82              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:J:510:TRP:CZ3  | 1:J:772:LEU:HD21 | 2.13                     | 0.82              |
| 1:A:499:GLU:OE1  | 1:A:766:PHE:HZ   | 1.62                     | 0.82              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:HD13 | 2.09                     | 0.82              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:CG1  | 2.10                     | 0.82              |
| 2:H:114:LYS:HA   | 2:H:146:GLY:C    | 2.02                     | 0.82              |
| 1:J:757:GLN:HG2  | 1:J:776:GLU:HG3  | 0.82                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:286:ASP:OD1  | 4:V:203:THR:CG2  | 2.26                     | 0.82              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:HB2   | 1.56                     | 0.82              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CG    | 2.09                     | 0.82              |
| 1:G:643:GLY:N    | 4:V:24:ASP:HA    | 1.94                     | 0.82              |
| 1:J:599:ASN:CA   | 1:J:649:VAL:CB   | 2.53                     | 0.82              |
| 1:J:643:GLY:N    | 4:W:24:ASP:HA    | 1.93                     | 0.82              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:NE2  | 2.43                     | 0.82              |
| 4:0:247:VAL:H    | 4:Y:324:THR:CG2  | 1.92                     | 0.82              |
| 1:A:641:LYS:HG2  | 1:A:647:GLN:HG3  | 1.60                     | 0.82              |
| 1:D:629:GLU:HA   | 1:D:643:GLY:C    | 2.05                     | 0.82              |
| 1:D:724:TYR:O    | 1:D:782:MLY:HH11 | 1.79                     | 0.82              |
| 1:G:279:LEU:HB2  | 1:G:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:G:578:HIS:HB3  | 1:G:592:ILE:HD12 | 1.62                     | 0.82              |
| 1:G:730:SER:O    | 1:G:734:GLU:HG3  | 1.78                     | 0.82              |
| 1:J:725:ARG:CD   | 1:J:733:PRO:HB3  | 2.07                     | 0.82              |
| 1:J:734:GLU:O    | 1:J:738:MET:CG   | 2.28                     | 0.82              |
| 1:J:816:ILE:HD11 | 2:K:100:ALA:HB1  | 1.59                     | 0.82              |
| 4:8:237:GLU:HA   | 4:8:251:GLY:HA2  | 1.60                     | 0.82              |
| 4:Z:237:GLU:HA   | 4:Z:251:GLY:HA2  | 1.60                     | 0.82              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:A:730:SER:O    | 1:A:734:GLU:HG3  | 1.78                     | 0.82              |
| 1:G:534:SER:O    | 4:V:351:THR:HG23 | 1.12                     | 0.82              |
| 1:J:93:MET:SD    | 1:J:716:LEU:CD1  | 2.66                     | 0.82              |
| 4:1:237:GLU:HA   | 4:1:251:GLY:HA2  | 1.60                     | 0.82              |
| 4:1:287:ILE:HG21 | 4:3:202:THR:C    | 2.05                     | 0.82              |
| 1:A:640:LYS:CB   | 1:A:645:SER:OG   | 2.25                     | 0.81              |
| 1:A:643:GLY:N    | 4:8:24:ASP:HA    | 1.93                     | 0.81              |
| 1:D:218:LEU:HB3  | 1:D:221:GLN:HG3  | 1.61                     | 0.81              |
| 1:D:549:SER:O    | 4:W:46:GLY:CA    | 2.27                     | 0.81              |
| 1:D:734:GLU:O    | 1:D:738:MET:CG   | 2.28                     | 0.81              |
| 1:D:797:PHE:HE2  | 3:F:126:LEU:CD2  | 1.92                     | 0.81              |
| 1:J:629:GLU:HA   | 1:J:643:GLY:C    | 2.05                     | 0.81              |
| 1:A:553:MLY:CB   | 4:V:46:GLY:CA    | 2.32                     | 0.81              |
| 1:A:831:TRP:CZ3  | 2:B:50:THR:HG21  | 2.15                     | 0.81              |
| 1:D:571:ALA:O    | 1:D:572:LYS:CG   | 2.28                     | 0.81              |
| 1:D:643:GLY:N    | 4:9:24:ASP:HA    | 1.93                     | 0.81              |
| 1:G:95:THR:OG1   | 1:G:713:SER:HB3  | 1.80                     | 0.81              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:HD22 | 1.45                     | 0.81              |
| 4:V:237:GLU:HA   | 4:V:251:GLY:HA2  | 1.60                     | 0.81              |
| 1:A:549:SER:O    | 4:V:46:GLY:CA    | 2.27                     | 0.81              |
| 1:A:789:ALA:CB   | 3:C:87:PHE:HE2   | 1.94                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:795:ARG:NH1  | 3:C:43:ASN:H     | 1.79                     | 0.81              |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:HD2  | 1.44                     | 0.81              |
| 1:D:557:GLU:N    | 4:W:48:GLY:HA2   | 1.90                     | 0.81              |
| 1:D:578:HIS:HD2  | 1:D:591:ASN:HA   | 1.45                     | 0.81              |
| 1:D:723:ARG:O    | 1:D:782:MLY:CE   | 2.29                     | 0.81              |
| 1:D:733:PRO:C    | 1:D:737:PHE:HD1  | 1.88                     | 0.81              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:N    | 1.94                     | 0.81              |
| 1:D:792:ALA:CB   | 3:F:40:ASN:O     | 2.28                     | 0.81              |
| 1:G:232:PHE:CZ   | 1:G:287:ILE:HD13 | 2.16                     | 0.81              |
| 1:G:733:PRO:C    | 1:G:737:PHE:HD1  | 1.88                     | 0.81              |
| 1:G:734:GLU:O    | 1:G:738:MET:CG   | 2.28                     | 0.81              |
| 2:K:111:SER:OG   | 2:K:148:VAL:C    | 2.15                     | 0.81              |
| 2:K:121:LEU:CG   | 2:K:128:PHE:CA   | 2.48                     | 0.81              |
| 4:X:237:GLU:HA   | 4:X:251:GLY:HA2  | 1.60                     | 0.81              |
| 1:A:538:GLU:CA   | 4:8:351:THR:H    | 1.93                     | 0.81              |
| 1:D:550:PHE:CA   | 4:W:46:GLY:CA    | 2.59                     | 0.81              |
| 1:D:809:ARG:CZ   | 2:E:124:GLY:HA3  | 2.11                     | 0.81              |
| 1:D:822:SER:CB   | 2:E:88:LEU:CD2   | 2.51                     | 0.81              |
| 1:J:797:PHE:HB2  | 3:L:149:VAL:CG1  | 2.11                     | 0.81              |
| 1:D:818:TYR:CB   | 2:E:90:GLY:N     | 2.44                     | 0.81              |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:HD2  | 1.45                     | 0.81              |
| 1:G:641:LYS:HG2  | 1:G:647:GLN:HG3  | 1.61                     | 0.81              |
| 1:J:578:HIS:HB3  | 1:J:592:ILE:HD12 | 1.62                     | 0.81              |
| 1:A:629:GLU:HA   | 1:A:643:GLY:C    | 2.05                     | 0.81              |
| 1:D:538:GLU:CA   | 4:9:351:THR:H    | 1.93                     | 0.81              |
| 1:D:542:PHE:CA   | 4:9:143:TYR:HE1  | 1.92                     | 0.81              |
| 1:D:641:LYS:HD2  | 4:9:348:SER:CA   | 2.09                     | 0.81              |
| 1:J:733:PRO:C    | 1:J:737:PHE:HD1  | 1.88                     | 0.81              |
| 4:9:290:ARG:NH1  | 4:W:202:THR:HG21 | 1.94                     | 0.81              |
| 1:A:798:LEU:HD12 | 3:C:126:LEU:HD21 | 1.58                     | 0.81              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:HG2  | 2.10                     | 0.81              |
| 2:E:114:LYS:HA   | 2:E:146:GLY:C    | 2.03                     | 0.81              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:HD22 | 1.45                     | 0.81              |
| 1:G:629:GLU:HA   | 1:G:643:GLY:C    | 2.05                     | 0.81              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:CD   | 2.54                     | 0.81              |
| 1:J:721:LYS:HG2  | 1:J:736:GLN:CD   | 1.86                     | 0.81              |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:CD1  | 2.10                     | 0.81              |
| 4:9:223:PHE:HE1  | 4:9:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:HG2  | 1.62                     | 0.81              |
| 1:A:734:GLU:O    | 1:A:738:MET:CG   | 2.28                     | 0.81              |
| 1:D:831:TRP:CH2  | 2:E:34:ILE:CG2   | 2.62                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:641:LYS:HD2  | 4:V:348:SER:CA   | 2.09                     | 0.81              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:NE2  | 2.43                     | 0.81              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:HG2  | 2.10                     | 0.81              |
| 1:J:641:LYS:HD2  | 4:W:348:SER:CA   | 2.09                     | 0.81              |
| 4:2:290:ARG:HH21 | 4:4:202:THR:HG23 | 1.41                     | 0.81              |
| 4:7:223:PHE:HE1  | 4:7:255:PHE:HB2  | 1.46                     | 0.81              |
| 4:8:223:PHE:HE1  | 4:8:255:PHE:HB2  | 1.46                     | 0.81              |
| 4:W:223:PHE:HE1  | 4:W:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:A:232:PHE:CZ   | 1:A:287:ILE:HD13 | 2.16                     | 0.81              |
| 1:A:721:LYS:HG2  | 1:A:736:GLN:CD   | 1.86                     | 0.81              |
| 1:A:752:ASP:O    | 1:A:778:MET:SD   | 2.39                     | 0.81              |
| 2:B:121:LEU:CG   | 2:B:128:PHE:CA   | 2.48                     | 0.81              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:HG2  | 1.62                     | 0.81              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:CE    | 2.59                     | 0.81              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:HD21 | 2.14                     | 0.81              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:NE2  | 2.43                     | 0.81              |
| 1:G:829:TRP:CH2  | 2:H:87:LYS:CE    | 2.63                     | 0.81              |
| 1:J:578:HIS:HD2  | 1:J:591:ASN:HA   | 1.45                     | 0.81              |
| 2:K:114:LYS:HA   | 2:K:146:GLY:C    | 2.03                     | 0.81              |
| 2:B:144:VAL:CA   | 2:B:153:ILE:HD11 | 2.11                     | 0.80              |
| 1:D:529:PRO:C    | 4:9:354:GLN:CB   | 2.49                     | 0.80              |
| 1:G:571:ALA:O    | 1:G:572:LYS:CG   | 2.28                     | 0.80              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:HD21 | 2.14                     | 0.80              |
| 1:J:84:MLY:HE2   | 1:J:719:ASP:CB   | 1.63                     | 0.80              |
| 1:J:538:GLU:CA   | 4:W:351:THR:H    | 1.93                     | 0.80              |
| 1:A:550:PHE:CA   | 4:V:46:GLY:CA    | 2.59                     | 0.80              |
| 1:A:725:ARG:CZ   | 1:A:733:PRO:HB3  | 2.06                     | 0.80              |
| 1:D:374:GLN:HG3  | 1:D:375:ALA:N    | 1.96                     | 0.80              |
| 1:G:836:PHE:CZ   | 2:H:159:HIS:HA   | 2.15                     | 0.80              |
| 1:J:510:TRP:CZ2  | 1:J:768:MLY:CH1  | 2.59                     | 0.80              |
| 1:A:502:GLU:C    | 1:A:761:GLY:CA   | 2.55                     | 0.80              |
| 1:A:641:LYS:HD2  | 4:8:348:SER:CA   | 2.10                     | 0.80              |
| 2:B:114:LYS:HA   | 2:B:146:GLY:C    | 2.03                     | 0.80              |
| 1:D:215:GLN:N    | 1:D:340:ILE:CD1  | 2.44                     | 0.80              |
| 1:D:723:ARG:O    | 1:D:782:MLY:NZ   | 2.14                     | 0.80              |
| 1:G:538:GLU:CA   | 4:V:351:THR:H    | 1.92                     | 0.80              |
| 2:H:150:TYR:C    | 2:H:151:LYS:CG   | 2.48                     | 0.80              |
| 1:J:215:GLN:N    | 1:J:340:ILE:CD1  | 2.44                     | 0.80              |
| 1:J:798:LEU:CD2  | 3:L:126:LEU:CG   | 2.59                     | 0.80              |
| 2:K:141:PRO:CB   | 2:K:142:PRO:HD2  | 2.11                     | 0.80              |
| 4:V:325:MET:SD   | 4:X:244:ASP:HB3  | 2.19                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:141:PRO:CB   | 2:B:142:PRO:HD2  | 2.11                     | 0.80              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HG3   | 1.63                     | 0.80              |
| 1:J:374:GLN:HG3  | 1:J:375:ALA:N    | 1.96                     | 0.80              |
| 4:0:223:PHE:HE1  | 4:0:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD13 | 0.91                     | 0.80              |
| 1:D:792:ALA:HB1  | 3:F:40:ASN:HB3   | 1.64                     | 0.80              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:CB   | 2.10                     | 0.80              |
| 4:X:223:PHE:HE1  | 4:X:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:215:GLN:N    | 1:A:340:ILE:CD1  | 2.44                     | 0.80              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:HD22 | 1.45                     | 0.80              |
| 1:A:578:HIS:HD2  | 1:A:591:ASN:HA   | 1.44                     | 0.80              |
| 1:A:709:LYS:O    | 1:A:710:GLY:HA3  | 1.81                     | 0.80              |
| 1:A:768:MLY:C    | 1:A:771:LEU:CB   | 2.59                     | 0.80              |
| 1:G:599:ASN:CA   | 1:G:649:VAL:CB   | 2.53                     | 0.80              |
| 2:K:141:PRO:HB2  | 2:K:142:PRO:CD   | 2.11                     | 0.80              |
| 4:0:167:GLU:CD   | 4:2:43:VAL:O     | 2.25                     | 0.80              |
| 4:2:223:PHE:HE1  | 4:2:255:PHE:HB2  | 1.46                     | 0.80              |
| 4:X:291:LYS:HE3  | 4:Z:243:PRO:HB2  | 0.80                     | 0.80              |
| 1:A:502:GLU:CD   | 1:A:763:THR:H    | 1.88                     | 0.80              |
| 1:A:757:GLN:HB2  | 1:A:771:LEU:HD11 | 1.57                     | 0.80              |
| 1:D:578:HIS:HB3  | 1:D:592:ILE:HD12 | 1.62                     | 0.80              |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:HD12 | 0.81                     | 0.80              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:CB   | 2.37                     | 0.80              |
| 4:0:245:GLY:CA   | 4:Y:324:THR:O    | 2.29                     | 0.80              |
| 1:D:232:PHE:CZ   | 1:D:287:ILE:HD13 | 2.16                     | 0.80              |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:HD12 | 0.81                     | 0.80              |
| 1:G:542:PHE:CA   | 4:V:143:TYR:HE1  | 1.93                     | 0.80              |
| 1:G:578:HIS:HD2  | 1:G:591:ASN:HA   | 1.44                     | 0.80              |
| 1:J:571:ALA:O    | 1:J:572:LYS:CG   | 2.28                     | 0.80              |
| 2:K:144:VAL:CA   | 2:K:153:ILE:HD11 | 2.11                     | 0.80              |
| 3:L:49:ILE:N     | 3:L:52:ASN:ND2   | 2.29                     | 0.80              |
| 4:V:223:PHE:HE1  | 4:V:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:374:GLN:HG3  | 1:A:375:ALA:N    | 1.96                     | 0.80              |
| 1:D:724:TYR:CZ   | 1:D:778:MET:SD   | 2.75                     | 0.80              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:HB2  | 1.51                     | 0.80              |
| 1:D:830:PRO:HB2  | 2:E:51:PHE:CE2   | 2.16                     | 0.80              |
| 1:G:215:GLN:N    | 1:G:340:ILE:CD1  | 2.44                     | 0.80              |
| 4:1:287:ILE:HG13 | 4:3:202:THR:HA   | 1.64                     | 0.80              |
| 4:5:223:PHE:HE1  | 4:5:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:793:ARG:HE   | 3:C:147:MET:CG   | 1.95                     | 0.80              |
| 3:F:49:ILE:N     | 3:F:52:ASN:ND2   | 2.29                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:93:MET:CE    | 1:G:763:THR:HG22 | 2.02                     | 0.80              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:HG2  | 1.62                     | 0.80              |
| 1:G:374:GLN:HG3  | 1:G:375:ALA:N    | 1.96                     | 0.80              |
| 4:0:290:ARG:HH22 | 4:2:202:THR:HG22 | 1.42                     | 0.80              |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:HD12 | 0.81                     | 0.79              |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:CD1  | 2.10                     | 0.79              |
| 1:G:798:LEU:CD2  | 3:I:122:GLU:HB3  | 2.10                     | 0.79              |
| 1:J:232:PHE:CZ   | 1:J:287:ILE:HD13 | 2.16                     | 0.79              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:HD13 | 1.34                     | 0.79              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD13 | 0.91                     | 0.79              |
| 4:0:201:VAL:HG23 | 4:Y:287:ILE:CG2  | 2.11                     | 0.79              |
| 1:A:571:ALA:O    | 1:A:572:LYS:CG   | 2.28                     | 0.79              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CB   | 1.84                     | 0.79              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:HE3  | 1.97                     | 0.79              |
| 3:C:49:ILE:N     | 3:C:52:ASN:ND2   | 2.29                     | 0.79              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:HD22 | 1.45                     | 0.79              |
| 1:D:793:ARG:HA   | 3:F:40:ASN:ND2   | 1.96                     | 0.79              |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:HD12 | 0.81                     | 0.79              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:CB   | 2.31                     | 0.79              |
| 4:0:166:TYR:CE2  | 4:2:64:ILE:CG2   | 2.59                     | 0.79              |
| 4:1:288:ASP:N    | 4:3:203:THR:CG2  | 2.45                     | 0.79              |
| 1:A:599:ASN:CA   | 1:A:649:VAL:CB   | 2.53                     | 0.79              |
| 2:E:144:VAL:CA   | 2:E:153:ILE:HD11 | 2.11                     | 0.79              |
| 1:J:784:ALA:O    | 1:J:788:THR:N    | 2.14                     | 0.79              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:CG   | 1.86                     | 0.79              |
| 4:4:223:PHE:HE1  | 4:4:255:PHE:HB2  | 1.46                     | 0.79              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CG   | 2.60                     | 0.79              |
| 1:A:817:GLN:HB2  | 2:B:127:ARG:NH1  | 1.96                     | 0.79              |
| 2:E:150:TYR:C    | 2:E:151:LYS:CG   | 2.48                     | 0.79              |
| 2:H:121:LEU:CG   | 2:H:128:PHE:CA   | 2.49                     | 0.79              |
| 2:H:144:VAL:CA   | 2:H:153:ILE:HD11 | 2.11                     | 0.79              |
| 3:I:49:ILE:N     | 3:I:52:ASN:ND2   | 2.29                     | 0.79              |
| 4:8:287:ILE:HB   | 4:V:204:ALA:N    | 1.97                     | 0.79              |
| 1:A:174:SER:CB   | 1:A:667:THR:HG21 | 2.13                     | 0.79              |
| 2:H:141:PRO:CB   | 2:H:142:PRO:HD2  | 2.11                     | 0.79              |
| 4:0:112:PRO:HB3  | 4:1:195:GLU:O    | 1.82                     | 0.79              |
| 4:3:223:PHE:HE1  | 4:3:255:PHE:HB2  | 1.46                     | 0.79              |
| 1:A:557:GLU:N    | 4:V:48:GLY:HA2   | 1.90                     | 0.79              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:HB2  | 2.13                     | 0.79              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CB   | 1.84                     | 0.79              |
| 1:G:800:ARG:HD2  | 3:I:149:VAL:HG22 | 1.63                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:92:ALA:O     | 1:J:714:ARG:CG   | 2.31                     | 0.79              |
| 4:1:203:THR:H    | 4:Z:287:ILE:HB   | 1.45                     | 0.79              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:HD2  | 2.11                     | 0.79              |
| 1:G:728:ASN:ND2  | 3:I:113:THR:OG1  | 2.16                     | 0.79              |
| 1:J:407:GLY:HA2  | 1:J:412:ALA:HA   | 1.65                     | 0.79              |
| 4:0:243:PRO:C    | 4:Y:291:LYS:HD2  | 2.07                     | 0.79              |
| 4:1:203:THR:N    | 4:Z:287:ILE:HG21 | 1.98                     | 0.79              |
| 1:A:409:GLY:N    | 1:A:636:LYS:CG   | 2.44                     | 0.79              |
| 1:A:550:PHE:N    | 4:V:46:GLY:HA3   | 1.97                     | 0.79              |
| 1:D:537:GLU:O    | 4:9:350:SER:N    | 2.16                     | 0.79              |
| 1:D:550:PHE:HA   | 4:W:46:GLY:HA2   | 1.64                     | 0.79              |
| 1:D:830:PRO:HD2  | 2:E:67:MET:CE    | 2.10                     | 0.79              |
| 2:E:141:PRO:HB2  | 2:E:142:PRO:CD   | 2.12                     | 0.79              |
| 1:G:174:SER:CB   | 1:G:667:THR:HG21 | 2.13                     | 0.79              |
| 1:G:537:GLU:O    | 4:V:350:SER:N    | 2.16                     | 0.79              |
| 1:G:641:LYS:HD2  | 4:V:348:SER:HB2  | 1.54                     | 0.79              |
| 4:Y:223:PHE:HE1  | 4:Y:255:PHE:HB2  | 1.46                     | 0.79              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:HG2  | 2.10                     | 0.79              |
| 1:A:537:GLU:O    | 4:8:350:SER:N    | 2.16                     | 0.79              |
| 2:B:141:PRO:HB2  | 2:B:142:PRO:CD   | 2.12                     | 0.79              |
| 1:D:407:GLY:HA2  | 1:D:412:ALA:HA   | 1.65                     | 0.79              |
| 1:D:409:GLY:N    | 1:D:636:LYS:CG   | 2.44                     | 0.79              |
| 1:G:93:MET:HE2   | 1:G:763:THR:HB   | 1.58                     | 0.79              |
| 1:A:641:LYS:HD2  | 4:8:348:SER:HB2  | 1.54                     | 0.79              |
| 1:A:721:LYS:CB   | 1:A:736:GLN:CD   | 2.56                     | 0.79              |
| 1:A:813:ILE:HG23 | 2:B:127:ARG:CD   | 1.96                     | 0.79              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:HG2  | 2.10                     | 0.79              |
| 1:G:567:LYS:HZ3  | 4:X:92:ASN:HD22  | 1.28                     | 0.79              |
| 1:J:797:PHE:HA   | 3:L:149:VAL:CG1  | 2.12                     | 0.79              |
| 1:A:553:MLY:NZ   | 4:V:45:VAL:HA    | 1.84                     | 0.78              |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:CD1  | 2.09                     | 0.78              |
| 1:D:291:ILE:HA   | 1:D:331:LEU:HD11 | 1.64                     | 0.78              |
| 1:J:639:GLY:CA   | 4:W:345:ILE:N    | 2.46                     | 0.78              |
| 1:J:642:LYS:CG   | 4:W:23:GLY:H     | 1.77                     | 0.78              |
| 1:J:817:GLN:OE1  | 2:K:127:ARG:HD2  | 1.83                     | 0.78              |
| 4:1:202:THR:CB   | 4:Z:287:ILE:HG21 | 2.13                     | 0.78              |
| 4:Z:223:PHE:HE1  | 4:Z:255:PHE:HB2  | 1.46                     | 0.78              |
| 1:A:534:SER:C    | 4:8:351:THR:CA   | 2.47                     | 0.78              |
| 1:D:792:ALA:CA   | 3:F:40:ASN:HB3   | 2.12                     | 0.78              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:HD2  | 1.73                     | 0.78              |
| 2:E:162:ASP:HB3  | 2:K:20:ASP:HB2   | 1.63                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:819:ASN:ND2  | 2:H:92:ASP:HB2   | 1.97                     | 0.78              |
| 1:J:409:GLY:N    | 1:J:636:LYS:CG   | 2.44                     | 0.78              |
| 4:0:112:PRO:CB   | 4:1:195:GLU:O    | 2.32                     | 0.78              |
| 1:A:542:PHE:CA   | 4:8:143:TYR:HE1  | 1.92                     | 0.78              |
| 1:A:550:PHE:HA   | 4:V:46:GLY:HA2   | 1.65                     | 0.78              |
| 1:A:642:LYS:HG2  | 4:8:22:ALA:HA    | 1.66                     | 0.78              |
| 1:A:733:PRO:C    | 1:A:737:PHE:HD1  | 1.88                     | 0.78              |
| 1:D:481:ASN:HD22 | 1:D:481:ASN:N    | 1.82                     | 0.78              |
| 1:G:407:GLY:HA2  | 1:G:412:ALA:HA   | 1.65                     | 0.78              |
| 1:G:642:LYS:HG2  | 4:V:22:ALA:HA    | 1.65                     | 0.78              |
| 1:J:291:ILE:HA   | 1:J:331:LEU:HD11 | 1.64                     | 0.78              |
| 1:A:51:THR:O     | 1:A:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:D:550:PHE:N    | 4:W:46:GLY:HA3   | 1.97                     | 0.78              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:HB2  | 2.13                     | 0.78              |
| 1:J:795:ARG:HE   | 3:L:118:MET:CE   | 1.87                     | 0.78              |
| 1:D:166:MET:HE1  | 1:D:254:PHE:CD2  | 2.19                     | 0.78              |
| 1:G:93:MET:SD    | 1:G:763:THR:HG22 | 2.23                     | 0.78              |
| 1:G:646:PHE:HE2  | 1:G:652:LEU:CD2  | 1.97                     | 0.78              |
| 1:J:174:SER:CB   | 1:J:667:THR:HG21 | 2.13                     | 0.78              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:CD2  | 1.97                     | 0.78              |
| 4:1:223:PHE:HE1  | 4:1:255:PHE:HB2  | 1.46                     | 0.78              |
| 4:7:287:ILE:HB   | 4:9:204:ALA:N    | 1.98                     | 0.78              |
| 4:9:287:ILE:HB   | 4:W:204:ALA:N    | 1.97                     | 0.78              |
| 1:A:166:MET:HE1  | 1:A:254:PHE:CD2  | 2.19                     | 0.78              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CG    | 2.66                     | 0.78              |
| 1:G:51:THR:O     | 1:G:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:J:537:GLU:O    | 4:W:350:SER:N    | 2.16                     | 0.78              |
| 4:0:287:ILE:HB   | 4:2:203:THR:HG21 | 1.63                     | 0.78              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:HB2  | 1.65                     | 0.78              |
| 1:A:131:TRP:C    | 1:A:132:LEU:HD12 | 2.09                     | 0.78              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HB1  | 1.84                     | 0.78              |
| 1:A:795:ARG:CB   | 3:C:35:ARG:NH2   | 2.42                     | 0.78              |
| 2:B:121:LEU:CG   | 2:B:128:PHE:HA   | 2.14                     | 0.78              |
| 1:D:721:LYS:CB   | 1:D:736:GLN:CD   | 2.56                     | 0.78              |
| 1:D:809:ARG:CZ   | 2:E:124:GLY:CA   | 2.61                     | 0.78              |
| 1:G:166:MET:HE1  | 1:G:254:PHE:CD2  | 2.19                     | 0.78              |
| 1:G:291:ILE:HA   | 1:G:331:LEU:HD11 | 1.64                     | 0.78              |
| 1:G:727:LEU:O    | 3:I:113:THR:OG1  | 2.02                     | 0.78              |
| 1:J:51:THR:O     | 1:J:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:J:84:MLY:HH11  | 1:J:715:VAL:HG11 | 1.66                     | 0.78              |
| 1:J:166:MET:HE1  | 1:J:254:PHE:CD2  | 2.19                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:530:MET:CG   | 4:W:354:GLN:CB   | 2.30                     | 0.78              |
| 4:1:203:THR:N    | 4:Z:287:ILE:CG2  | 2.45                     | 0.78              |
| 1:A:496:PHE:CD2  | 1:A:514:ASP:HA   | 2.19                     | 0.78              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:HD21 | 2.14                     | 0.78              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HB1  | 1.84                     | 0.78              |
| 1:G:219:GLU:O    | 1:G:223:ILE:HG13 | 1.84                     | 0.78              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD13 | 0.91                     | 0.78              |
| 4:1:324:THR:HG23 | 4:3:244:ASP:CA   | 2.14                     | 0.78              |
| 4:3:288:ASP:N    | 4:5:203:THR:CG2  | 2.46                     | 0.78              |
| 4:3:322:PRO:HB3  | 4:5:244:ASP:CB   | 2.10                     | 0.78              |
| 3:C:49:ILE:N     | 3:C:52:ASN:HD22  | 1.82                     | 0.78              |
| 1:G:836:PHE:CZ   | 2:H:160:GLY:N    | 2.49                     | 0.78              |
| 1:J:798:LEU:HD21 | 3:L:126:LEU:CG   | 2.14                     | 0.78              |
| 4:0:244:ASP:OD2  | 4:Y:325:MET:CE   | 2.32                     | 0.78              |
| 1:A:789:ALA:HB1  | 3:C:87:PHE:CE2   | 2.18                     | 0.78              |
| 1:D:508:ILE:HA   | 1:D:761:GLY:HA3  | 1.64                     | 0.78              |
| 1:D:530:MET:HE2  | 4:9:354:GLN:HG3  | 1.61                     | 0.78              |
| 1:G:496:PHE:CD2  | 1:G:514:ASP:HA   | 2.19                     | 0.78              |
| 1:G:733:PRO:C    | 1:G:737:PHE:CD1  | 2.62                     | 0.78              |
| 1:J:496:PHE:CD2  | 1:J:514:ASP:HA   | 2.19                     | 0.78              |
| 1:J:831:TRP:CH2  | 2:K:47:LEU:CD2   | 2.67                     | 0.78              |
| 4:3:322:PRO:CB   | 4:5:244:ASP:CG   | 2.54                     | 0.78              |
| 4:4:223:PHE:HD2  | 4:4:312:ARG:HH21 | 1.32                     | 0.78              |
| 1:A:219:GLU:O    | 1:A:223:ILE:HG13 | 1.84                     | 0.77              |
| 1:A:407:GLY:HA2  | 1:A:412:ALA:HA   | 1.65                     | 0.77              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:HD21 | 1.47                     | 0.77              |
| 1:D:815:CYS:SG   | 2:E:92:ASP:HB2   | 2.24                     | 0.77              |
| 1:G:409:GLY:N    | 1:G:636:LYS:CG   | 2.44                     | 0.77              |
| 1:G:639:GLY:CA   | 4:V:345:ILE:N    | 2.47                     | 0.77              |
| 4:1:202:THR:HA   | 4:Z:287:ILE:HG12 | 1.67                     | 0.77              |
| 4:1:203:THR:HG22 | 4:Z:288:ASP:N    | 1.99                     | 0.77              |
| 4:5:223:PHE:HD2  | 4:5:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:D:496:PHE:CD2  | 1:D:514:ASP:HA   | 2.19                     | 0.77              |
| 1:D:639:GLY:CA   | 4:9:345:ILE:N    | 2.47                     | 0.77              |
| 1:G:93:MET:CA    | 1:G:764:MLY:NZ   | 2.36                     | 0.77              |
| 1:D:51:THR:O     | 1:D:62:VAL:HG13  | 1.84                     | 0.77              |
| 1:J:116:TYR:O    | 1:J:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:J:567:LYS:HZ1  | 4:Y:92:ASN:HD22  | 1.32                     | 0.77              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:HD21 | 1.47                     | 0.77              |
| 4:W:223:PHE:HD2  | 4:W:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:A:529:PRO:C    | 4:8:354:GLN:CB   | 2.49                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:641:LYS:CE   | 1:G:647:GLN:HB2  | 2.13                     | 0.77              |
| 3:I:49:ILE:N     | 3:I:52:ASN:HD22  | 1.82                     | 0.77              |
| 4:0:223:PHE:HD2  | 4:0:312:ARG:HH21 | 1.33                     | 0.77              |
| 4:1:324:THR:CB   | 4:3:244:ASP:HA   | 2.14                     | 0.77              |
| 4:9:223:PHE:HD2  | 4:9:312:ARG:HH21 | 1.32                     | 0.77              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:CA   | 2.61                     | 0.77              |
| 1:A:291:ILE:HA   | 1:A:331:LEU:HD11 | 1.64                     | 0.77              |
| 1:A:639:GLY:CA   | 4:8:345:ILE:N    | 2.47                     | 0.77              |
| 1:D:94:MET:CE    | 1:D:101:ALA:HB1  | 2.15                     | 0.77              |
| 1:D:831:TRP:HA   | 2:E:51:PHE:HE1   | 1.47                     | 0.77              |
| 1:G:116:TYR:O    | 1:G:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB1  | 1.27                     | 0.77              |
| 1:J:725:ARG:HG3  | 1:J:733:PRO:HA   | 1.67                     | 0.77              |
| 2:K:121:LEU:CG   | 2:K:128:PHE:HA   | 2.14                     | 0.77              |
| 4:1:324:THR:CG2  | 4:3:244:ASP:CA   | 2.59                     | 0.77              |
| 4:X:291:LYS:HE2  | 4:Z:243:PRO:O    | 1.82                     | 0.77              |
| 4:Y:223:PHE:HD2  | 4:Y:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:HB2  | 1.51                     | 0.77              |
| 1:D:174:SER:CB   | 1:D:667:THR:HG21 | 2.13                     | 0.77              |
| 3:I:3:SER:O      | 3:I:4:LYS:HB2    | 1.84                     | 0.77              |
| 1:J:530:MET:HE2  | 4:W:354:GLN:HG3  | 1.62                     | 0.77              |
| 1:D:116:TYR:O    | 1:D:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:CD2  | 1.97                     | 0.77              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG12 | 1.66                     | 0.77              |
| 4:0:203:THR:N    | 4:Y:286:ASP:OD1  | 2.17                     | 0.77              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:HG21 | 1.60                     | 0.77              |
| 4:7:223:PHE:HD2  | 4:7:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:A:502:GLU:CG   | 1:A:764:MLY:O    | 2.32                     | 0.77              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:HB2  | 2.13                     | 0.77              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:CD2  | 1.97                     | 0.77              |
| 1:G:721:LYS:CB   | 1:G:736:GLN:CD   | 2.56                     | 0.77              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:HD13 | 1.34                     | 0.77              |
| 1:J:131:TRP:C    | 1:J:132:LEU:HD12 | 2.09                     | 0.77              |
| 1:J:219:GLU:O    | 1:J:223:ILE:HG13 | 1.84                     | 0.77              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:HD21 | 2.14                     | 0.77              |
| 1:J:721:LYS:CB   | 1:J:736:GLN:CD   | 2.56                     | 0.77              |
| 4:3:324:THR:CG2  | 4:5:244:ASP:C    | 2.55                     | 0.77              |
| 4:Z:223:PHE:HD2  | 4:Z:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:NE2  | 2.43                     | 0.77              |
| 1:A:725:ARG:HG3  | 1:A:733:PRO:HA   | 1.67                     | 0.77              |
| 1:D:818:TYR:CG   | 2:E:89:LYS:HB2   | 2.20                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:93:MET:CE    | 1:G:764:MLY:HE3  | 2.15                     | 0.77              |
| 1:G:290:GLN:C    | 1:G:331:LEU:HD12 | 2.09                     | 0.77              |
| 1:G:751:GLY:CA   | 3:I:114:LEU:HD13 | 2.14                     | 0.77              |
| 2:H:141:PRO:HB2  | 2:H:142:PRO:CD   | 2.11                     | 0.77              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG12 | 1.67                     | 0.77              |
| 3:L:3:SER:O      | 3:L:4:LYS:HB2    | 1.84                     | 0.77              |
| 4:3:223:PHE:HD2  | 4:3:312:ARG:HH21 | 1.32                     | 0.77              |
| 4:3:288:ASP:H    | 4:5:203:THR:CG2  | 1.98                     | 0.77              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:OE1  | 2.33                     | 0.77              |
| 1:A:732:ILE:N    | 1:A:733:PRO:HD2  | 2.00                     | 0.77              |
| 1:D:290:GLN:C    | 1:D:331:LEU:HD12 | 2.09                     | 0.77              |
| 1:D:635:GLY:HA3  | 4:9:341:ILE:CD1  | 2.14                     | 0.77              |
| 1:D:642:LYS:HG2  | 4:9:22:ALA:HA    | 1.65                     | 0.77              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:OE1  | 2.33                     | 0.77              |
| 1:G:725:ARG:HG3  | 1:G:733:PRO:HA   | 1.67                     | 0.77              |
| 1:G:732:ILE:N    | 1:G:733:PRO:HD2  | 2.00                     | 0.77              |
| 1:J:95:THR:HA    | 1:J:713:SER:HA   | 1.67                     | 0.77              |
| 4:8:223:PHE:HD2  | 4:8:312:ARG:HH21 | 1.33                     | 0.77              |
| 4:X:223:PHE:HD2  | 4:X:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:D:599:ASN:CA   | 1:D:649:VAL:CB   | 2.53                     | 0.76              |
| 1:D:831:TRP:HZ3  | 2:E:34:ILE:HG23  | 1.43                     | 0.76              |
| 3:F:49:ILE:N     | 3:F:52:ASN:HD22  | 1.82                     | 0.76              |
| 1:G:534:SER:C    | 4:V:351:THR:CA   | 2.48                     | 0.76              |
| 1:J:635:GLY:HA3  | 4:W:341:ILE:CD1  | 2.14                     | 0.76              |
| 1:A:94:MET:CE    | 1:A:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:A:290:GLN:C    | 1:A:331:LEU:HD12 | 2.09                     | 0.76              |
| 1:D:217:THR:C    | 1:D:221:GLN:HE21 | 1.92                     | 0.76              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:CG   | 2.60                     | 0.76              |
| 1:D:834:LEU:HG   | 2:E:54:MET:CG    | 2.04                     | 0.76              |
| 1:J:94:MET:CE    | 1:J:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:CG   | 2.60                     | 0.76              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CE2   | 2.52                     | 0.76              |
| 4:0:287:ILE:CG2  | 4:2:203:THR:H    | 1.96                     | 0.76              |
| 4:1:223:PHE:HD2  | 4:1:312:ARG:HH21 | 1.32                     | 0.76              |
| 4:1:288:ASP:OD1  | 4:3:203:THR:HG23 | 1.84                     | 0.76              |
| 4:2:223:PHE:HD2  | 4:2:312:ARG:HH21 | 1.33                     | 0.76              |
| 1:A:793:ARG:HE   | 3:C:147:MET:HA   | 1.48                     | 0.76              |
| 1:A:836:PHE:HZ   | 2:B:160:GLY:N    | 1.78                     | 0.76              |
| 1:D:219:GLU:O    | 1:D:223:ILE:HG13 | 1.84                     | 0.76              |
| 1:D:793:ARG:HE   | 3:F:147:MET:HA   | 1.49                     | 0.76              |
| 2:E:121:LEU:CG   | 2:E:128:PHE:HA   | 2.14                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:131:TRP:C    | 1:G:132:LEU:HD12 | 2.09                     | 0.76              |
| 1:G:218:LEU:HB2  | 1:G:221:GLN:CG   | 2.09                     | 0.76              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:OE1  | 1.80                     | 0.76              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:OE1  | 2.33                     | 0.76              |
| 1:J:757:GLN:HG3  | 1:J:776:GLU:HG3  | 1.63                     | 0.76              |
| 4:2:324:THR:HG21 | 4:4:243:PRO:C    | 2.11                     | 0.76              |
| 4:V:223:PHE:HD2  | 4:V:312:ARG:HH21 | 1.32                     | 0.76              |
| 1:A:217:THR:C    | 1:A:221:GLN:HE21 | 1.93                     | 0.76              |
| 1:A:623:PHE:CG   | 1:A:623:PHE:CA   | 2.68                     | 0.76              |
| 1:D:131:TRP:C    | 1:D:132:LEU:HD12 | 2.09                     | 0.76              |
| 1:D:534:SER:O    | 4:9:351:THR:N    | 2.19                     | 0.76              |
| 1:D:732:ILE:N    | 1:D:733:PRO:HD2  | 2.00                     | 0.76              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:CB   | 2.63                     | 0.76              |
| 2:H:121:LEU:CG   | 2:H:128:PHE:HA   | 2.14                     | 0.76              |
| 1:J:290:GLN:C    | 1:J:331:LEU:HD12 | 2.09                     | 0.76              |
| 1:J:732:ILE:N    | 1:J:733:PRO:HD2  | 2.01                     | 0.76              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG12 | 1.67                     | 0.76              |
| 1:A:502:GLU:CB   | 1:A:761:GLY:HA3  | 2.16                     | 0.76              |
| 1:D:831:TRP:N    | 2:E:51:PHE:CZ    | 2.54                     | 0.76              |
| 1:G:530:MET:CG   | 4:V:354:GLN:CB   | 2.30                     | 0.76              |
| 1:G:831:TRP:CZ2  | 2:H:47:LEU:HD22  | 2.18                     | 0.76              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:CH2  | 2.33                     | 0.76              |
| 4:1:202:THR:C    | 4:Z:287:ILE:HG21 | 2.09                     | 0.76              |
| 1:D:623:PHE:CG   | 1:D:623:PHE:CA   | 2.68                     | 0.76              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HD2  | 1.52                     | 0.76              |
| 1:J:481:ASN:HD22 | 1:J:481:ASN:N    | 1.82                     | 0.76              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:CA   | 2.68                     | 0.76              |
| 4:0:244:ASP:H    | 4:Y:291:LYS:HD2  | 1.51                     | 0.76              |
| 1:G:217:THR:C    | 1:G:221:GLN:HE21 | 1.92                     | 0.76              |
| 1:G:769:ALA:HB2  | 1:G:770:GLY:CA   | 2.16                     | 0.76              |
| 1:G:797:PHE:HD1  | 3:I:149:VAL:CB   | 1.97                     | 0.76              |
| 1:J:217:THR:C    | 1:J:221:GLN:HE21 | 1.92                     | 0.76              |
| 4:1:287:ILE:HG13 | 4:3:202:THR:CA   | 2.16                     | 0.76              |
| 4:9:290:ARG:NH1  | 4:W:202:THR:CG2  | 2.49                     | 0.76              |
| 4:W:291:LYS:HB3  | 4:Y:244:ASP:HB3  | 1.66                     | 0.76              |
| 1:A:116:TYR:O    | 1:A:153:PRO:HB2  | 1.85                     | 0.76              |
| 1:A:218:LEU:HB2  | 1:A:221:GLN:CG   | 2.09                     | 0.76              |
| 1:A:218:LEU:HB3  | 1:A:221:GLN:HG3  | 1.60                     | 0.76              |
| 1:A:831:TRP:HH2  | 2:B:50:THR:CB    | 1.99                     | 0.76              |
| 1:D:553:MLY:NZ   | 4:W:45:VAL:HA    | 1.84                     | 0.76              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:CB   | 2.64                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:664:LEU:O    | 1:D:667:THR:HB   | 1.86                     | 0.76              |
| 1:D:769:ALA:CA   | 1:D:771:LEU:HA   | 2.15                     | 0.76              |
| 1:D:818:TYR:HB2  | 2:E:90:GLY:CA    | 2.16                     | 0.76              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:HD21 | 1.47                     | 0.76              |
| 1:J:754:ASP:CG   | 1:J:776:GLU:CA   | 2.59                     | 0.76              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:CB   | 2.64                     | 0.76              |
| 4:3:324:THR:CG2  | 4:5:244:ASP:N    | 2.31                     | 0.76              |
| 4:8:290:ARG:NH1  | 4:V:202:THR:CG2  | 2.49                     | 0.76              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:CB   | 1.98                     | 0.76              |
| 1:D:550:PHE:HA   | 4:W:46:GLY:HA3   | 1.66                     | 0.76              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:CG   | 2.60                     | 0.76              |
| 3:L:49:ILE:N     | 3:L:52:ASN:HD22  | 1.82                     | 0.76              |
| 1:A:505:MLY:HB2  | 1:A:761:GLY:C    | 2.11                     | 0.75              |
| 1:D:733:PRO:C    | 1:D:737:PHE:CD1  | 2.62                     | 0.75              |
| 1:G:94:MET:CE    | 1:G:101:ALA:HB1  | 2.15                     | 0.75              |
| 1:G:481:ASN:HD22 | 1:G:481:ASN:N    | 1.82                     | 0.75              |
| 1:G:534:SER:O    | 4:V:351:THR:N    | 2.20                     | 0.75              |
| 1:G:538:GLU:OE2  | 4:V:355:MET:HE2  | 1.87                     | 0.75              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:CB   | 2.64                     | 0.75              |
| 1:A:664:LEU:O    | 1:A:667:THR:HB   | 1.85                     | 0.75              |
| 1:A:795:ARG:NH1  | 3:C:43:ASN:N     | 2.32                     | 0.75              |
| 1:D:537:GLU:HG3  | 4:9:350:SER:O    | 1.79                     | 0.75              |
| 4:W:324:THR:CG2  | 4:Y:247:VAL:HG22 | 2.17                     | 0.75              |
| 1:A:757:GLN:HG3  | 1:A:771:LEU:HD11 | 1.69                     | 0.75              |
| 1:G:795:ARG:CD   | 3:I:35:ARG:NH2   | 2.17                     | 0.75              |
| 1:J:541:MET:O    | 4:W:143:TYR:CZ   | 2.40                     | 0.75              |
| 1:J:820:VAL:HG11 | 2:K:136:MET:CE   | 2.17                     | 0.75              |
| 4:X:287:ILE:CG1  | 4:Z:201:VAL:CG2  | 2.63                     | 0.75              |
| 1:D:642:LYS:CG   | 4:9:23:GLY:H     | 1.77                     | 0.75              |
| 1:G:721:LYS:HG2  | 1:G:736:GLN:CD   | 1.86                     | 0.75              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:OE1  | 2.33                     | 0.75              |
| 1:J:642:LYS:HG2  | 4:W:22:ALA:HA    | 1.65                     | 0.75              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:CB   | 2.64                     | 0.75              |
| 1:J:752:ASP:O    | 1:J:780:ASP:CG   | 2.30                     | 0.75              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:CE   | 2.50                     | 0.75              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:HG22 | 0.92                     | 0.75              |
| 3:C:3:SER:O      | 3:C:4:LYS:HB2    | 1.84                     | 0.75              |
| 1:G:623:PHE:CG   | 1:G:623:PHE:CA   | 2.68                     | 0.75              |
| 1:A:530:MET:CG   | 4:8:354:GLN:CB   | 2.30                     | 0.75              |
| 1:A:636:LYS:O    | 1:A:637:LYS:HB2  | 1.86                     | 0.75              |
| 1:D:725:ARG:HG3  | 1:D:733:PRO:HA   | 1.67                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:350:ALA:O    | 1:J:354:LEU:HB2  | 1.87                     | 0.75              |
| 1:J:797:PHE:CA   | 3:L:149:VAL:CG1  | 2.65                     | 0.75              |
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:HD2  | 1.68                     | 0.75              |
| 4:1:287:ILE:CB   | 4:3:203:THR:HG22 | 2.13                     | 0.75              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:HG22 | 1.97                     | 0.75              |
| 4:3:322:PRO:CB   | 4:5:244:ASP:HB2  | 2.14                     | 0.75              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:HE2  | 1.69                     | 0.75              |
| 1:A:350:ALA:O    | 1:A:354:LEU:HB2  | 1.87                     | 0.75              |
| 1:A:534:SER:O    | 4:8:351:THR:N    | 2.18                     | 0.75              |
| 1:A:795:ARG:HE   | 3:C:118:MET:CE   | 1.99                     | 0.75              |
| 1:D:538:GLU:O    | 4:9:349:LEU:HG   | 1.86                     | 0.75              |
| 1:D:724:TYR:HA   | 1:D:782:MLY:CH1  | 2.16                     | 0.75              |
| 1:D:831:TRP:HA   | 2:E:51:PHE:CE1   | 2.22                     | 0.75              |
| 1:G:817:GLN:HG3  | 2:H:128:PHE:CE1  | 2.22                     | 0.75              |
| 1:J:310:TYR:CE2  | 1:J:320:ILE:HD11 | 2.22                     | 0.75              |
| 1:J:664:LEU:O    | 1:J:667:THR:HB   | 1.86                     | 0.75              |
| 1:J:768:MLY:CD   | 1:J:772:LEU:HB2  | 2.17                     | 0.75              |
| 1:A:481:ASN:HD22 | 1:A:481:ASN:N    | 1.82                     | 0.75              |
| 1:A:793:ARG:NE   | 3:C:147:MET:HA   | 2.02                     | 0.75              |
| 3:F:3:SER:O      | 3:F:4:LYS:HB2    | 1.84                     | 0.75              |
| 1:G:541:MET:O    | 4:V:143:TYR:CZ   | 2.40                     | 0.75              |
| 1:G:664:LEU:O    | 1:G:667:THR:HB   | 1.86                     | 0.75              |
| 4:1:253:GLU:HA   | 4:1:256:ARG:HG3  | 1.69                     | 0.75              |
| 1:D:732:ILE:N    | 1:D:733:PRO:CD   | 2.50                     | 0.74              |
| 1:G:783:LEU:O    | 1:G:787:ILE:CB   | 2.35                     | 0.74              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:N    | 2.02                     | 0.74              |
| 4:5:253:GLU:HA   | 4:5:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:7:288:ASP:H    | 4:9:203:THR:HG22 | 1.52                     | 0.74              |
| 4:X:287:ILE:HG23 | 4:Z:201:VAL:HG23 | 1.68                     | 0.74              |
| 1:A:502:GLU:CA   | 1:A:761:GLY:CA   | 2.66                     | 0.74              |
| 1:A:541:MET:O    | 4:8:143:TYR:CZ   | 2.40                     | 0.74              |
| 1:D:272:MLY:HH13 | 1:D:435:GLU:OE1  | 1.87                     | 0.74              |
| 1:D:769:ALA:CA   | 1:D:770:GLY:C    | 2.60                     | 0.74              |
| 1:G:798:LEU:HD22 | 3:I:126:LEU:HD11 | 1.68                     | 0.74              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:HD21 | 1.47                     | 0.74              |
| 1:J:818:TYR:CZ   | 2:K:127:ARG:NH2  | 2.55                     | 0.74              |
| 4:9:288:ASP:H    | 4:W:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:215:GLN:NE2  | 1:A:336:SER:O    | 2.20                     | 0.74              |
| 1:A:732:ILE:N    | 1:A:733:PRO:CD   | 2.51                     | 0.74              |
| 1:D:350:ALA:O    | 1:D:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:D:726:VAL:H    | 1:D:782:MLY:CH2  | 2.00                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:831:TRP:CG   | 2:E:51:PHE:CZ    | 2.76                     | 0.74              |
| 1:G:350:ALA:O    | 1:G:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:G:636:LYS:O    | 1:G:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB1  | 1.26                     | 0.74              |
| 1:J:739:ASP:CB   | 1:J:742:LYS:HB3  | 2.12                     | 0.74              |
| 4:O:253:GLU:HA   | 4:O:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:1:202:THR:HB   | 4:Z:287:ILE:HG23 | 0.76                     | 0.74              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:OD2  | 2.26                     | 0.74              |
| 4:3:253:GLU:HA   | 4:3:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:7:290:ARG:HH22 | 4:9:202:THR:HG23 | 1.50                     | 0.74              |
| 4:9:253:GLU:HA   | 4:9:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:W:253:GLU:HA   | 4:W:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:A:538:GLU:O    | 4:8:349:LEU:HG   | 1.86                     | 0.74              |
| 1:A:831:TRP:CD2  | 2:B:51:PHE:CE1   | 2.75                     | 0.74              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:HE   | 1.89                     | 0.74              |
| 1:G:218:LEU:HB3  | 1:G:221:GLN:HG3  | 1.60                     | 0.74              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:G:556:ASP:OD2  | 4:X:47:MET:HE3   | 1.85                     | 0.74              |
| 1:G:735:GLY:CA   | 1:G:743:ALA:HA   | 2.17                     | 0.74              |
| 1:J:90:ASP:HB3   | 1:J:764:MLY:HH21 | 1.70                     | 0.74              |
| 1:J:636:LYS:O    | 1:J:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:J:733:PRO:C    | 1:J:737:PHE:CD1  | 2.62                     | 0.74              |
| 4:8:288:ASP:H    | 4:V:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:436:MLY:HE3  | 1:A:626:TYR:CE1  | 2.22                     | 0.74              |
| 1:A:733:PRO:C    | 1:A:737:PHE:CD1  | 2.62                     | 0.74              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG12 | 1.67                     | 0.74              |
| 1:D:310:TYR:CE2  | 1:D:320:ILE:HD11 | 2.22                     | 0.74              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:OE1  | 1.81                     | 0.74              |
| 1:D:215:GLN:NE2  | 1:D:336:SER:O    | 2.20                     | 0.74              |
| 1:D:541:MET:O    | 4:9:143:TYR:CZ   | 2.40                     | 0.74              |
| 1:D:636:LYS:O    | 1:D:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:HE2  | 1.69                     | 0.74              |
| 1:J:95:THR:HG1   | 1:J:713:SER:HB3  | 1.48                     | 0.74              |
| 1:J:534:SER:O    | 4:W:351:THR:N    | 2.19                     | 0.74              |
| 1:A:409:GLY:HA3  | 4:8:333:PRO:N    | 2.02                     | 0.74              |
| 1:A:635:GLY:HA3  | 4:8:341:ILE:CD1  | 2.14                     | 0.74              |
| 1:G:310:TYR:CE2  | 1:G:320:ILE:HD11 | 2.22                     | 0.74              |
| 3:I:4:LYS:N      | 3:I:5:ALA:O      | 2.16                     | 0.74              |
| 1:J:272:MLY:HH13 | 1:J:435:GLU:OE1  | 1.87                     | 0.74              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:HD12 | 0.74                     | 0.74              |
| 4:X:253:GLU:HA   | 4:X:256:ARG:HG3  | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:253:GLU:HA   | 4:Y:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:HD12 | 0.74                     | 0.74              |
| 4:X:287:ILE:HG13 | 4:Z:201:VAL:HG23 | 1.69                     | 0.74              |
| 4:Z:253:GLU:HA   | 4:Z:256:ARG:HG3  | 1.70                     | 0.74              |
| 1:A:486:MLY:HH13 | 1:A:527:GLU:OE1  | 1.88                     | 0.74              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CB   | 2.18                     | 0.74              |
| 1:D:640:LYS:O    | 4:9:23:GLY:O     | 2.06                     | 0.74              |
| 1:G:731:ALA:HB2  | 3:I:109:HIS:ND1  | 2.02                     | 0.74              |
| 1:J:538:GLU:O    | 4:W:349:LEU:HG   | 1.86                     | 0.74              |
| 4:1:202:THR:OG1  | 4:Z:287:ILE:HG23 | 1.88                     | 0.74              |
| 4:7:253:GLU:HA   | 4:7:256:ARG:HG3  | 1.70                     | 0.74              |
| 1:A:530:MET:CE   | 4:8:355:MET:SD   | 2.76                     | 0.74              |
| 1:D:436:MLY:HE3  | 1:D:626:TYR:CE1  | 2.23                     | 0.74              |
| 1:D:530:MET:CG   | 4:9:354:GLN:CB   | 2.30                     | 0.74              |
| 1:D:789:ALA:HB2  | 3:F:81:GLN:HG2   | 1.70                     | 0.74              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:CG   | 2.66                     | 0.74              |
| 3:I:24:LYS:CA    | 3:I:63:ILE:O     | 2.36                     | 0.74              |
| 1:J:820:VAL:CG1  | 2:K:136:MET:HE1  | 2.18                     | 0.74              |
| 4:0:201:VAL:HG23 | 4:Y:287:ILE:HG23 | 1.70                     | 0.74              |
| 4:8:290:ARG:HH22 | 4:V:202:THR:HG23 | 1.50                     | 0.74              |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:CG2  | 2.18                     | 0.74              |
| 1:A:499:GLU:OE1  | 1:A:766:PHE:CZ   | 2.41                     | 0.73              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:HE2  | 1.69                     | 0.73              |
| 1:G:732:ILE:N    | 1:G:733:PRO:CD   | 2.51                     | 0.73              |
| 1:J:735:GLY:CA   | 1:J:743:ALA:HA   | 2.18                     | 0.73              |
| 1:J:790:THR:N    | 3:L:87:PHE:CE2   | 2.56                     | 0.73              |
| 2:K:130:PRO:O    | 2:K:132:GLU:N    | 2.21                     | 0.73              |
| 4:1:202:THR:HA   | 4:Z:287:ILE:CG1  | 2.18                     | 0.73              |
| 1:J:486:MLY:HH13 | 1:J:527:GLU:OE1  | 1.87                     | 0.73              |
| 4:V:253:GLU:HA   | 4:V:256:ARG:HG3  | 1.69                     | 0.73              |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:HG23 | 1.70                     | 0.73              |
| 1:A:542:PHE:CD2  | 4:8:143:TYR:CE1  | 2.76                     | 0.73              |
| 1:A:709:LYS:O    | 1:A:710:GLY:CA   | 2.37                     | 0.73              |
| 3:C:48:LYS:C     | 3:C:52:ASN:HD21  | 1.97                     | 0.73              |
| 1:D:487:LEU:O    | 1:D:490:PHE:HB3  | 1.88                     | 0.73              |
| 1:D:534:SER:CA   | 4:9:351:THR:HA   | 2.18                     | 0.73              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:SD    | 2.61                     | 0.73              |
| 1:A:310:TYR:CE2  | 1:A:320:ILE:HD11 | 2.22                     | 0.73              |
| 1:D:409:GLY:HA3  | 4:9:333:PRO:N    | 2.03                     | 0.73              |
| 1:G:215:GLN:NE2  | 1:G:336:SER:O    | 2.20                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:409:GLY:HA3  | 4:V:333:PRO:N    | 2.03                     | 0.73              |
| 2:H:130:PRO:O    | 2:H:132:GLU:N    | 2.21                     | 0.73              |
| 1:J:441:MET:O    | 1:J:445:ILE:HG13 | 1.88                     | 0.73              |
| 1:J:534:SER:CA   | 4:W:351:THR:HA   | 2.18                     | 0.73              |
| 4:0:243:PRO:C    | 4:Y:291:LYS:CE   | 2.62                     | 0.73              |
| 4:8:253:GLU:HA   | 4:8:256:ARG:HG3  | 1.69                     | 0.73              |
| 1:A:237:THR:HG22 | 1:A:239:ARG:H    | 1.53                     | 0.73              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:SD    | 2.29                     | 0.73              |
| 2:B:130:PRO:O    | 2:B:132:GLU:N    | 2.21                     | 0.73              |
| 2:E:130:PRO:O    | 2:E:132:GLU:N    | 2.21                     | 0.73              |
| 1:G:486:MLY:HH13 | 1:G:527:GLU:OE1  | 1.87                     | 0.73              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:HH12 | 1.70                     | 0.73              |
| 1:J:487:LEU:O    | 1:J:490:PHE:HB3  | 1.88                     | 0.73              |
| 1:J:530:MET:CE   | 4:W:355:MET:SD   | 2.77                     | 0.73              |
| 4:0:287:ILE:CG2  | 4:2:202:THR:HB   | 2.18                     | 0.73              |
| 1:D:538:GLU:OE2  | 4:9:355:MET:HE2  | 1.86                     | 0.73              |
| 1:D:542:PHE:CD2  | 4:9:143:TYR:CE1  | 2.77                     | 0.73              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:CD   | 2.61                     | 0.73              |
| 3:F:24:LYS:CA    | 3:F:63:ILE:O     | 2.36                     | 0.73              |
| 1:G:487:LEU:O    | 1:G:490:PHE:HB3  | 1.88                     | 0.73              |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CZ   | 2.24                     | 0.73              |
| 1:G:769:ALA:O    | 1:G:773:GLY:CA   | 2.37                     | 0.73              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:HH11 | 2.01                     | 0.73              |
| 1:J:436:MLY:HE3  | 1:J:626:TYR:CE1  | 2.23                     | 0.73              |
| 4:1:43:VAL:O     | 4:Z:167:GLU:OE1  | 2.06                     | 0.73              |
| 1:A:538:GLU:OE2  | 4:8:355:MET:HE2  | 1.86                     | 0.73              |
| 1:A:640:LYS:O    | 4:8:23:GLY:O     | 2.06                     | 0.73              |
| 1:D:530:MET:CE   | 4:9:355:MET:SD   | 2.77                     | 0.73              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:N    | 2.03                     | 0.73              |
| 1:D:802:GLU:O    | 1:D:806:MET:HG3  | 1.89                     | 0.73              |
| 1:G:190:MLY:HE3  | 1:G:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:G:410:ASN:OD1  | 4:V:335:ARG:N    | 2.21                     | 0.73              |
| 1:G:635:GLY:HA3  | 4:V:341:ILE:CD1  | 2.14                     | 0.73              |
| 2:H:144:VAL:CB   | 2:H:153:ILE:HD11 | 2.19                     | 0.73              |
| 1:J:295:MLY:HG3  | 1:J:332:MET:HE2  | 1.69                     | 0.73              |
| 1:J:640:LYS:O    | 1:J:645:SER:OG   | 2.06                     | 0.73              |
| 4:2:253:GLU:HA   | 4:2:256:ARG:HG3  | 1.70                     | 0.73              |
| 4:3:288:ASP:CB   | 4:5:203:THR:CG2  | 2.66                     | 0.73              |
| 1:A:410:ASN:OD1  | 4:8:335:ARG:N    | 2.22                     | 0.73              |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CZ   | 2.24                     | 0.73              |
| 1:A:735:GLY:CA   | 1:A:743:ALA:HA   | 2.17                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:839:MLY:CD   | 2:B:159:HIS:CB   | 2.66                     | 0.73              |
| 1:D:557:GLU:N    | 4:W:48:GLY:HA3   | 1.90                     | 0.73              |
| 1:D:831:TRP:CH2  | 2:E:47:LEU:CA    | 2.41                     | 0.73              |
| 1:J:190:MLY:HE3  | 1:J:230:GLU:OE2  | 1.89                     | 0.73              |
| 4:1:204:ALA:N    | 4:Z:287:ILE:HG21 | 2.03                     | 0.73              |
| 1:D:441:MET:O    | 1:D:445:ILE:HG13 | 1.88                     | 0.73              |
| 1:D:486:MLY:HH13 | 1:D:527:GLU:OE1  | 1.88                     | 0.73              |
| 1:J:21:GLU:O     | 1:J:25:ILE:HG13  | 1.88                     | 0.73              |
| 1:J:640:LYS:O    | 4:W:23:GLY:O     | 2.06                     | 0.73              |
| 1:J:732:ILE:N    | 1:J:733:PRO:CD   | 2.51                     | 0.73              |
| 4:2:288:ASP:H    | 4:4:203:THR:CG2  | 1.98                     | 0.73              |
| 4:9:290:ARG:HH22 | 4:W:202:THR:HG23 | 1.50                     | 0.73              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:C    | 2.31                     | 0.73              |
| 1:D:190:MLY:HE3  | 1:D:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:D:214:MET:HA   | 1:D:340:ILE:HD11 | 1.71                     | 0.73              |
| 1:D:237:THR:HG22 | 1:D:239:ARG:H    | 1.54                     | 0.73              |
| 1:D:410:ASN:OD1  | 4:9:335:ARG:N    | 2.22                     | 0.73              |
| 1:D:618:THR:O    | 1:D:622:LEU:HD13 | 1.89                     | 0.73              |
| 1:D:640:LYS:O    | 1:D:645:SER:OG   | 2.06                     | 0.73              |
| 1:G:21:GLU:O     | 1:G:25:ILE:HG13  | 1.88                     | 0.73              |
| 1:G:272:MLY:HH13 | 1:G:435:GLU:OE1  | 1.88                     | 0.73              |
| 1:G:436:MLY:HE3  | 1:G:626:TYR:CE1  | 2.23                     | 0.73              |
| 1:G:538:GLU:O    | 4:V:349:LEU:HG   | 1.87                     | 0.73              |
| 1:G:730:SER:CB   | 3:I:109:HIS:NE2  | 2.52                     | 0.73              |
| 1:J:84:MLY:CH1   | 1:J:715:VAL:HG12 | 2.16                     | 0.73              |
| 1:J:215:GLN:NE2  | 1:J:336:SER:O    | 2.20                     | 0.73              |
| 1:J:237:THR:HG22 | 1:J:239:ARG:H    | 1.54                     | 0.73              |
| 1:D:36:SER:O     | 1:D:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:HA3  | 1.71                     | 0.72              |
| 2:E:144:VAL:CB   | 2:E:153:ILE:HD11 | 2.19                     | 0.72              |
| 1:G:640:LYS:O    | 4:V:23:GLY:O     | 2.06                     | 0.72              |
| 1:G:802:GLU:O    | 1:G:806:MET:HG3  | 1.89                     | 0.72              |
| 1:J:36:SER:O     | 1:J:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:J:93:MET:HA    | 1:J:714:ARG:HG3  | 1.71                     | 0.72              |
| 1:J:410:ASN:OD1  | 4:W:335:ARG:N    | 2.21                     | 0.72              |
| 1:J:618:THR:O    | 1:J:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:A:441:MET:O    | 1:A:445:ILE:HG13 | 1.88                     | 0.72              |
| 1:A:802:GLU:O    | 1:A:806:MET:HG3  | 1.89                     | 0.72              |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CZ   | 2.24                     | 0.72              |
| 1:D:735:GLY:CA   | 1:D:743:ALA:HA   | 2.18                     | 0.72              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:HH21  | 1.90                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:510:TRP:CZ3  | 1:J:768:MLY:HH12 | 2.23                     | 0.72              |
| 1:J:542:PHE:CD2  | 4:W:143:TYR:CE1  | 2.77                     | 0.72              |
| 1:J:823:PHE:CE1  | 2:K:156:VAL:HG12 | 2.23                     | 0.72              |
| 4:4:253:GLU:HA   | 4:4:256:ARG:HG3  | 1.69                     | 0.72              |
| 1:A:534:SER:CA   | 4:8:351:THR:HA   | 2.18                     | 0.72              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:CZ   | 2.18                     | 0.72              |
| 3:C:24:LYS:CA    | 3:C:63:ILE:O     | 2.37                     | 0.72              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:CE   | 2.19                     | 0.72              |
| 1:J:214:MET:HA   | 1:J:340:ILE:HD11 | 1.70                     | 0.72              |
| 1:J:295:MLY:HG3  | 1:J:332:MET:CE   | 2.19                     | 0.72              |
| 1:J:802:GLU:O    | 1:J:806:MET:HG3  | 1.88                     | 0.72              |
| 3:L:24:LYS:CA    | 3:L:63:ILE:O     | 2.37                     | 0.72              |
| 4:2:3:ASP:HA     | 4:2:6:THR:CB     | 2.18                     | 0.72              |
| 1:A:272:MLY:HH13 | 1:A:435:GLU:OE1  | 1.88                     | 0.72              |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:OE1  | 1.81                     | 0.72              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:NZ   | 2.51                     | 0.72              |
| 1:G:618:THR:O    | 1:G:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:HB2  | 2.17                     | 0.72              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:CD   | 2.53                     | 0.72              |
| 3:I:48:LYS:C     | 3:I:52:ASN:HD21  | 1.96                     | 0.72              |
| 1:J:409:GLY:HA3  | 4:W:333:PRO:N    | 2.03                     | 0.72              |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CZ   | 2.24                     | 0.72              |
| 1:J:538:GLU:OE2  | 4:W:355:MET:HE2  | 1.86                     | 0.72              |
| 1:J:754:ASP:HB3  | 1:J:757:GLN:HG2  | 1.72                     | 0.72              |
| 3:L:4:LYS:N      | 3:L:5:ALA:O      | 2.16                     | 0.72              |
| 4:3:287:ILE:HB   | 4:5:203:THR:HG22 | 1.69                     | 0.72              |
| 1:A:36:SER:O     | 1:A:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:A:519:LEU:HD12 | 1:A:519:LEU:N    | 2.04                     | 0.72              |
| 1:G:176:LEU:HD12 | 1:G:176:LEU:N    | 2.05                     | 0.72              |
| 1:G:214:MET:HA   | 1:G:340:ILE:HD11 | 1.70                     | 0.72              |
| 1:G:552:ASN:C    | 4:X:47:MET:HE1   | 2.14                     | 0.72              |
| 1:G:754:ASP:HB3  | 1:G:757:GLN:HG2  | 1.72                     | 0.72              |
| 1:J:510:TRP:CE3  | 1:J:768:MLY:CH1  | 2.71                     | 0.72              |
| 1:J:800:ARG:CG   | 3:L:149:VAL:HG23 | 2.12                     | 0.72              |
| 2:K:144:VAL:CB   | 2:K:153:ILE:HD11 | 2.19                     | 0.72              |
| 4:2:287:ILE:CD1  | 4:4:203:THR:HB   | 2.19                     | 0.72              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:HB3  | 1.70                     | 0.72              |
| 1:A:21:GLU:O     | 1:A:25:ILE:HG13  | 1.88                     | 0.72              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:NH2   | 2.01                     | 0.72              |
| 1:D:817:GLN:OE1  | 2:E:127:ARG:NE   | 2.22                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:237:THR:HG22 | 1:G:239:ARG:H    | 1.53                     | 0.72              |
| 1:G:530:MET:CE   | 4:V:355:MET:SD   | 2.78                     | 0.72              |
| 4:1:3:ASP:HA     | 4:1:6:THR:CB     | 2.17                     | 0.72              |
| 4:8:3:ASP:HA     | 4:8:6:THR:CB     | 2.18                     | 0.72              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:CA   | 2.70                     | 0.72              |
| 1:D:21:GLU:O     | 1:D:25:ILE:HG13  | 1.88                     | 0.72              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:OE1  | 1.81                     | 0.72              |
| 1:G:441:MET:O    | 1:G:445:ILE:HG13 | 1.88                     | 0.72              |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:OE2  | 1.90                     | 0.72              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CA   | 2.19                     | 0.72              |
| 4:0:287:ILE:HB   | 4:2:203:THR:CB   | 2.19                     | 0.72              |
| 4:1:288:ASP:H    | 4:3:203:THR:HG22 | 1.54                     | 0.72              |
| 4:3:3:ASP:HA     | 4:3:6:THR:CB     | 2.18                     | 0.72              |
| 4:V:286:ASP:OD1  | 4:X:203:THR:N    | 2.23                     | 0.72              |
| 4:V:287:ILE:HD11 | 4:X:201:VAL:O    | 1.75                     | 0.72              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:HB3  | 2.20                     | 0.72              |
| 1:A:800:ARG:CZ   | 3:C:149:VAL:C    | 2.62                     | 0.72              |
| 2:B:144:VAL:CB   | 2:B:153:ILE:HD11 | 2.19                     | 0.72              |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:D:754:ASP:HB3  | 1:D:757:GLN:HG2  | 1.72                     | 0.72              |
| 1:D:817:GLN:HG3  | 2:E:127:ARG:CD   | 2.18                     | 0.72              |
| 1:G:14:ALA:HB3   | 1:G:15:PRO:HD3   | 1.72                     | 0.72              |
| 2:K:150:TYR:C    | 2:K:151:LYS:CG   | 2.48                     | 0.72              |
| 4:1:203:THR:CB   | 4:Z:287:ILE:HB   | 2.19                     | 0.72              |
| 4:7:290:ARG:NH1  | 4:9:202:THR:CG2  | 2.49                     | 0.72              |
| 1:D:769:ALA:CA   | 1:D:771:LEU:CA   | 2.60                     | 0.72              |
| 1:G:739:ASP:CB   | 1:G:742:LYS:HB3  | 2.12                     | 0.72              |
| 1:G:798:LEU:HD13 | 3:I:126:LEU:HD21 | 0.73                     | 0.72              |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:OE2  | 1.90                     | 0.72              |
| 2:K:136:MET:O    | 2:K:140:PHE:HB2  | 1.90                     | 0.72              |
| 4:1:287:ILE:HG21 | 4:3:202:THR:OG1  | 1.89                     | 0.72              |
| 4:X:324:THR:HB   | 4:Z:246:GLN:CA   | 2.20                     | 0.72              |
| 4:X:324:THR:HB   | 4:Z:247:VAL:H    | 1.55                     | 0.72              |
| 1:A:14:ALA:HB3   | 1:A:15:PRO:HD3   | 1.72                     | 0.72              |
| 1:D:176:LEU:HD12 | 1:D:176:LEU:N    | 2.05                     | 0.72              |
| 1:D:519:LEU:HD12 | 1:D:519:LEU:N    | 2.04                     | 0.72              |
| 1:D:829:TRP:CD1  | 2:E:67:MET:HG2   | 2.25                     | 0.72              |
| 1:J:176:LEU:HD12 | 1:J:176:LEU:N    | 2.05                     | 0.72              |
| 1:J:818:TYR:CE1  | 2:K:127:ARG:NH1  | 2.58                     | 0.72              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:N    | 2.52                     | 0.72              |
| 1:A:217:THR:O    | 1:A:220:ASP:HB2  | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:754:ASP:HB3  | 1:A:757:GLN:HG2  | 1.72                     | 0.71              |
| 1:A:831:TRP:CZ3  | 2:B:50:THR:CG2   | 2.72                     | 0.71              |
| 1:D:834:LEU:HD12 | 2:E:54:MET:HB2   | 1.72                     | 0.71              |
| 2:E:136:MET:O    | 2:E:140:PHE:HB2  | 1.90                     | 0.71              |
| 1:G:36:SER:O     | 1:G:52:ILE:HG12  | 1.90                     | 0.71              |
| 1:G:519:LEU:HD12 | 1:G:519:LEU:N    | 2.04                     | 0.71              |
| 1:G:542:PHE:CD2  | 4:V:143:TYR:CE1  | 2.77                     | 0.71              |
| 1:G:640:LYS:O    | 1:G:645:SER:OG   | 2.06                     | 0.71              |
| 4:9:3:ASP:HA     | 4:9:6:THR:CB     | 2.18                     | 0.71              |
| 1:A:190:MLY:HE3  | 1:A:230:GLU:OE2  | 1.89                     | 0.71              |
| 1:A:487:LEU:O    | 1:A:490:PHE:HB3  | 1.88                     | 0.71              |
| 1:D:217:THR:O    | 1:D:220:ASP:HB2  | 1.90                     | 0.71              |
| 1:G:534:SER:CA   | 4:V:351:THR:HA   | 2.19                     | 0.71              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CB   | 1.85                     | 0.71              |
| 1:J:95:THR:CB    | 1:J:713:SER:HB3  | 2.20                     | 0.71              |
| 1:J:826:VAL:CG2  | 2:K:88:LEU:HD21  | 2.12                     | 0.71              |
| 1:A:214:MET:HA   | 1:A:340:ILE:HD11 | 1.71                     | 0.71              |
| 1:A:640:LYS:O    | 1:A:645:SER:OG   | 2.06                     | 0.71              |
| 1:A:707:CYS:CA   | 1:A:714:ARG:NH1  | 2.50                     | 0.71              |
| 1:D:530:MET:HE3  | 4:9:355:MET:SD   | 2.30                     | 0.71              |
| 1:D:789:ALA:C    | 3:F:87:PHE:CE2   | 2.67                     | 0.71              |
| 1:G:537:GLU:C    | 4:V:351:THR:H    | 1.99                     | 0.71              |
| 1:A:530:MET:HE3  | 4:8:355:MET:SD   | 2.29                     | 0.71              |
| 2:B:136:MET:O    | 2:B:140:PHE:HB2  | 1.90                     | 0.71              |
| 1:D:86:ASP:OD2   | 1:D:87:MLY:HH13  | 1.91                     | 0.71              |
| 1:D:795:ARG:CZ   | 3:F:43:ASN:CG    | 2.63                     | 0.71              |
| 1:D:831:TRP:CD1  | 2:E:51:PHE:HZ    | 2.08                     | 0.71              |
| 1:G:557:GLU:HB2  | 4:X:47:MET:C     | 2.16                     | 0.71              |
| 1:G:752:ASP:C    | 1:G:779:ARG:HH12 | 1.97                     | 0.71              |
| 1:J:72:VAL:HG13  | 1:J:76:GLN:CB    | 2.19                     | 0.71              |
| 1:J:816:ILE:HD11 | 2:K:100:ALA:CB   | 2.19                     | 0.71              |
| 4:1:287:ILE:HG23 | 4:3:202:THR:HB   | 0.88                     | 0.71              |
| 4:2:287:ILE:CG2  | 4:4:204:ALA:H    | 2.04                     | 0.71              |
| 4:X:3:ASP:HA     | 4:X:6:THR:CB     | 2.17                     | 0.71              |
| 4:Z:3:ASP:HA     | 4:Z:6:THR:CB     | 2.18                     | 0.71              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:CE   | 2.19                     | 0.71              |
| 1:A:618:THR:O    | 1:A:622:LEU:HD13 | 1.89                     | 0.71              |
| 1:A:793:ARG:HG3  | 3:C:146:ILE:CG2  | 2.21                     | 0.71              |
| 1:A:818:TYR:CB   | 2:B:89:LYS:C     | 2.63                     | 0.71              |
| 1:D:56:GLU:CB    | 1:D:59:MLY:HB3   | 2.19                     | 0.71              |
| 1:D:245:ARG:HD3  | 1:D:271:GLU:OE1  | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:789:ALA:HB1  | 3:F:81:GLN:O     | 1.91                     | 0.71              |
| 1:G:93:MET:SD    | 1:G:716:LEU:HD11 | 2.30                     | 0.71              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:N    | 2.17                     | 0.71              |
| 4:2:287:ILE:HB   | 4:4:204:ALA:H    | 1.54                     | 0.71              |
| 4:5:3:ASP:HA     | 4:5:6:THR:CB     | 2.18                     | 0.71              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:CA    | 2.21                     | 0.71              |
| 1:D:726:VAL:H    | 1:D:782:MLY:HH22 | 1.53                     | 0.71              |
| 1:D:789:ALA:CB   | 3:F:81:GLN:O     | 2.38                     | 0.71              |
| 3:F:4:LYS:N      | 3:F:5:ALA:O      | 2.16                     | 0.71              |
| 1:J:519:LEU:HD12 | 1:J:519:LEU:N    | 2.04                     | 0.71              |
| 1:D:14:ALA:HB3   | 1:D:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:D:831:TRP:CD1  | 2:E:51:PHE:CZ    | 2.79                     | 0.71              |
| 1:G:166:MET:HE1  | 1:G:254:PHE:HB2  | 1.73                     | 0.71              |
| 1:G:274:ARG:NH2  | 1:G:282:GLU:OE1  | 2.24                     | 0.71              |
| 1:G:792:ALA:HA   | 3:I:35:ARG:NH1   | 2.04                     | 0.71              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:HH12  | 1.55                     | 0.71              |
| 3:L:48:LYS:C     | 3:L:52:ASN:HD21  | 1.96                     | 0.71              |
| 4:X:286:ASP:OD1  | 4:Z:203:THR:N    | 2.24                     | 0.71              |
| 1:A:537:GLU:C    | 4:8:351:THR:H    | 1.99                     | 0.71              |
| 1:G:557:GLU:HA   | 4:X:48:GLY:CA    | 2.18                     | 0.71              |
| 1:J:749:GLY:C    | 3:L:114:LEU:HD21 | 2.15                     | 0.71              |
| 1:J:762:HIS:H    | 1:J:762:HIS:CD2  | 2.07                     | 0.71              |
| 1:A:166:MET:HE1  | 1:A:254:PHE:HB2  | 1.73                     | 0.71              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:HG23 | 0.71                     | 0.71              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CG   | 2.20                     | 0.71              |
| 1:D:537:GLU:C    | 4:9:351:THR:H    | 1.98                     | 0.71              |
| 3:F:48:LYS:O     | 3:F:52:ASN:CG    | 2.34                     | 0.71              |
| 1:G:86:ASP:OD2   | 1:G:87:MLY:HH13  | 1.91                     | 0.71              |
| 1:G:245:ARG:HD3  | 1:G:271:GLU:OE1  | 1.90                     | 0.71              |
| 1:J:14:ALA:HB3   | 1:J:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:J:56:GLU:CB    | 1:J:59:MLY:HB3   | 2.19                     | 0.71              |
| 1:J:274:ARG:NH2  | 1:J:282:GLU:OE1  | 2.24                     | 0.71              |
| 4:7:3:ASP:HA     | 4:7:6:THR:CB     | 2.18                     | 0.71              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:C    | 2.16                     | 0.71              |
| 1:A:814:PHE:HD1  | 2:B:127:ARG:NH2  | 1.69                     | 0.71              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:CE   | 2.20                     | 0.71              |
| 1:J:245:ARG:HD3  | 1:J:271:GLU:OE1  | 1.90                     | 0.71              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:N    | 2.54                     | 0.71              |
| 1:J:800:ARG:HB2  | 3:L:149:VAL:CG2  | 2.06                     | 0.71              |
| 1:G:84:MLY:HH11  | 1:G:715:VAL:HG11 | 1.71                     | 0.70              |
| 1:J:787:ILE:HG22 | 1:J:788:THR:N    | 2.06                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:3:ASP:HA     | 4:V:6:THR:CB     | 2.18                     | 0.70              |
| 1:A:72:VAL:HG13  | 1:A:76:GLN:CB    | 2.19                     | 0.70              |
| 1:A:176:LEU:N    | 1:A:176:LEU:HD12 | 2.05                     | 0.70              |
| 1:A:787:ILE:HG22 | 1:A:788:THR:N    | 2.07                     | 0.70              |
| 1:A:818:TYR:HB3  | 2:B:89:LYS:C     | 2.16                     | 0.70              |
| 1:A:819:ASN:N    | 2:B:90:GLY:CA    | 2.54                     | 0.70              |
| 1:D:166:MET:HE1  | 1:D:254:PHE:HB2  | 1.73                     | 0.70              |
| 1:D:577:ALA:O    | 1:D:578:HIS:CG   | 2.44                     | 0.70              |
| 1:D:579:PHE:HD2  | 1:D:592:ILE:HD11 | 1.56                     | 0.70              |
| 1:D:834:LEU:HD13 | 2:E:51:PHE:HD1   | 1.56                     | 0.70              |
| 1:G:537:GLU:HG3  | 4:V:350:SER:O    | 1.79                     | 0.70              |
| 1:J:166:MET:HE1  | 1:J:254:PHE:HB2  | 1.73                     | 0.70              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:HG23 | 0.71                     | 0.70              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:C    | 2.16                     | 0.70              |
| 4:3:1:ASP:HA     | 4:3:4:GLU:HB3    | 1.74                     | 0.70              |
| 1:A:245:ARG:HD3  | 1:A:271:GLU:OE1  | 1.90                     | 0.70              |
| 1:A:274:ARG:NH2  | 1:A:282:GLU:OE1  | 2.24                     | 0.70              |
| 2:B:150:TYR:C    | 2:B:151:LYS:CG   | 2.49                     | 0.70              |
| 3:C:48:LYS:HB3   | 3:C:52:ASN:HD21  | 1.57                     | 0.70              |
| 1:D:800:ARG:CD   | 3:F:149:VAL:HG22 | 2.21                     | 0.70              |
| 3:I:48:LYS:O     | 3:I:52:ASN:CG    | 2.34                     | 0.70              |
| 1:J:86:ASP:OD2   | 1:J:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:J:217:THR:O    | 1:J:220:ASP:HB2  | 1.91                     | 0.70              |
| 1:J:530:MET:HE3  | 4:W:355:MET:SD   | 2.30                     | 0.70              |
| 1:A:86:ASP:OD2   | 1:A:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:D:723:ARG:NH2  | 1:D:783:LEU:HD11 | 2.05                     | 0.70              |
| 1:D:792:ALA:CB   | 3:F:40:ASN:HB3   | 2.20                     | 0.70              |
| 3:F:48:LYS:C     | 3:F:52:ASN:HD21  | 1.96                     | 0.70              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:C    | 2.16                     | 0.70              |
| 1:G:810:ARG:HG2  | 1:G:810:ARG:HH11 | 1.56                     | 0.70              |
| 2:H:136:MET:O    | 2:H:140:PHE:HB2  | 1.90                     | 0.70              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:HH21 | 2.16                     | 0.70              |
| 1:J:537:GLU:C    | 4:W:351:THR:H    | 1.98                     | 0.70              |
| 1:J:786:ILE:CG1  | 3:L:86:ASP:HB3   | 2.21                     | 0.70              |
| 1:D:72:VAL:HG13  | 1:D:76:GLN:CB    | 2.19                     | 0.70              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:OD1  | 1.92                     | 0.70              |
| 1:D:274:ARG:NH2  | 1:D:282:GLU:OE1  | 2.24                     | 0.70              |
| 1:D:641:LYS:HD2  | 4:9:348:SER:HA   | 1.73                     | 0.70              |
| 1:D:818:TYR:CB   | 2:E:89:LYS:C     | 2.64                     | 0.70              |
| 1:D:830:PRO:CB   | 2:E:51:PHE:CZ    | 2.66                     | 0.70              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HB3   | 2.23                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:217:THR:O    | 1:G:220:ASP:HB2  | 1.91                     | 0.70              |
| 1:G:757:GLN:CD   | 1:G:772:LEU:HG   | 2.16                     | 0.70              |
| 1:G:800:ARG:NH1  | 3:I:149:VAL:C    | 2.50                     | 0.70              |
| 1:J:84:MLY:CH2   | 1:J:716:LEU:O    | 2.39                     | 0.70              |
| 1:J:213:LYS:HA   | 1:J:220:ASP:OD1  | 1.92                     | 0.70              |
| 1:J:630:ALA:O    | 4:W:25:ASP:HB2   | 1.91                     | 0.70              |
| 1:J:641:LYS:HD2  | 4:W:348:SER:HA   | 1.72                     | 0.70              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:A:502:GLU:HA   | 1:A:761:GLY:C    | 2.16                     | 0.70              |
| 1:A:839:MLY:CD   | 2:B:159:HIS:CG   | 2.70                     | 0.70              |
| 1:G:56:GLU:CB    | 1:G:59:MLY:HB3   | 2.19                     | 0.70              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:CG   | 2.20                     | 0.70              |
| 1:G:579:PHE:HD2  | 1:G:592:ILE:HD11 | 1.57                     | 0.70              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:CD1   | 2.75                     | 0.70              |
| 4:O:247:VAL:H    | 4:Y:324:THR:HB   | 1.56                     | 0.70              |
| 4:W:324:THR:HG23 | 4:Y:247:VAL:HG22 | 1.70                     | 0.70              |
| 4:X:1:ASP:HA     | 4:X:4:GLU:HB3    | 1.74                     | 0.70              |
| 1:A:579:PHE:HD2  | 1:A:592:ILE:HD11 | 1.56                     | 0.70              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:NH1  | 2.06                     | 0.70              |
| 3:F:25:ILE:O     | 3:F:63:ILE:HB    | 1.92                     | 0.70              |
| 3:F:48:LYS:HB3   | 3:F:52:ASN:HD21  | 1.57                     | 0.70              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:J:810:ARG:HG2  | 1:J:810:ARG:HH11 | 1.57                     | 0.70              |
| 1:J:831:TRP:HH2  | 2:K:34:ILE:HG21  | 1.56                     | 0.70              |
| 4:Y:3:ASP:HA     | 4:Y:6:THR:CB     | 2.18                     | 0.70              |
| 1:A:546:THR:HG22 | 1:A:548:THR:N    | 2.05                     | 0.70              |
| 1:A:802:GLU:OE1  | 1:A:802:GLU:HA   | 1.92                     | 0.70              |
| 2:B:111:SER:OG   | 2:B:148:VAL:HG12 | 1.92                     | 0.70              |
| 1:D:630:ALA:O    | 4:9:25:ASP:HB2   | 1.92                     | 0.70              |
| 1:D:769:ALA:CA   | 1:D:771:LEU:N    | 2.54                     | 0.70              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:G:166:MET:HE1  | 1:G:254:PHE:HD2  | 1.56                     | 0.70              |
| 1:G:530:MET:HE3  | 4:V:355:MET:SD   | 2.31                     | 0.70              |
| 1:J:577:ALA:O    | 1:J:578:HIS:CG   | 2.44                     | 0.70              |
| 3:L:25:ILE:O     | 3:L:63:ILE:HB    | 1.92                     | 0.70              |
| 4:O:290:ARG:NH2  | 4:2:202:THR:HG21 | 1.87                     | 0.70              |
| 4:1:287:ILE:CG2  | 4:3:203:THR:N    | 2.55                     | 0.70              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:C    | 2.16                     | 0.70              |
| 1:D:782:MLY:C    | 1:D:783:LEU:HD12 | 2.22                     | 0.70              |
| 1:G:546:THR:HG22 | 1:G:548:THR:N    | 2.05                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:762:HIS:H    | 1:G:762:HIS:CD2  | 2.08                     | 0.70              |
| 1:G:782:MLY:C    | 1:G:783:LEU:HD12 | 2.22                     | 0.70              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD11 | 0.73                     | 0.70              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CD1  | 2.20                     | 0.70              |
| 4:W:324:THR:HG23 | 4:Y:247:VAL:H    | 1.45                     | 0.70              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:CG   | 2.75                     | 0.70              |
| 1:A:166:MET:HE1  | 1:A:254:PHE:HD2  | 1.56                     | 0.69              |
| 1:A:818:TYR:CB   | 2:B:90:GLY:N     | 2.55                     | 0.69              |
| 1:D:810:ARG:HG2  | 1:D:810:ARG:HH11 | 1.57                     | 0.69              |
| 1:G:798:LEU:HD23 | 3:I:122:GLU:CB   | 2.20                     | 0.69              |
| 3:I:25:ILE:O     | 3:I:63:ILE:HB    | 1.92                     | 0.69              |
| 2:K:111:SER:OG   | 2:K:148:VAL:HG12 | 1.92                     | 0.69              |
| 1:D:218:LEU:HB2  | 1:D:221:GLN:CG   | 2.09                     | 0.69              |
| 1:D:797:PHE:CE2  | 3:F:126:LEU:CD2  | 2.74                     | 0.69              |
| 1:J:93:MET:SD    | 1:J:764:MLY:CH2  | 2.67                     | 0.69              |
| 1:J:215:GLN:CA   | 1:J:340:ILE:CG2  | 2.62                     | 0.69              |
| 3:L:48:LYS:HB3   | 3:L:52:ASN:HD21  | 1.57                     | 0.69              |
| 1:A:577:ALA:O    | 1:A:578:HIS:CG   | 2.44                     | 0.69              |
| 1:A:636:LYS:HG3  | 4:8:334:GLU:CD   | 2.17                     | 0.69              |
| 1:A:782:MLY:C    | 1:A:783:LEU:HD12 | 2.22                     | 0.69              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:OD1  | 2.39                     | 0.69              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CA   | 2.20                     | 0.69              |
| 1:G:643:GLY:N    | 4:V:24:ASP:CA    | 2.47                     | 0.69              |
| 1:G:793:ARG:NH1  | 3:I:40:ASN:HD21  | 1.91                     | 0.69              |
| 2:H:111:SER:OG   | 2:H:148:VAL:HG12 | 1.92                     | 0.69              |
| 1:J:84:MLY:CH1   | 1:J:715:VAL:HG11 | 2.17                     | 0.69              |
| 1:J:90:ASP:OD1   | 1:J:764:MLY:HH11 | 1.91                     | 0.69              |
| 1:J:579:PHE:HD2  | 1:J:592:ILE:HD11 | 1.56                     | 0.69              |
| 1:J:636:LYS:HG3  | 4:W:334:GLU:CD   | 2.17                     | 0.69              |
| 4:1:1:ASP:HA     | 4:1:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:V:1:ASP:HA     | 4:V:4:GLU:HB3    | 1.74                     | 0.69              |
| 3:C:3:SER:O      | 3:C:4:LYS:CB     | 2.41                     | 0.69              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:HG23 | 0.70                     | 0.69              |
| 1:G:787:ILE:HG22 | 1:G:788:THR:N    | 2.07                     | 0.69              |
| 1:J:630:ALA:O    | 4:W:25:ASP:CB    | 2.41                     | 0.69              |
| 3:L:48:LYS:O     | 3:L:52:ASN:CG    | 2.34                     | 0.69              |
| 4:0:1:ASP:HA     | 4:0:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:7:1:ASP:HA     | 4:7:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:A:641:LYS:HD2  | 4:8:348:SER:HA   | 1.73                     | 0.69              |
| 1:D:636:LYS:HG3  | 4:9:334:GLU:CD   | 2.17                     | 0.69              |
| 1:G:72:VAL:HG13  | 1:G:76:GLN:CB    | 2.19                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:823:PHE:CD1  | 2:K:156:VAL:O    | 2.45                     | 0.69              |
| 1:A:793:ARG:CG   | 3:C:146:ILE:HG22 | 2.21                     | 0.69              |
| 1:A:810:ARG:HG2  | 1:A:810:ARG:HH11 | 1.57                     | 0.69              |
| 1:A:834:LEU:CD2  | 2:B:54:MET:HG3   | 2.22                     | 0.69              |
| 1:D:541:MET:CG   | 4:9:345:ILE:O    | 2.41                     | 0.69              |
| 1:D:818:TYR:HB2  | 2:E:89:LYS:C     | 2.17                     | 0.69              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:HG23 | 0.70                     | 0.69              |
| 1:G:751:GLY:HA2  | 3:I:114:LEU:CD1  | 2.21                     | 0.69              |
| 1:G:815:CYS:O    | 1:G:819:ASN:HB2  | 1.93                     | 0.69              |
| 1:J:218:LEU:HB2  | 1:J:221:GLN:CG   | 2.09                     | 0.69              |
| 1:J:807:VAL:O    | 1:J:810:ARG:HB2  | 1.93                     | 0.69              |
| 4:Y:1:ASP:HA     | 4:Y:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:CD1  | 2.23                     | 0.69              |
| 1:A:553:MLY:HG2  | 4:V:47:MET:N     | 2.07                     | 0.69              |
| 1:A:642:LYS:HB3  | 4:8:21:PHE:O     | 1.92                     | 0.69              |
| 1:D:642:LYS:HB3  | 4:9:21:PHE:O     | 1.92                     | 0.69              |
| 1:G:93:MET:CE    | 1:G:763:THR:CA   | 2.66                     | 0.69              |
| 1:G:577:ALA:O    | 1:G:578:HIS:CG   | 2.45                     | 0.69              |
| 1:G:800:ARG:HD2  | 3:I:149:VAL:HG23 | 1.71                     | 0.69              |
| 3:I:48:LYS:C     | 3:I:52:ASN:HD22  | 1.96                     | 0.69              |
| 1:J:818:TYR:CE1  | 2:K:127:ARG:CZ   | 2.76                     | 0.69              |
| 3:L:3:SER:O      | 3:L:4:LYS:CB     | 2.41                     | 0.69              |
| 4:0:287:ILE:CG2  | 4:2:203:THR:CG2  | 2.61                     | 0.69              |
| 4:9:1:ASP:HA     | 4:9:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:W:3:ASP:HA     | 4:W:6:THR:CB     | 2.18                     | 0.69              |
| 1:A:537:GLU:HG3  | 4:8:350:SER:O    | 1.79                     | 0.69              |
| 1:A:839:MLY:HD2  | 2:B:159:HIS:CB   | 2.22                     | 0.69              |
| 1:D:166:MET:HE1  | 1:D:254:PHE:HD2  | 1.56                     | 0.69              |
| 1:D:553:MLY:HG2  | 4:W:47:MET:N     | 2.07                     | 0.69              |
| 1:D:556:ASP:HA   | 4:W:49:GLN:O     | 1.70                     | 0.69              |
| 1:D:807:VAL:O    | 1:D:810:ARG:HB2  | 1.93                     | 0.69              |
| 2:E:140:PHE:O    | 2:E:141:PRO:C    | 2.33                     | 0.69              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG2   | 2.21                     | 0.69              |
| 1:G:636:LYS:HG3  | 4:V:334:GLU:CD   | 2.18                     | 0.69              |
| 1:G:641:LYS:HD2  | 4:V:348:SER:HA   | 1.73                     | 0.69              |
| 1:G:791:GLN:CD   | 3:I:116:GLU:HB2  | 2.18                     | 0.69              |
| 1:J:90:ASP:HB2   | 1:J:764:MLY:HH21 | 1.73                     | 0.69              |
| 1:J:707:CYS:CA   | 1:J:714:ARG:HH22 | 2.06                     | 0.69              |
| 1:J:802:GLU:OE1  | 1:J:802:GLU:HA   | 1.93                     | 0.69              |
| 4:0:3:ASP:HA     | 4:0:6:THR:CB     | 2.18                     | 0.69              |
| 4:4:1:ASP:HA     | 4:4:4:GLU:HB3    | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:3:ASP:HA     | 4:4:6:THR:CB     | 2.17                     | 0.69              |
| 4:8:1:ASP:HA     | 4:8:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:W:1:ASP:HA     | 4:W:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:A:550:PHE:HA   | 4:V:46:GLY:HA3   | 1.66                     | 0.69              |
| 1:A:630:ALA:O    | 4:8:25:ASP:HB2   | 1.92                     | 0.69              |
| 3:C:48:LYS:O     | 3:C:52:ASN:CG    | 2.34                     | 0.69              |
| 1:D:630:ALA:O    | 4:9:25:ASP:CB    | 2.41                     | 0.69              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:CD1  | 2.23                     | 0.69              |
| 1:J:537:GLU:C    | 4:W:351:THR:N    | 2.51                     | 0.69              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:NE   | 1.89                     | 0.69              |
| 4:0:287:ILE:CB   | 4:2:203:THR:CG2  | 2.33                     | 0.69              |
| 1:A:815:CYS:O    | 1:A:819:ASN:HB2  | 1.93                     | 0.69              |
| 1:A:830:PRO:HG2  | 2:B:67:MET:CE    | 2.23                     | 0.69              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:C    | 2.36                     | 0.69              |
| 1:G:556:ASP:OD2  | 4:X:47:MET:CE    | 2.39                     | 0.69              |
| 1:G:820:VAL:CG1  | 2:H:136:MET:HE1  | 2.22                     | 0.69              |
| 3:I:3:SER:O      | 3:I:4:LYS:CB     | 2.41                     | 0.69              |
| 1:J:546:THR:HG22 | 1:J:548:THR:N    | 2.05                     | 0.69              |
| 4:V:325:MET:CE   | 4:X:244:ASP:OD2  | 2.34                     | 0.69              |
| 1:A:800:ARG:CG   | 3:C:149:VAL:CG2  | 2.61                     | 0.68              |
| 1:D:537:GLU:C    | 4:9:351:THR:N    | 2.51                     | 0.68              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:CG2  | 2.22                     | 0.68              |
| 1:D:815:CYS:O    | 1:D:819:ASN:HB2  | 1.93                     | 0.68              |
| 1:D:831:TRP:CG   | 2:E:51:PHE:HZ    | 2.12                     | 0.68              |
| 2:E:111:SER:OG   | 2:E:148:VAL:HG12 | 1.92                     | 0.68              |
| 1:G:652:LEU:O    | 1:G:655:GLU:N    | 2.27                     | 0.68              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:HD11 | 1.26                     | 0.68              |
| 1:J:754:ASP:CG   | 1:J:776:GLU:HA   | 2.18                     | 0.68              |
| 4:2:1:ASP:HA     | 4:2:4:GLU:HB3    | 1.74                     | 0.68              |
| 4:3:160:THR:HG21 | 4:3:274:ILE:HD11 | 1.75                     | 0.68              |
| 4:9:160:THR:HG21 | 4:9:274:ILE:HD11 | 1.75                     | 0.68              |
| 1:A:52:ILE:HD13  | 1:A:52:ILE:N     | 2.08                     | 0.68              |
| 1:A:817:GLN:HE21 | 2:B:127:ARG:HG2  | 1.58                     | 0.68              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CA   | 2.20                     | 0.68              |
| 1:D:62:VAL:HG12  | 1:D:63:MLY:O     | 1.93                     | 0.68              |
| 1:G:807:VAL:O    | 1:G:810:ARG:HB2  | 1.93                     | 0.68              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:CG2  | 2.34                     | 0.68              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:SD    | 2.33                     | 0.68              |
| 4:7:160:THR:HG21 | 4:7:274:ILE:HD11 | 1.75                     | 0.68              |
| 4:W:160:THR:HG21 | 4:W:274:ILE:HD11 | 1.75                     | 0.68              |
| 4:Y:160:THR:HG21 | 4:Y:274:ILE:HD11 | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:LYS:HA   | 1:A:220:ASP:OD1  | 1.92                     | 0.68              |
| 1:A:793:ARG:HE   | 3:C:147:MET:CA   | 2.05                     | 0.68              |
| 1:D:510:TRP:CH2  | 1:D:711:PHE:HE2  | 2.11                     | 0.68              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD11 | 0.72                     | 0.68              |
| 1:D:817:GLN:CG   | 2:E:127:ARG:HD3  | 2.21                     | 0.68              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:OD1  | 2.39                     | 0.68              |
| 1:G:819:ASN:OD1  | 2:H:90:GLY:O     | 2.11                     | 0.68              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:OD1  | 2.39                     | 0.68              |
| 1:J:541:MET:CG   | 4:W:345:ILE:O    | 2.40                     | 0.68              |
| 4:1:244:ASP:CB   | 4:Z:322:PRO:CB   | 2.65                     | 0.68              |
| 4:5:1:ASP:HA     | 4:5:4:GLU:HB3    | 1.74                     | 0.68              |
| 4:Z:1:ASP:HA     | 4:Z:4:GLU:HB3    | 1.74                     | 0.68              |
| 1:A:769:ALA:N    | 1:A:771:LEU:HB2  | 2.08                     | 0.68              |
| 1:D:787:ILE:HG22 | 1:D:788:THR:N    | 2.07                     | 0.68              |
| 3:F:3:SER:O      | 3:F:4:LYS:CB     | 2.41                     | 0.68              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:OD1  | 1.92                     | 0.68              |
| 1:G:533:PHE:O    | 1:G:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:G:792:ALA:HB3  | 3:I:40:ASN:HB3   | 1.75                     | 0.68              |
| 1:J:642:LYS:CG   | 4:W:22:ALA:C     | 2.67                     | 0.68              |
| 4:0:243:PRO:C    | 4:Y:291:LYS:HE2  | 2.19                     | 0.68              |
| 1:A:652:LEU:O    | 1:A:655:GLU:N    | 2.27                     | 0.68              |
| 1:D:762:HIS:H    | 1:D:762:HIS:CD2  | 2.08                     | 0.68              |
| 2:E:117:LEU:HD11 | 2:E:147:ASN:HB3  | 1.75                     | 0.68              |
| 1:G:642:LYS:CG   | 4:V:22:ALA:C     | 2.66                     | 0.68              |
| 1:G:754:ASP:CG   | 1:G:776:GLU:OE2  | 2.35                     | 0.68              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CA   | 2.19                     | 0.68              |
| 4:0:287:ILE:HG22 | 4:2:203:THR:HG22 | 1.72                     | 0.68              |
| 3:C:25:ILE:O     | 3:C:63:ILE:HB    | 1.92                     | 0.68              |
| 1:D:534:SER:C    | 4:9:351:THR:CA   | 2.47                     | 0.68              |
| 1:G:52:ILE:HD13  | 1:G:52:ILE:N     | 2.09                     | 0.68              |
| 1:G:550:PHE:HE2  | 1:G:592:ILE:HG23 | 1.59                     | 0.68              |
| 3:I:48:LYS:HB3   | 3:I:52:ASN:HD21  | 1.56                     | 0.68              |
| 1:J:533:PHE:O    | 1:J:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:HD11 | 1.26                     | 0.68              |
| 1:A:798:LEU:HD21 | 3:C:122:GLU:HB3  | 1.74                     | 0.68              |
| 1:A:807:VAL:O    | 1:A:810:ARG:HB2  | 1.93                     | 0.68              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:CD1  | 2.23                     | 0.68              |
| 1:D:533:PHE:O    | 1:D:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:D:802:GLU:OE1  | 1:D:802:GLU:HA   | 1.93                     | 0.68              |
| 1:D:834:LEU:HD13 | 2:E:51:PHE:HA    | 1.74                     | 0.68              |
| 2:E:162:ASP:O    | 2:K:21:GLU:CB    | 2.41                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:HB3  | 4:V:21:PHE:O     | 1.92                     | 0.68              |
| 1:J:537:GLU:HG3  | 4:W:350:SER:O    | 1.78                     | 0.68              |
| 1:A:408:VAL:HG12 | 4:8:332:PRO:HB3  | 1.76                     | 0.68              |
| 1:A:537:GLU:C    | 4:8:351:THR:N    | 2.52                     | 0.68              |
| 1:D:550:PHE:HE2  | 1:D:592:ILE:HG23 | 1.59                     | 0.68              |
| 1:G:408:VAL:HG12 | 4:V:332:PRO:HB3  | 1.76                     | 0.68              |
| 1:G:541:MET:CG   | 4:V:345:ILE:O    | 2.41                     | 0.68              |
| 4:2:153:LEU:HD11 | 4:2:274:ILE:HG13 | 1.76                     | 0.68              |
| 4:V:325:MET:CE   | 4:X:244:ASP:CB   | 2.70                     | 0.68              |
| 1:A:502:GLU:HG2  | 1:A:764:MLY:O    | 1.94                     | 0.68              |
| 1:D:652:LEU:O    | 1:D:655:GLU:N    | 2.26                     | 0.68              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CE    | 2.24                     | 0.68              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:HB3  | 2.24                     | 0.68              |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:HD1  | 1.59                     | 0.68              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:HA3  | 1.68                     | 0.68              |
| 1:J:818:TYR:HB3  | 2:K:90:GLY:HA2   | 1.74                     | 0.68              |
| 4:0:247:VAL:N    | 4:Y:324:THR:CG2  | 2.57                     | 0.68              |
| 4:0:287:ILE:HD13 | 4:2:203:THR:HB   | 1.75                     | 0.68              |
| 4:4:153:LEU:HD11 | 4:4:274:ILE:HG13 | 1.76                     | 0.68              |
| 4:5:160:THR:HG21 | 4:5:274:ILE:HD11 | 1.75                     | 0.68              |
| 4:X:160:THR:HG21 | 4:X:274:ILE:HD11 | 1.75                     | 0.68              |
| 1:A:58:GLY:HA2   | 1:A:74:GLU:OE1   | 1.94                     | 0.68              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:HA   | 2.26                     | 0.68              |
| 1:D:215:GLN:HA   | 1:D:340:ILE:CB   | 2.23                     | 0.68              |
| 1:D:642:LYS:CG   | 4:9:22:ALA:C     | 2.67                     | 0.68              |
| 1:G:537:GLU:C    | 4:V:351:THR:N    | 2.51                     | 0.68              |
| 1:J:62:VAL:HG12  | 1:J:63:MLY:O     | 1.93                     | 0.68              |
| 1:J:782:MLY:C    | 1:J:783:LEU:HD12 | 2.22                     | 0.68              |
| 1:J:815:CYS:O    | 1:J:819:ASN:HB2  | 1.93                     | 0.68              |
| 4:0:202:THR:C    | 4:Y:286:ASP:OD1  | 2.35                     | 0.68              |
| 1:A:56:GLU:CB    | 1:A:59:MLY:HB3   | 2.20                     | 0.67              |
| 1:A:541:MET:CG   | 4:8:345:ILE:O    | 2.41                     | 0.67              |
| 1:A:630:ALA:O    | 4:8:25:ASP:CB    | 2.41                     | 0.67              |
| 1:A:762:HIS:H    | 1:A:762:HIS:CD2  | 2.08                     | 0.67              |
| 1:G:553:MLY:CD   | 4:X:45:VAL:HG12  | 2.23                     | 0.67              |
| 1:G:643:GLY:H    | 4:V:23:GLY:C     | 2.02                     | 0.67              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:CD1  | 2.23                     | 0.67              |
| 1:J:642:LYS:HB3  | 4:W:21:PHE:O     | 1.92                     | 0.67              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:OD1  | 2.39                     | 0.67              |
| 4:1:322:PRO:CB   | 4:3:244:ASP:HB2  | 2.23                     | 0.67              |
| 1:A:546:THR:H    | 1:A:549:SER:HB3  | 1.59                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:141:PRO:O    | 2:B:145:ALA:CB   | 2.43                     | 0.67              |
| 1:D:52:ILE:HD13  | 1:D:52:ILE:N     | 2.09                     | 0.67              |
| 1:G:832:MET:SD   | 2:H:84:PHE:HE2   | 2.18                     | 0.67              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:HB3  | 2.24                     | 0.67              |
| 3:I:24:LYS:HA    | 3:I:63:ILE:O     | 1.95                     | 0.67              |
| 1:J:546:THR:H    | 1:J:549:SER:HB3  | 1.59                     | 0.67              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:N    | 2.43                     | 0.67              |
| 4:O:153:LEU:HD11 | 4:O:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:2:160:THR:HG21 | 4:2:274:ILE:HD11 | 1.75                     | 0.67              |
| 4:3:288:ASP:CB   | 4:5:203:THR:HG21 | 2.25                     | 0.67              |
| 4:Y:153:LEU:HD11 | 4:Y:274:ILE:HG13 | 1.76                     | 0.67              |
| 1:D:546:THR:H    | 1:D:549:SER:HB3  | 1.59                     | 0.67              |
| 1:D:724:TYR:C    | 1:D:782:MLY:CH2  | 2.64                     | 0.67              |
| 1:D:795:ARG:C    | 3:F:35:ARG:HD3   | 2.20                     | 0.67              |
| 1:D:831:TRP:NE1  | 2:E:47:LEU:CD2   | 2.35                     | 0.67              |
| 1:G:217:THR:O    | 1:G:221:GLN:HG2  | 1.94                     | 0.67              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:C    | 2.36                     | 0.67              |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:HD1  | 1.59                     | 0.67              |
| 1:A:217:THR:O    | 1:A:221:GLN:HG2  | 1.94                     | 0.67              |
| 1:A:830:PRO:HG2  | 2:B:67:MET:HE1   | 1.76                     | 0.67              |
| 2:B:149:ASP:OD2  | 2:B:150:TYR:C    | 2.36                     | 0.67              |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:CD1  | 1.55                     | 0.67              |
| 1:D:831:TRP:CZ3  | 2:E:50:THR:HB    | 2.30                     | 0.67              |
| 1:G:58:GLY:HA2   | 1:G:74:GLU:OE1   | 1.95                     | 0.67              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:HB3  | 2.24                     | 0.67              |
| 4:1:160:THR:HG21 | 4:1:274:ILE:HD11 | 1.76                     | 0.67              |
| 4:V:153:LEU:HD11 | 4:V:274:ILE:HG13 | 1.76                     | 0.67              |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:HD1  | 1.59                     | 0.67              |
| 1:D:546:THR:HG22 | 1:D:548:THR:N    | 2.05                     | 0.67              |
| 1:D:730:SER:C    | 1:D:733:PRO:HD2  | 2.20                     | 0.67              |
| 1:G:529:PRO:C    | 4:V:354:GLN:CB   | 2.50                     | 0.67              |
| 1:G:784:ALA:O    | 1:G:788:THR:HB   | 1.94                     | 0.67              |
| 1:J:374:GLN:HG3  | 1:J:375:ALA:H    | 1.59                     | 0.67              |
| 1:J:652:LEU:O    | 1:J:655:GLU:N    | 2.26                     | 0.67              |
| 1:J:750:GLY:HA2  | 3:L:114:LEU:CD2  | 2.25                     | 0.67              |
| 1:J:823:PHE:CZ   | 2:K:156:VAL:HG12 | 2.29                     | 0.67              |
| 4:V:160:THR:HG21 | 4:V:274:ILE:HD11 | 1.75                     | 0.67              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HD13 | 2.19                     | 0.67              |
| 1:J:58:GLY:HA2   | 1:J:74:GLU:OE1   | 1.94                     | 0.67              |
| 1:J:84:MLY:NZ    | 1:J:719:ASP:O    | 2.12                     | 0.67              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:ND2  | 2.09                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:643:GLY:N    | 4:W:24:ASP:CA    | 2.46                     | 0.67              |
| 4:8:153:LEU:HD11 | 4:8:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:W:153:LEU:HD11 | 4:W:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:X:287:ILE:C    | 4:Z:205:GLU:OE1  | 2.37                     | 0.67              |
| 1:A:502:GLU:CD   | 1:A:764:MLY:O    | 2.37                     | 0.67              |
| 3:C:24:LYS:HA    | 3:C:63:ILE:O     | 1.95                     | 0.67              |
| 1:G:62:VAL:HG12  | 1:G:63:MLY:O     | 1.94                     | 0.67              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:NH1   | 2.54                     | 0.67              |
| 1:J:798:LEU:HD21 | 3:L:126:LEU:CD1  | 2.22                     | 0.67              |
| 1:J:831:TRP:CH2  | 2:K:47:LEU:HD23  | 2.30                     | 0.67              |
| 1:D:131:TRP:O    | 1:D:132:LEU:HD12 | 1.95                     | 0.67              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:ND2  | 2.09                     | 0.67              |
| 1:D:642:LYS:CD   | 4:9:24:ASP:O     | 2.42                     | 0.67              |
| 1:G:84:MLY:HH12  | 1:G:715:VAL:HG12 | 1.67                     | 0.67              |
| 1:G:202:SER:HA   | 1:G:207:LYS:HE3  | 1.72                     | 0.67              |
| 1:G:556:ASP:CG   | 4:X:47:MET:HE2   | 1.84                     | 0.67              |
| 1:G:802:GLU:OE1  | 1:G:802:GLU:HA   | 1.93                     | 0.67              |
| 1:J:131:TRP:O    | 1:J:132:LEU:HD12 | 1.95                     | 0.67              |
| 1:J:290:GLN:O    | 1:J:331:LEU:HD12 | 1.95                     | 0.67              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:HE1   | 2.24                     | 0.67              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:C    | 2.36                     | 0.67              |
| 1:A:533:PHE:O    | 1:A:537:GLU:HG2  | 1.93                     | 0.67              |
| 1:D:58:GLY:HA2   | 1:D:74:GLU:OE1   | 1.95                     | 0.67              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:N    | 2.43                     | 0.67              |
| 1:G:290:GLN:O    | 1:G:331:LEU:HD12 | 1.95                     | 0.67              |
| 1:G:546:THR:H    | 1:G:549:SER:HB3  | 1.59                     | 0.67              |
| 1:G:730:SER:C    | 1:G:733:PRO:HD2  | 2.20                     | 0.67              |
| 2:H:141:PRO:O    | 2:H:145:ALA:CB   | 2.43                     | 0.67              |
| 2:K:141:PRO:O    | 2:K:145:ALA:CB   | 2.43                     | 0.67              |
| 3:L:24:LYS:HA    | 3:L:63:ILE:O     | 1.95                     | 0.67              |
| 4:X:153:LEU:HD11 | 4:X:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:X:291:LYS:HD2  | 4:Z:243:PRO:C    | 2.10                     | 0.67              |
| 1:A:61:THR:HG23  | 1:A:71:THR:OG1   | 1.94                     | 0.67              |
| 1:A:62:VAL:HG12  | 1:A:63:MLY:O     | 1.93                     | 0.67              |
| 1:A:550:PHE:HE2  | 1:A:592:ILE:HG23 | 1.59                     | 0.67              |
| 1:D:374:GLN:HG3  | 1:D:375:ALA:H    | 1.60                     | 0.67              |
| 1:D:648:THR:CB   | 4:9:350:SER:OG   | 2.43                     | 0.67              |
| 1:G:61:THR:HG23  | 1:G:71:THR:OG1   | 1.94                     | 0.67              |
| 1:G:78:PHE:HB3   | 1:G:98:HIS:CD2   | 2.30                     | 0.67              |
| 1:J:166:MET:HE1  | 1:J:254:PHE:HD2  | 1.56                     | 0.67              |
| 1:J:408:VAL:HG12 | 4:W:332:PRO:HB3  | 1.75                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:541:MET:O    | 4:W:143:TYR:OH   | 2.13                     | 0.67              |
| 1:J:730:SER:C    | 1:J:733:PRO:HD2  | 2.19                     | 0.67              |
| 1:J:754:ASP:HB2  | 1:J:776:GLU:CB   | 2.13                     | 0.67              |
| 1:J:795:ARG:HB3  | 3:L:35:ARG:NH2   | 2.09                     | 0.67              |
| 1:J:798:LEU:HD23 | 3:L:122:GLU:HB3  | 1.76                     | 0.67              |
| 4:8:160:THR:HG21 | 4:8:274:ILE:HD11 | 1.76                     | 0.67              |
| 4:Z:153:LEU:HD11 | 4:Z:274:ILE:HG13 | 1.76                     | 0.67              |
| 1:A:541:MET:C    | 4:8:143:TYR:CZ   | 2.73                     | 0.66              |
| 1:A:797:PHE:CD2  | 3:C:126:LEU:HD22 | 2.30                     | 0.66              |
| 1:D:418:THR:HG22 | 1:D:419:VAL:N    | 2.11                     | 0.66              |
| 1:D:541:MET:C    | 4:9:143:TYR:CZ   | 2.73                     | 0.66              |
| 1:D:739:ASP:CB   | 1:D:742:LYS:HB3  | 2.12                     | 0.66              |
| 2:E:141:PRO:O    | 2:E:145:ALA:CB   | 2.43                     | 0.66              |
| 1:G:131:TRP:O    | 1:G:132:LEU:HD12 | 1.94                     | 0.66              |
| 1:G:783:LEU:O    | 1:G:787:ILE:CA   | 2.42                     | 0.66              |
| 1:J:635:GLY:O    | 4:W:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:J:817:GLN:HG3  | 2:K:128:PHE:CE1  | 2.31                     | 0.66              |
| 2:K:117:LEU:HD11 | 2:K:147:ASN:HB3  | 1.76                     | 0.66              |
| 4:4:160:THR:HG21 | 4:4:274:ILE:HD11 | 1.75                     | 0.66              |
| 4:W:324:THR:HG22 | 4:Y:247:VAL:HG13 | 1.77                     | 0.66              |
| 1:A:78:PHE:HB3   | 1:A:98:HIS:CD2   | 2.30                     | 0.66              |
| 1:A:642:LYS:CG   | 4:8:22:ALA:C     | 2.67                     | 0.66              |
| 1:A:648:THR:CB   | 4:8:350:SER:OG   | 2.43                     | 0.66              |
| 1:A:730:SER:C    | 1:A:733:PRO:HD2  | 2.20                     | 0.66              |
| 3:C:4:LYS:N      | 3:C:5:ALA:O      | 2.17                     | 0.66              |
| 1:D:834:LEU:CD1  | 2:E:51:PHE:HA    | 2.24                     | 0.66              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:N    | 2.29                     | 0.66              |
| 1:J:52:ILE:HD13  | 1:J:52:ILE:N     | 2.09                     | 0.66              |
| 1:J:550:PHE:HE2  | 1:J:592:ILE:HG23 | 1.59                     | 0.66              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:C    | 2.68                     | 0.66              |
| 4:9:153:LEU:HD11 | 4:9:274:ILE:HG13 | 1.76                     | 0.66              |
| 4:X:287:ILE:O    | 4:Z:205:GLU:CD   | 2.38                     | 0.66              |
| 1:A:174:SER:O    | 1:A:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:A:418:THR:HG22 | 1:A:419:VAL:N    | 2.11                     | 0.66              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:HB3  | 2.24                     | 0.66              |
| 1:D:339:ASP:OD1  | 1:D:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:D:788:THR:HG23 | 3:F:42:THR:CG2   | 2.21                     | 0.66              |
| 1:G:174:SER:O    | 1:G:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:G:648:THR:CB   | 4:V:350:SER:OG   | 2.44                     | 0.66              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:CD1  | 2.26                     | 0.66              |
| 1:J:541:MET:C    | 4:W:143:TYR:CZ   | 2.72                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:0:160:THR:HG21 | 4:0:274:ILE:HD11 | 1.76                     | 0.66              |
| 1:A:504:MLY:C    | 1:A:762:HIS:NE2  | 2.58                     | 0.66              |
| 1:D:408:VAL:HG12 | 4:9:332:PRO:HB3  | 1.76                     | 0.66              |
| 1:D:831:TRP:HE1  | 2:E:47:LEU:HD22  | 1.55                     | 0.66              |
| 1:G:541:MET:C    | 4:V:143:TYR:CZ   | 2.73                     | 0.66              |
| 1:J:174:SER:O    | 1:J:670:HIS:HB2  | 1.95                     | 0.66              |
| 1:J:339:ASP:OD1  | 1:J:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:J:707:CYS:CB   | 1:J:714:ARG:HH22 | 2.08                     | 0.66              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HG3   | 1.77                     | 0.66              |
| 2:B:141:PRO:O    | 2:B:145:ALA:HB2  | 1.95                     | 0.66              |
| 1:D:174:SER:O    | 1:D:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:D:507:GLY:O    | 1:D:762:HIS:N    | 2.29                     | 0.66              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:N    | 2.28                     | 0.66              |
| 1:D:724:TYR:HE1  | 1:D:778:MET:CG   | 2.08                     | 0.66              |
| 1:G:374:GLN:HG3  | 1:G:375:ALA:H    | 1.60                     | 0.66              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:N    | 2.42                     | 0.66              |
| 1:G:639:GLY:N    | 4:V:344:SER:C    | 2.54                     | 0.66              |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:HD1  | 1.59                     | 0.66              |
| 1:J:648:THR:CB   | 4:W:350:SER:OG   | 2.43                     | 0.66              |
| 4:0:243:PRO:HB3  | 4:Y:291:LYS:CE   | 2.02                     | 0.66              |
| 1:A:131:TRP:O    | 1:A:132:LEU:HD12 | 1.94                     | 0.66              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:ND2  | 2.09                     | 0.66              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:N    | 2.43                     | 0.66              |
| 1:A:642:LYS:CD   | 4:8:24:ASP:O     | 2.42                     | 0.66              |
| 1:D:226:ASN:HB2  | 1:D:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:D:290:GLN:O    | 1:D:331:LEU:HD12 | 1.95                     | 0.66              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HE3   | 1.76                     | 0.66              |
| 2:E:141:PRO:O    | 2:E:145:ALA:HB2  | 1.96                     | 0.66              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:ND2  | 2.35                     | 0.66              |
| 1:J:78:PHE:HB3   | 1:J:98:HIS:CD2   | 2.30                     | 0.66              |
| 1:J:831:TRP:CE3  | 2:K:34:ILE:CD1   | 2.78                     | 0.66              |
| 4:0:166:TYR:CZ   | 4:2:64:ILE:HG21  | 2.29                     | 0.66              |
| 4:0:247:VAL:H    | 4:Y:324:THR:CB   | 2.08                     | 0.66              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:CD1  | 2.26                     | 0.66              |
| 1:D:541:MET:O    | 4:9:143:TYR:OH   | 2.14                     | 0.66              |
| 2:E:146:GLY:O    | 2:E:147:ASN:HB2  | 1.96                     | 0.66              |
| 1:G:226:ASN:HB2  | 1:G:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:J:226:ASN:HB2  | 1:J:227:PRO:HD3  | 1.77                     | 0.66              |
| 1:J:639:GLY:N    | 4:W:344:SER:C    | 2.53                     | 0.66              |
| 2:K:141:PRO:O    | 2:K:145:ALA:HB2  | 1.96                     | 0.66              |
| 4:1:153:LEU:HD11 | 4:1:274:ILE:HG13 | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:153:LEU:HD11 | 4:7:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:A:161:ASN:O    | 1:A:165:PHE:HB2  | 1.96                     | 0.66              |
| 1:A:296:MLY:HH11 | 1:A:348:MLY:HH21 | 1.78                     | 0.66              |
| 1:A:530:MET:CG   | 4:8:354:GLN:CG   | 2.71                     | 0.66              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:HB3  | 1.78                     | 0.66              |
| 1:A:818:TYR:HB3  | 2:B:90:GLY:N     | 2.11                     | 0.66              |
| 1:G:751:GLY:N    | 3:I:114:LEU:CD1  | 2.59                     | 0.66              |
| 2:H:146:GLY:O    | 2:H:147:ASN:HB2  | 1.96                     | 0.66              |
| 1:J:643:GLY:H    | 4:W:23:GLY:C     | 2.02                     | 0.66              |
| 4:1:288:ASP:H    | 4:3:203:THR:CG2  | 2.08                     | 0.66              |
| 4:V:288:ASP:H    | 4:X:204:ALA:H    | 1.43                     | 0.66              |
| 1:A:144:ARG:NH1  | 1:A:160:ASP:OD1  | 2.29                     | 0.66              |
| 1:A:556:ASP:HA   | 4:V:49:GLN:O     | 1.70                     | 0.66              |
| 1:A:643:GLY:N    | 4:8:24:ASP:CA    | 2.46                     | 0.66              |
| 1:D:635:GLY:O    | 4:9:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:G:161:ASN:O    | 1:G:165:PHE:HB2  | 1.96                     | 0.66              |
| 1:G:635:GLY:O    | 4:V:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:J:61:THR:HG23  | 1:J:71:THR:OG1   | 1.94                     | 0.66              |
| 1:J:790:THR:CA   | 3:L:87:PHE:CE2   | 2.79                     | 0.66              |
| 1:J:795:ARG:HH11 | 3:L:35:ARG:CZ    | 2.08                     | 0.66              |
| 1:J:831:TRP:HH2  | 2:K:47:LEU:HD23  | 1.60                     | 0.66              |
| 2:K:146:GLY:O    | 2:K:147:ASN:HB2  | 1.96                     | 0.66              |
| 4:2:287:ILE:HG22 | 4:4:204:ALA:HB3  | 1.76                     | 0.66              |
| 4:5:153:LEU:HD11 | 4:5:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:A:339:ASP:OD1  | 1:A:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:A:530:MET:CA   | 4:8:354:GLN:CB   | 2.74                     | 0.66              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:NH1   | 2.44                     | 0.66              |
| 1:D:217:THR:C    | 1:D:221:GLN:HG2  | 2.21                     | 0.66              |
| 1:J:144:ARG:NH1  | 1:J:160:ASP:OD1  | 2.29                     | 0.66              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:N    | 2.29                     | 0.66              |
| 1:J:691:VAL:O    | 1:J:695:LEU:HD13 | 1.96                     | 0.66              |
| 3:L:45:GLU:O     | 3:L:49:ILE:HG13  | 1.96                     | 0.66              |
| 4:0:202:THR:OG1  | 4:Y:286:ASP:OD1  | 2.14                     | 0.66              |
| 4:Z:160:THR:HG21 | 4:Z:274:ILE:HD11 | 1.76                     | 0.66              |
| 3:C:45:GLU:O     | 3:C:49:ILE:HG13  | 1.96                     | 0.65              |
| 1:D:61:THR:HG23  | 1:D:71:THR:OG1   | 1.94                     | 0.65              |
| 1:D:217:THR:O    | 1:D:221:GLN:HG2  | 1.94                     | 0.65              |
| 1:D:466:GLY:HA2  | 1:D:484:ASN:HD21 | 1.61                     | 0.65              |
| 1:D:691:VAL:O    | 1:D:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:G:144:ARG:NH1  | 1:G:160:ASP:OD1  | 2.29                     | 0.65              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:N    | 2.11                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:480:ILE:HG22 | 1:G:481:ASN:ND2  | 2.10                     | 0.65              |
| 1:G:541:MET:O    | 4:V:143:TYR:OH   | 2.13                     | 0.65              |
| 2:H:141:PRO:O    | 2:H:145:ALA:HB2  | 1.96                     | 0.65              |
| 1:J:217:THR:O    | 1:J:221:GLN:HG2  | 1.95                     | 0.65              |
| 1:J:567:LYS:HZ3  | 4:Y:92:ASN:ND2   | 1.94                     | 0.65              |
| 4:O:287:ILE:CG1  | 4:2:203:THR:HB   | 2.27                     | 0.65              |
| 1:A:217:THR:C    | 1:A:221:GLN:HG2  | 2.21                     | 0.65              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:CB   | 2.24                     | 0.65              |
| 1:D:643:GLY:H    | 4:9:23:GLY:C     | 2.02                     | 0.65              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:HE3   | 2.27                     | 0.65              |
| 3:F:24:LYS:HA    | 3:F:63:ILE:O     | 1.95                     | 0.65              |
| 1:G:691:VAL:O    | 1:G:695:LEU:HD13 | 1.96                     | 0.65              |
| 2:H:117:LEU:HD11 | 2:H:147:ASN:HB3  | 1.76                     | 0.65              |
| 1:J:665:ARG:C    | 1:J:667:THR:H    | 2.05                     | 0.65              |
| 1:A:94:MET:HE1   | 1:A:101:ALA:HB1  | 1.79                     | 0.65              |
| 1:G:84:MLY:HH11  | 1:G:720:PHE:N    | 2.12                     | 0.65              |
| 1:G:296:MLY:HH11 | 1:G:348:MLY:HH21 | 1.78                     | 0.65              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:N    | 2.58                     | 0.65              |
| 1:G:820:VAL:HG11 | 2:H:136:MET:CE   | 2.26                     | 0.65              |
| 3:I:45:GLU:O     | 3:I:49:ILE:HG13  | 1.97                     | 0.65              |
| 1:J:161:ASN:O    | 1:J:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:J:642:LYS:HA   | 4:W:21:PHE:O     | 1.96                     | 0.65              |
| 4:1:202:THR:HB   | 4:Z:287:ILE:CG1  | 2.26                     | 0.65              |
| 4:1:203:THR:N    | 4:Z:287:ILE:HB   | 2.04                     | 0.65              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:CA   | 2.44                     | 0.65              |
| 1:A:635:GLY:O    | 4:8:341:ILE:HG21 | 1.95                     | 0.65              |
| 1:D:78:PHE:HB3   | 1:D:98:HIS:CD2   | 2.30                     | 0.65              |
| 1:D:530:MET:CG   | 4:9:354:GLN:CG   | 2.71                     | 0.65              |
| 1:D:721:LYS:HG2  | 1:D:736:GLN:CD   | 1.85                     | 0.65              |
| 3:F:45:GLU:O     | 3:F:49:ILE:HG13  | 1.97                     | 0.65              |
| 1:G:339:ASP:OD1  | 1:G:348:MLY:HH13 | 1.95                     | 0.65              |
| 1:G:818:TYR:CD1  | 2:H:127:ARG:NH1  | 2.64                     | 0.65              |
| 4:O:243:PRO:C    | 4:Y:291:LYS:HG3  | 2.21                     | 0.65              |
| 4:3:153:LEU:HD11 | 4:3:274:ILE:HG13 | 1.76                     | 0.65              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:N    | 2.11                     | 0.65              |
| 1:A:502:GLU:HA   | 1:A:761:GLY:CA   | 2.26                     | 0.65              |
| 1:A:643:GLY:H    | 4:8:23:GLY:C     | 2.02                     | 0.65              |
| 1:A:665:ARG:C    | 1:A:667:THR:H    | 2.05                     | 0.65              |
| 1:A:691:VAL:O    | 1:A:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:A:739:ASP:CB   | 1:A:742:LYS:HB3  | 2.12                     | 0.65              |
| 1:D:94:MET:HE1   | 1:D:101:ALA:HB1  | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:530:MET:CA   | 4:9:354:GLN:CB   | 2.74                     | 0.65              |
| 1:D:822:SER:O    | 1:D:825:ASN:HB2  | 1.97                     | 0.65              |
| 1:G:410:ASN:CG   | 4:V:334:GLU:C    | 2.64                     | 0.65              |
| 1:G:466:GLY:HA2  | 1:G:484:ASN:HD21 | 1.61                     | 0.65              |
| 1:G:822:SER:O    | 1:G:825:ASN:HB2  | 1.97                     | 0.65              |
| 1:J:217:THR:C    | 1:J:221:GLN:HG2  | 2.21                     | 0.65              |
| 1:J:567:LYS:NZ   | 4:Y:92:ASN:HA    | 2.10                     | 0.65              |
| 4:0:245:GLY:C    | 4:Y:324:THR:O    | 2.39                     | 0.65              |
| 1:A:226:ASN:HB2  | 1:A:227:PRO:HD3  | 1.78                     | 0.65              |
| 1:A:322:VAL:HB   | 1:A:325:ILE:CD1  | 2.26                     | 0.65              |
| 1:A:374:GLN:HG3  | 1:A:375:ALA:H    | 1.59                     | 0.65              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:N    | 2.29                     | 0.65              |
| 3:C:49:ILE:HA    | 3:C:52:ASN:ND2   | 2.05                     | 0.65              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:N    | 1.94                     | 0.65              |
| 1:G:530:MET:CG   | 4:V:354:GLN:CG   | 2.71                     | 0.65              |
| 1:G:725:ARG:NE   | 1:G:737:PHE:HE1  | 1.95                     | 0.65              |
| 1:J:418:THR:HG22 | 1:J:419:VAL:N    | 2.11                     | 0.65              |
| 1:J:725:ARG:NE   | 1:J:737:PHE:HE1  | 1.95                     | 0.65              |
| 1:A:290:GLN:O    | 1:A:331:LEU:HD12 | 1.95                     | 0.65              |
| 1:A:822:SER:O    | 1:A:825:ASN:HB2  | 1.97                     | 0.65              |
| 1:D:725:ARG:NE   | 1:D:737:PHE:HE1  | 1.95                     | 0.65              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:OE1  | 2.28                     | 0.65              |
| 1:D:831:TRP:CH2  | 2:E:47:LEU:HD23  | 2.28                     | 0.65              |
| 1:G:418:THR:HG22 | 1:G:419:VAL:N    | 2.11                     | 0.65              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:CB    | 2.56                     | 0.65              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:HH13 | 1.96                     | 0.65              |
| 1:J:530:MET:CA   | 4:W:354:GLN:CB   | 2.74                     | 0.65              |
| 4:0:244:ASP:N    | 4:Y:291:LYS:HG3  | 2.05                     | 0.65              |
| 1:A:466:GLY:HA2  | 1:A:484:ASN:ND2  | 2.11                     | 0.65              |
| 1:A:642:LYS:HA   | 4:8:21:PHE:O     | 1.96                     | 0.65              |
| 1:A:817:GLN:HE21 | 2:B:127:ARG:CG   | 2.10                     | 0.65              |
| 1:D:479:CYS:HB3  | 1:D:653:PHE:CE2  | 2.32                     | 0.65              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:CD2  | 2.80                     | 0.65              |
| 1:D:639:GLY:N    | 4:9:344:SER:C    | 2.54                     | 0.65              |
| 1:D:665:ARG:C    | 1:D:667:THR:H    | 2.04                     | 0.65              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:CZ   | 2.69                     | 0.65              |
| 1:J:793:ARG:HG3  | 3:L:146:ILE:HG22 | 1.78                     | 0.65              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HD13 | 2.20                     | 0.65              |
| 4:0:247:VAL:N    | 4:Y:324:THR:HG21 | 2.11                     | 0.65              |
| 4:3:288:ASP:OD2  | 4:5:203:THR:CB   | 2.42                     | 0.65              |
| 4:V:324:THR:HG23 | 4:X:247:VAL:H    | 1.60                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:287:ILE:CG1  | 4:Z:201:VAL:CB   | 2.75                     | 0.65              |
| 1:A:217:THR:HB   | 1:A:220:ASP:OD2  | 1.97                     | 0.65              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:HZ1  | 1.62                     | 0.65              |
| 1:G:107:MLY:HB3  | 1:G:686:MET:CE   | 2.26                     | 0.65              |
| 1:G:322:VAL:HB   | 1:G:325:ILE:CD1  | 2.26                     | 0.65              |
| 1:G:466:GLY:HA2  | 1:G:484:ASN:ND2  | 2.12                     | 0.65              |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:CD1  | 1.55                     | 0.65              |
| 1:J:819:ASN:N    | 2:K:90:GLY:O     | 2.28                     | 0.65              |
| 1:J:822:SER:O    | 1:J:825:ASN:HB2  | 1.97                     | 0.65              |
| 4:1:287:ILE:HG21 | 4:3:204:ALA:N    | 2.11                     | 0.65              |
| 1:A:466:GLY:HA2  | 1:A:484:ASN:HD21 | 1.61                     | 0.65              |
| 1:D:144:ARG:NH1  | 1:D:160:ASP:OD1  | 2.29                     | 0.65              |
| 1:D:161:ASN:O    | 1:D:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:D:202:SER:CA   | 1:D:207:LYS:HE3  | 2.27                     | 0.65              |
| 1:D:642:LYS:CD   | 4:9:340:TRP:CZ3  | 2.79                     | 0.65              |
| 1:D:830:PRO:HG2  | 2:E:67:MET:HE1   | 0.65                     | 0.65              |
| 1:G:217:THR:C    | 1:G:221:GLN:HG2  | 2.21                     | 0.65              |
| 1:J:466:GLY:HA2  | 1:J:484:ASN:ND2  | 2.11                     | 0.65              |
| 1:A:642:LYS:CD   | 4:8:340:TRP:CZ3  | 2.79                     | 0.64              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:N    | 2.11                     | 0.64              |
| 1:D:636:LYS:O    | 1:D:637:LYS:CB   | 2.45                     | 0.64              |
| 1:D:642:LYS:HA   | 4:9:21:PHE:O     | 1.96                     | 0.64              |
| 1:J:95:THR:CA    | 1:J:713:SER:HB3  | 2.27                     | 0.64              |
| 1:D:806:MET:O    | 1:D:809:ARG:HB2  | 1.98                     | 0.64              |
| 1:G:553:MLY:O    | 4:X:46:GLY:CA    | 2.45                     | 0.64              |
| 1:G:642:LYS:CD   | 4:V:24:ASP:O     | 2.43                     | 0.64              |
| 1:G:665:ARG:C    | 1:G:667:THR:H    | 2.05                     | 0.64              |
| 1:J:49:MLY:HH23  | 1:J:80:MET:HE3   | 1.80                     | 0.64              |
| 1:J:768:MLY:HH21 | 1:J:772:LEU:HD22 | 1.66                     | 0.64              |
| 4:2:148:THR:HG21 | 4:4:45:VAL:CG2   | 2.26                     | 0.64              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:N    | 1.94                     | 0.64              |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:HH21 | 1.78                     | 0.64              |
| 1:D:466:GLY:HA2  | 1:D:484:ASN:ND2  | 2.11                     | 0.64              |
| 1:D:537:GLU:HB3  | 1:D:648:THR:HB   | 1.80                     | 0.64              |
| 1:D:709:LYS:O    | 1:D:710:GLY:HA2  | 1.97                     | 0.64              |
| 1:G:642:LYS:HA   | 4:V:21:PHE:O     | 1.97                     | 0.64              |
| 1:J:94:MET:HE1   | 1:J:101:ALA:HB1  | 1.79                     | 0.64              |
| 1:J:133:PRO:O    | 1:J:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:HH21 | 1.78                     | 0.64              |
| 1:J:410:ASN:CG   | 4:W:334:GLU:C    | 2.65                     | 0.64              |
| 1:J:479:CYS:HB3  | 1:J:653:PHE:CE2  | 2.32                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:287:ILE:CB   | 4:Z:201:VAL:HG23 | 2.27                     | 0.64              |
| 1:A:133:PRO:O    | 1:A:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:A:202:SER:CA   | 1:A:207:LYS:HE3  | 2.27                     | 0.64              |
| 1:A:218:LEU:CD2  | 1:A:222:ILE:HG12 | 2.28                     | 0.64              |
| 1:A:557:GLU:N    | 4:V:48:GLY:HA3   | 1.90                     | 0.64              |
| 1:D:107:MLY:HB3  | 1:D:686:MET:CE   | 2.26                     | 0.64              |
| 1:D:217:THR:HB   | 1:D:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:HG23 | 1.68                     | 0.64              |
| 1:G:217:THR:HB   | 1:G:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:HB3  | 1.79                     | 0.64              |
| 1:G:829:TRP:CZ2  | 2:H:87:LYS:HE2   | 2.33                     | 0.64              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:N    | 1.94                     | 0.64              |
| 1:J:783:LEU:HD12 | 1:J:783:LEU:N    | 2.13                     | 0.64              |
| 1:A:501:GLU:O    | 1:A:762:HIS:CG   | 2.49                     | 0.64              |
| 1:A:642:LYS:CA   | 4:8:21:PHE:O     | 2.46                     | 0.64              |
| 1:A:822:SER:HG   | 2:B:88:LEU:HA    | 1.61                     | 0.64              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:D:49:MLY:HH23  | 1:D:80:MET:HE3   | 1.80                     | 0.64              |
| 1:G:133:PRO:O    | 1:G:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:J:217:THR:HB   | 1:J:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:J:466:GLY:HA2  | 1:J:484:ASN:HD21 | 1.61                     | 0.64              |
| 1:J:556:ASP:O    | 4:Y:48:GLY:N     | 2.29                     | 0.64              |
| 1:J:792:ALA:HB1  | 3:L:40:ASN:HB3   | 0.72                     | 0.64              |
| 1:J:806:MET:O    | 1:J:809:ARG:HB2  | 1.98                     | 0.64              |
| 2:K:140:PHE:HB3  | 2:K:144:VAL:CG1  | 2.27                     | 0.64              |
| 4:1:167:GLU:OE1  | 4:3:44:MET:HA    | 1.98                     | 0.64              |
| 4:2:288:ASP:N    | 4:4:203:THR:CG2  | 2.56                     | 0.64              |
| 1:A:93:MET:O     | 1:A:713:SER:HB3  | 1.97                     | 0.64              |
| 1:A:479:CYS:HB3  | 1:A:653:PHE:CE2  | 2.32                     | 0.64              |
| 1:A:553:MLY:CE   | 4:V:45:VAL:CA    | 2.49                     | 0.64              |
| 1:A:725:ARG:NE   | 1:A:737:PHE:HE1  | 1.95                     | 0.64              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:C     | 2.72                     | 0.64              |
| 1:G:218:LEU:CD2  | 1:G:222:ILE:HG12 | 2.28                     | 0.64              |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:N    | 2.13                     | 0.64              |
| 1:G:530:MET:CA   | 4:V:354:GLN:CB   | 2.75                     | 0.64              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:N    | 1.94                     | 0.64              |
| 2:H:140:PHE:HB3  | 2:H:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:CD   | 2.11                     | 0.64              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:HB3  | 1.78                     | 0.64              |
| 1:J:642:LYS:CA   | 4:W:21:PHE:O     | 2.45                     | 0.64              |
| 1:A:636:LYS:O    | 1:A:637:LYS:CB   | 2.45                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:541:MET:HG2  | 4:V:345:ILE:O    | 1.98                     | 0.64              |
| 1:G:642:LYS:CA   | 4:V:21:PHE:O     | 2.46                     | 0.64              |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:CD   | 2.11                     | 0.64              |
| 1:G:769:ALA:HB2  | 1:G:770:GLY:N    | 2.11                     | 0.64              |
| 1:G:829:TRP:CH2  | 2:H:87:LYS:NZ    | 2.65                     | 0.64              |
| 1:J:636:LYS:O    | 1:J:637:LYS:CB   | 2.45                     | 0.64              |
| 1:J:642:LYS:CD   | 4:W:340:TRP:CZ3  | 2.79                     | 0.64              |
| 1:J:817:GLN:CD   | 2:K:127:ARG:CD   | 2.58                     | 0.64              |
| 2:K:144:VAL:HA   | 2:K:153:ILE:HD11 | 1.80                     | 0.64              |
| 4:O:190:MET:SD   | 4:O:209:VAL:HG11 | 2.38                     | 0.64              |
| 4:1:287:ILE:HG13 | 4:3:202:THR:CB   | 2.26                     | 0.64              |
| 4:8:190:MET:SD   | 4:8:209:VAL:HG11 | 2.38                     | 0.64              |
| 4:X:291:LYS:HG3  | 4:Z:243:PRO:C    | 2.22                     | 0.64              |
| 1:A:541:MET:O    | 4:8:143:TYR:OH   | 2.14                     | 0.64              |
| 1:G:94:MET:HE1   | 1:G:101:ALA:HB1  | 1.79                     | 0.64              |
| 1:G:479:CYS:HB3  | 1:G:653:PHE:CE2  | 2.33                     | 0.64              |
| 1:G:724:TYR:HB3  | 1:G:727:LEU:HD12 | 1.80                     | 0.64              |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:N    | 2.13                     | 0.64              |
| 1:J:636:LYS:N    | 4:W:334:GLU:OE1  | 2.31                     | 0.64              |
| 4:O:247:VAL:HG22 | 4:Y:324:THR:HG22 | 0.67                     | 0.64              |
| 4:4:190:MET:SD   | 4:4:209:VAL:HG11 | 2.38                     | 0.64              |
| 4:Y:190:MET:SD   | 4:Y:209:VAL:HG11 | 2.38                     | 0.64              |
| 1:A:806:MET:O    | 1:A:809:ARG:HB2  | 1.98                     | 0.64              |
| 1:A:814:PHE:HA   | 2:B:127:ARG:HH22 | 1.55                     | 0.64              |
| 2:B:132:GLU:O    | 2:B:136:MET:HG2  | 1.98                     | 0.64              |
| 2:B:146:GLY:O    | 2:B:147:ASN:HB2  | 1.96                     | 0.64              |
| 2:E:140:PHE:HB3  | 2:E:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:G:84:MLY:CH1   | 1:G:719:ASP:C    | 2.49                     | 0.64              |
| 1:G:784:ALA:O    | 1:G:788:THR:CB   | 2.45                     | 0.64              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:HG   | 1.80                     | 0.64              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:N    | 2.11                     | 0.64              |
| 4:2:287:ILE:CB   | 4:4:204:ALA:H    | 2.11                     | 0.64              |
| 4:9:190:MET:SD   | 4:9:209:VAL:HG11 | 2.38                     | 0.64              |
| 1:A:502:GLU:OE2  | 1:A:764:MLY:N    | 2.31                     | 0.63              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:CG   | 2.27                     | 0.63              |
| 1:A:636:LYS:N    | 4:8:334:GLU:OE1  | 2.31                     | 0.63              |
| 1:A:724:TYR:HB3  | 1:A:727:LEU:HD12 | 1.80                     | 0.63              |
| 1:A:793:ARG:CZ   | 3:C:147:MET:HG2  | 2.28                     | 0.63              |
| 1:G:215:GLN:CA   | 1:G:340:ILE:CG2  | 2.62                     | 0.63              |
| 1:G:577:ALA:O    | 1:G:578:HIS:CD2  | 2.51                     | 0.63              |
| 1:G:783:LEU:HD12 | 1:G:783:LEU:N    | 2.13                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:797:PHE:CD1  | 3:I:149:VAL:HG12 | 2.26                     | 0.63              |
| 1:J:577:ALA:O    | 1:J:578:HIS:CD2  | 2.51                     | 0.63              |
| 4:1:203:THR:H    | 4:Z:287:ILE:CD1  | 2.05                     | 0.63              |
| 4:2:190:MET:SD   | 4:2:209:VAL:HG11 | 2.38                     | 0.63              |
| 2:B:144:VAL:HA   | 2:B:153:ILE:HD11 | 1.80                     | 0.63              |
| 1:D:218:LEU:CD2  | 1:D:222:ILE:HG12 | 2.28                     | 0.63              |
| 1:G:537:GLU:HB3  | 1:G:648:THR:HB   | 1.80                     | 0.63              |
| 3:I:49:ILE:HA    | 3:I:52:ASN:ND2   | 2.06                     | 0.63              |
| 1:J:725:ARG:NE   | 1:J:737:PHE:CE1  | 2.66                     | 0.63              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:HH12  | 2.12                     | 0.63              |
| 2:K:146:GLY:O    | 2:K:147:ASN:CB   | 2.46                     | 0.63              |
| 4:0:202:THR:CG2  | 4:Y:285:CYS:O    | 2.46                     | 0.63              |
| 1:A:724:TYR:HD1  | 1:A:727:LEU:HD11 | 1.64                     | 0.63              |
| 1:A:725:ARG:NE   | 1:A:737:PHE:CE1  | 2.67                     | 0.63              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:CB   | 2.76                     | 0.63              |
| 1:D:133:PRO:O    | 1:D:136:ASN:HB2  | 1.98                     | 0.63              |
| 1:D:577:ALA:O    | 1:D:578:HIS:CD2  | 2.51                     | 0.63              |
| 1:D:831:TRP:HH2  | 2:E:47:LEU:HA    | 1.48                     | 0.63              |
| 1:G:724:TYR:HD1  | 1:G:727:LEU:HD11 | 1.64                     | 0.63              |
| 4:1:202:THR:OG1  | 4:Z:287:ILE:CG2  | 2.42                     | 0.63              |
| 4:W:190:MET:SD   | 4:W:209:VAL:HG11 | 2.38                     | 0.63              |
| 4:X:324:THR:O    | 4:Z:245:GLY:HA3  | 1.98                     | 0.63              |
| 1:A:530:MET:HA   | 4:8:354:GLN:CB   | 2.29                     | 0.63              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:HB3  | 1.78                     | 0.63              |
| 1:D:783:LEU:HD12 | 1:D:783:LEU:N    | 2.13                     | 0.63              |
| 1:D:818:TYR:HD2  | 2:E:89:LYS:O     | 1.81                     | 0.63              |
| 1:D:830:PRO:HB2  | 2:E:67:MET:HE1   | 1.74                     | 0.63              |
| 3:F:24:LYS:HB3   | 3:F:63:ILE:H     | 1.64                     | 0.63              |
| 1:J:278:GLN:CG   | 1:J:317:GLU:HB2  | 2.27                     | 0.63              |
| 1:J:541:MET:CA   | 4:W:143:TYR:OH   | 2.46                     | 0.63              |
| 4:W:257:CYS:HB3  | 4:W:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:Y:257:CYS:HB3  | 4:Y:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:410:ASN:CG   | 4:8:334:GLU:C    | 2.65                     | 0.63              |
| 1:A:577:ALA:O    | 1:A:578:HIS:CD2  | 2.51                     | 0.63              |
| 1:A:831:TRP:CH2  | 2:B:34:ILE:HG23  | 2.33                     | 0.63              |
| 2:B:140:PHE:O    | 2:B:141:PRO:C    | 2.33                     | 0.63              |
| 2:E:132:GLU:O    | 2:E:136:MET:HG2  | 1.99                     | 0.63              |
| 1:G:636:LYS:O    | 1:G:637:LYS:CB   | 2.45                     | 0.63              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:CB   | 2.76                     | 0.63              |
| 1:J:141:LEU:H    | 1:J:141:LEU:HD12 | 1.64                     | 0.63              |
| 1:J:817:GLN:CG   | 2:K:127:ARG:CD   | 2.73                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:112:ILE:C    | 2:K:147:ASN:O    | 2.42                     | 0.63              |
| 4:0:257:CYS:HB3  | 4:0:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:CD   | 2.11                     | 0.63              |
| 1:A:795:ARG:CB   | 3:C:35:ARG:CZ    | 2.75                     | 0.63              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HE3   | 1.81                     | 0.63              |
| 2:E:146:GLY:O    | 2:E:147:ASN:CB   | 2.46                     | 0.63              |
| 1:G:771:LEU:O    | 1:G:774:LEU:N    | 2.32                     | 0.63              |
| 1:J:218:LEU:CD2  | 1:J:222:ILE:HG12 | 2.28                     | 0.63              |
| 1:J:537:GLU:HB3  | 1:J:648:THR:HB   | 1.80                     | 0.63              |
| 1:J:724:TYR:HB3  | 1:J:727:LEU:HD12 | 1.80                     | 0.63              |
| 3:L:49:ILE:HA    | 3:L:52:ASN:ND2   | 2.06                     | 0.63              |
| 4:2:257:CYS:HB3  | 4:2:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:7:257:CYS:HB3  | 4:7:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:542:PHE:CZ   | 1:A:553:MLY:HH11 | 2.34                     | 0.63              |
| 2:B:146:GLY:O    | 2:B:147:ASN:CB   | 2.46                     | 0.63              |
| 1:D:278:GLN:CG   | 1:D:317:GLU:HB2  | 2.26                     | 0.63              |
| 1:D:411:GLU:N    | 4:9:333:PRO:HB2  | 2.10                     | 0.63              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:CG   | 2.33                     | 0.63              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:CG   | 2.28                     | 0.63              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:O    | 1.98                     | 0.63              |
| 1:D:726:VAL:HB   | 1:D:782:MLY:HH13 | 0.82                     | 0.63              |
| 1:D:767:PHE:HB3  | 1:D:771:LEU:HD11 | 1.80                     | 0.63              |
| 1:G:90:ASP:O     | 1:G:764:MLY:CH2  | 2.46                     | 0.63              |
| 1:G:806:MET:O    | 1:G:809:ARG:HB2  | 1.98                     | 0.63              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:O    | 1.98                     | 0.63              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:CB   | 2.75                     | 0.63              |
| 2:K:132:GLU:O    | 2:K:136:MET:HG2  | 1.98                     | 0.63              |
| 4:0:287:ILE:CB   | 4:2:203:THR:H    | 2.12                     | 0.63              |
| 4:4:257:CYS:HB3  | 4:4:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:X:190:MET:SD   | 4:X:209:VAL:HG11 | 2.38                     | 0.63              |
| 4:X:324:THR:OG1  | 4:Z:246:GLN:HA   | 1.98                     | 0.63              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:O    | 1.98                     | 0.63              |
| 1:A:795:ARG:CD   | 3:C:118:MET:HE1  | 2.28                     | 0.63              |
| 1:A:831:TRP:HZ3  | 2:B:50:THR:CG2   | 2.11                     | 0.63              |
| 2:B:121:LEU:HA   | 2:B:128:PHE:CG   | 2.34                     | 0.63              |
| 3:C:24:LYS:HB3   | 3:C:63:ILE:H     | 1.64                     | 0.63              |
| 1:D:725:ARG:NE   | 1:D:737:PHE:CE1  | 2.66                     | 0.63              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:HB2  | 1.79                     | 0.63              |
| 1:D:771:LEU:O    | 1:D:774:LEU:N    | 2.32                     | 0.63              |
| 2:E:121:LEU:HA   | 2:E:128:PHE:CG   | 2.34                     | 0.63              |
| 1:G:141:LEU:H    | 1:G:141:LEU:HD12 | 1.64                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:251:ARG:HB2  | 1:G:264:ASP:CB   | 2.29                     | 0.63              |
| 1:G:541:MET:CA   | 4:V:143:TYR:OH   | 2.47                     | 0.63              |
| 1:J:823:PHE:CE2  | 2:K:140:PHE:CZ   | 2.87                     | 0.63              |
| 4:9:257:CYS:HB3  | 4:9:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:Z:190:MET:SD   | 4:Z:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:A:541:MET:CA   | 4:8:143:TYR:OH   | 2.47                     | 0.63              |
| 1:A:783:LEU:HD12 | 1:A:783:LEU:N    | 2.13                     | 0.63              |
| 1:G:636:LYS:N    | 4:V:334:GLU:OE1  | 2.31                     | 0.63              |
| 2:H:121:LEU:HA   | 2:H:128:PHE:CG   | 2.34                     | 0.63              |
| 1:J:107:MLY:HB3  | 1:J:686:MET:CE   | 2.27                     | 0.63              |
| 4:5:190:MET:SD   | 4:5:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:A:822:SER:CB   | 2:B:88:LEU:CD2   | 2.67                     | 0.62              |
| 1:D:210:GLN:O    | 1:D:211:SER:OG   | 2.15                     | 0.62              |
| 1:D:724:TYR:HD1  | 1:D:727:LEU:HD11 | 1.64                     | 0.62              |
| 1:G:725:ARG:NE   | 1:G:737:PHE:CE1  | 2.67                     | 0.62              |
| 1:G:792:ALA:HA   | 3:I:35:ARG:CZ    | 2.29                     | 0.62              |
| 1:J:278:GLN:HG3  | 1:J:318:GLY:N    | 2.14                     | 0.62              |
| 4:7:190:MET:SD   | 4:7:209:VAL:HG11 | 2.38                     | 0.62              |
| 4:V:361:GLU:HB3  | 4:V:369:ILE:HG12 | 1.81                     | 0.62              |
| 1:A:274:ARG:HB2  | 1:A:285:TYR:CE2  | 2.34                     | 0.62              |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:N    | 2.13                     | 0.62              |
| 1:A:578:HIS:CB   | 1:A:592:ILE:HD12 | 2.29                     | 0.62              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:CB   | 2.29                     | 0.62              |
| 1:D:551:MLY:C    | 4:W:46:GLY:O     | 2.47                     | 0.62              |
| 2:E:112:ILE:C    | 2:E:147:ASN:O    | 2.42                     | 0.62              |
| 1:G:202:SER:CA   | 1:G:207:LYS:HE3  | 2.28                     | 0.62              |
| 1:G:544:LYS:HB2  | 4:V:147:ARG:HA   | 1.80                     | 0.62              |
| 2:H:111:SER:OG   | 2:H:148:VAL:CG1  | 2.47                     | 0.62              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:CB   | 2.29                     | 0.62              |
| 4:5:257:CYS:HB3  | 4:5:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:V:190:MET:SD   | 4:V:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:CB   | 2.29                     | 0.62              |
| 1:A:501:GLU:CG   | 1:A:762:HIS:ND1  | 2.45                     | 0.62              |
| 1:A:506:GLU:N    | 1:A:761:GLY:HA2  | 2.13                     | 0.62              |
| 1:A:537:GLU:HB3  | 1:A:648:THR:HB   | 1.80                     | 0.62              |
| 1:A:542:PHE:N    | 4:8:143:TYR:OH   | 2.33                     | 0.62              |
| 1:A:544:LYS:HB2  | 4:8:147:ARG:HA   | 1.80                     | 0.62              |
| 1:A:551:MLY:C    | 4:V:46:GLY:O     | 2.47                     | 0.62              |
| 1:D:642:LYS:CA   | 4:9:21:PHE:O     | 2.46                     | 0.62              |
| 1:D:769:ALA:C    | 1:D:770:GLY:C    | 2.66                     | 0.62              |
| 1:G:791:GLN:OE1  | 3:I:116:GLU:CG   | 2.48                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:146:GLY:O    | 2:H:147:ASN:CB   | 2.46                     | 0.62              |
| 3:I:24:LYS:HB3   | 3:I:63:ILE:H     | 1.64                     | 0.62              |
| 1:J:724:TYR:HD1  | 1:J:727:LEU:HD11 | 1.64                     | 0.62              |
| 1:J:771:LEU:O    | 1:J:774:LEU:N    | 2.32                     | 0.62              |
| 3:L:24:LYS:HB3   | 3:L:63:ILE:H     | 1.64                     | 0.62              |
| 4:8:361:GLU:HB3  | 4:8:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:302:MET:HG2  | 1:A:303:LEU:CD1  | 2.30                     | 0.62              |
| 1:D:580:SER:HA   | 1:D:588:VAL:O    | 2.00                     | 0.62              |
| 1:D:636:LYS:N    | 4:9:334:GLU:OE1  | 2.31                     | 0.62              |
| 1:D:724:TYR:HB3  | 1:D:727:LEU:HD12 | 1.80                     | 0.62              |
| 1:G:49:MLY:HH23  | 1:G:80:MET:HE3   | 1.80                     | 0.62              |
| 1:G:542:PHE:N    | 4:V:143:TYR:OH   | 2.33                     | 0.62              |
| 1:J:544:LYS:HB2  | 4:W:147:ARG:HA   | 1.80                     | 0.62              |
| 1:J:580:SER:HA   | 1:J:588:VAL:O    | 2.00                     | 0.62              |
| 4:1:190:MET:SD   | 4:1:209:VAL:HG11 | 2.38                     | 0.62              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:HB2  | 2.26                     | 0.62              |
| 4:8:257:CYS:HB3  | 4:8:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:Y:361:GLU:HB3  | 4:Y:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:161:ASN:HA   | 1:A:164:GLN:HE21 | 1.63                     | 0.62              |
| 1:A:530:MET:HE1  | 4:8:355:MET:SD   | 2.39                     | 0.62              |
| 1:D:542:PHE:CZ   | 1:D:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:D:800:ARG:HB2  | 3:F:149:VAL:HG22 | 1.80                     | 0.62              |
| 2:E:111:SER:OG   | 2:E:148:VAL:CG1  | 2.48                     | 0.62              |
| 1:G:769:ALA:O    | 1:G:773:GLY:HA3  | 1.98                     | 0.62              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:CG   | 2.28                     | 0.62              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD11 | 0.73                     | 0.62              |
| 2:K:111:SER:OG   | 2:K:148:VAL:CG1  | 2.47                     | 0.62              |
| 4:2:361:GLU:HB3  | 4:2:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:9:361:GLU:HB3  | 4:9:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:X:361:GLU:HB3  | 4:X:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:520:ALA:O    | 1:A:524:GLU:HG2  | 2.00                     | 0.62              |
| 1:A:543:PRO:HG2  | 4:8:143:TYR:O    | 1.98                     | 0.62              |
| 1:D:578:HIS:CB   | 1:D:592:ILE:HD12 | 2.30                     | 0.62              |
| 1:G:580:SER:HA   | 1:G:588:VAL:O    | 2.00                     | 0.62              |
| 1:G:730:SER:CB   | 3:I:109:HIS:CD2  | 2.82                     | 0.62              |
| 1:J:161:ASN:HA   | 1:J:164:GLN:HE21 | 1.63                     | 0.62              |
| 1:J:530:MET:CG   | 4:W:354:GLN:CG   | 2.72                     | 0.62              |
| 4:1:288:ASP:CB   | 4:3:203:THR:HG21 | 2.29                     | 0.62              |
| 4:V:257:CYS:HB3  | 4:V:258:PRO:HD3  | 1.81                     | 0.62              |
| 1:A:49:MLY:HH23  | 1:A:80:MET:HE3   | 1.80                     | 0.62              |
| 1:A:107:MLY:HB3  | 1:A:686:MET:CE   | 2.26                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:580:SER:HA   | 1:A:588:VAL:O    | 2.00                     | 0.62              |
| 1:D:530:MET:HE1  | 4:9:355:MET:SD   | 2.39                     | 0.62              |
| 1:D:542:PHE:CB   | 4:9:143:TYR:HE1  | 2.13                     | 0.62              |
| 1:G:98:HIS:HB3   | 1:G:100:PRO:CD   | 2.25                     | 0.62              |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:CD   | 2.11                     | 0.62              |
| 1:G:543:PRO:HG2  | 4:V:143:TYR:O    | 1.98                     | 0.62              |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:HG2  | 0.79                     | 0.62              |
| 1:J:542:PHE:CZ   | 1:J:553:MLY:HH11 | 2.34                     | 0.62              |
| 2:K:121:LEU:HA   | 2:K:128:PHE:CG   | 2.34                     | 0.62              |
| 4:7:361:GLU:HB3  | 4:7:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:W:361:GLU:HB3  | 4:W:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:173:GLN:C    | 1:A:667:THR:HG23 | 2.25                     | 0.62              |
| 1:A:553:MLY:O    | 4:V:48:GLY:HA2   | 1.99                     | 0.62              |
| 1:A:643:GLY:O    | 1:A:644:SER:CB   | 2.48                     | 0.62              |
| 1:D:161:ASN:HA   | 1:D:164:GLN:HE21 | 1.64                     | 0.62              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:CD2  | 2.88                     | 0.62              |
| 1:G:173:GLN:C    | 1:G:667:THR:HG23 | 2.25                     | 0.62              |
| 1:G:542:PHE:CZ   | 1:G:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:G:599:ASN:CG   | 1:G:649:VAL:HB   | 2.24                     | 0.62              |
| 1:G:827:MLY:HH21 | 2:H:139:ALA:HB3  | 1.82                     | 0.62              |
| 4:3:190:MET:SD   | 4:3:209:VAL:HG11 | 2.38                     | 0.62              |
| 4:3:361:GLU:HB3  | 4:3:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:98:HIS:HB3   | 1:A:100:PRO:CD   | 2.25                     | 0.62              |
| 1:A:141:LEU:H    | 1:A:141:LEU:HD12 | 1.64                     | 0.62              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:N     | 2.15                     | 0.62              |
| 2:B:112:ILE:C    | 2:B:147:ASN:O    | 2.42                     | 0.62              |
| 1:D:520:ALA:O    | 1:D:524:GLU:HG2  | 2.00                     | 0.62              |
| 1:D:544:LYS:HB2  | 4:9:147:ARG:HA   | 1.80                     | 0.62              |
| 1:D:793:ARG:HE   | 3:F:147:MET:CA   | 2.13                     | 0.62              |
| 1:D:831:TRP:N    | 2:E:51:PHE:CE1   | 2.68                     | 0.62              |
| 1:G:278:GLN:HG3  | 1:G:318:GLY:N    | 2.14                     | 0.62              |
| 1:G:557:GLU:HB2  | 4:X:47:MET:N     | 2.11                     | 0.62              |
| 1:G:578:HIS:CB   | 1:G:592:ILE:HD12 | 2.30                     | 0.62              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:HB3   | 2.15                     | 0.62              |
| 1:J:534:SER:C    | 4:W:351:THR:CA   | 2.47                     | 0.62              |
| 1:J:707:CYS:HB3  | 1:J:714:ARG:NH2  | 2.14                     | 0.62              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:HB2  | 1.81                     | 0.62              |
| 4:1:257:CYS:HB3  | 4:1:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:X:257:CYS:HB3  | 4:X:258:PRO:HD3  | 1.81                     | 0.62              |
| 1:A:278:GLN:HG3  | 1:A:318:GLY:N    | 2.15                     | 0.62              |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:CD1  | 1.55                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:771:LEU:O    | 1:A:774:LEU:N    | 2.32                     | 0.62              |
| 3:C:50:LEU:O     | 3:C:53:PRO:HD2   | 2.00                     | 0.62              |
| 1:D:202:SER:HA   | 1:D:207:LYS:HE3  | 1.72                     | 0.62              |
| 1:D:278:GLN:HG3  | 1:D:318:GLY:N    | 2.15                     | 0.62              |
| 1:D:302:MET:HG2  | 1:D:303:LEU:CD1  | 2.30                     | 0.62              |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:N    | 2.13                     | 0.62              |
| 1:D:543:PRO:HG2  | 4:9:143:TYR:O    | 1.98                     | 0.62              |
| 1:G:302:MET:HG2  | 1:G:303:LEU:CD1  | 2.30                     | 0.62              |
| 1:G:797:PHE:CB   | 3:I:149:VAL:HG11 | 2.29                     | 0.62              |
| 3:I:50:LEU:O     | 3:I:53:PRO:HD2   | 2.00                     | 0.62              |
| 1:J:411:GLU:N    | 4:W:333:PRO:HB2  | 2.11                     | 0.62              |
| 1:J:510:TRP:CZ3  | 1:J:772:LEU:CD2  | 2.82                     | 0.62              |
| 1:J:557:GLU:HG3  | 1:J:557:GLU:O    | 2.00                     | 0.62              |
| 4:3:257:CYS:HB3  | 4:3:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:Z:257:CYS:HB3  | 4:Z:258:PRO:HD3  | 1.81                     | 0.62              |
| 1:A:81:ASN:OD1   | 1:A:96:HIS:HB2   | 2.00                     | 0.61              |
| 1:A:278:GLN:CG   | 1:A:317:GLU:HB2  | 2.27                     | 0.61              |
| 1:A:579:PHE:CE1  | 1:A:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:A:639:GLY:N    | 4:8:344:SER:C    | 2.54                     | 0.61              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:ND1  | 2.15                     | 0.61              |
| 1:D:830:PRO:C    | 2:E:51:PHE:CE1   | 2.78                     | 0.61              |
| 3:F:50:LEU:O     | 3:F:53:PRO:HD2   | 2.00                     | 0.61              |
| 2:H:132:GLU:O    | 2:H:136:MET:HG2  | 1.99                     | 0.61              |
| 1:J:84:MLY:HH11  | 1:J:715:VAL:HG12 | 1.77                     | 0.61              |
| 2:K:114:LYS:HG3  | 2:K:146:GLY:HA2  | 1.82                     | 0.61              |
| 4:2:324:THR:CG2  | 4:4:243:PRO:C    | 2.57                     | 0.61              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:D:141:LEU:H    | 1:D:141:LEU:HD12 | 1.64                     | 0.61              |
| 1:D:541:MET:CA   | 4:9:143:TYR:OH   | 2.47                     | 0.61              |
| 1:G:278:GLN:CG   | 1:G:317:GLU:HB2  | 2.26                     | 0.61              |
| 1:G:508:ILE:HG21 | 1:G:711:PHE:HZ   | 1.64                     | 0.61              |
| 1:G:730:SER:HG   | 3:I:109:HIS:CG   | 2.18                     | 0.61              |
| 1:G:798:LEU:HD21 | 3:I:122:GLU:O    | 2.00                     | 0.61              |
| 1:J:642:LYS:CD   | 4:W:24:ASP:O     | 2.43                     | 0.61              |
| 1:J:786:ILE:HG12 | 3:L:86:ASP:CB    | 2.28                     | 0.61              |
| 4:Z:361:GLU:HB3  | 4:Z:369:ILE:HG12 | 1.82                     | 0.61              |
| 1:A:99:GLU:OE2   | 1:A:696:ARG:NH2  | 2.30                     | 0.61              |
| 1:A:686:MET:HG3  | 1:A:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:A:798:LEU:HD23 | 3:C:122:GLU:HB3  | 1.83                     | 0.61              |
| 1:D:410:ASN:CG   | 4:9:334:GLU:C    | 2.65                     | 0.61              |
| 1:D:553:MLY:O    | 4:W:48:GLY:HA2   | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:599:ASN:CG   | 1:D:649:VAL:HB   | 2.25                     | 0.61              |
| 1:D:769:ALA:CB   | 1:D:771:LEU:N    | 2.63                     | 0.61              |
| 2:E:114:LYS:HG3  | 2:E:146:GLY:HA2  | 1.82                     | 0.61              |
| 1:G:210:GLN:O    | 1:G:211:SER:OG   | 2.15                     | 0.61              |
| 1:G:530:MET:HE1  | 4:V:355:MET:SD   | 2.41                     | 0.61              |
| 1:J:173:GLN:C    | 1:J:667:THR:HG23 | 2.25                     | 0.61              |
| 1:J:538:GLU:CG   | 4:W:351:THR:C    | 2.73                     | 0.61              |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:CD1  | 1.55                     | 0.61              |
| 3:L:52:ASN:N     | 3:L:53:PRO:HD2   | 2.15                     | 0.61              |
| 4:0:244:ASP:OD2  | 4:Y:325:MET:HE1  | 2.01                     | 0.61              |
| 4:1:202:THR:CB   | 4:Z:287:ILE:CG1  | 2.79                     | 0.61              |
| 4:1:203:THR:N    | 4:Z:287:ILE:CD1  | 2.62                     | 0.61              |
| 4:5:361:GLU:HB3  | 4:5:369:ILE:HG12 | 1.82                     | 0.61              |
| 4:7:190:MET:HE1  | 4:7:206:ARG:HA   | 1.83                     | 0.61              |
| 1:A:599:ASN:CG   | 1:A:649:VAL:HB   | 2.25                     | 0.61              |
| 1:D:173:GLN:C    | 1:D:667:THR:HG23 | 2.25                     | 0.61              |
| 1:D:274:ARG:HB2  | 1:D:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:D:793:ARG:NE   | 3:F:147:MET:HA   | 2.16                     | 0.61              |
| 1:G:81:ASN:OD1   | 1:G:96:HIS:HB2   | 2.00                     | 0.61              |
| 1:G:161:ASN:HA   | 1:G:164:GLN:HE21 | 1.63                     | 0.61              |
| 1:G:510:TRP:CE3  | 1:G:768:MLY:CH1  | 2.83                     | 0.61              |
| 1:G:553:MLY:HB2  | 4:X:46:GLY:HA3   | 1.83                     | 0.61              |
| 1:G:579:PHE:CE1  | 1:G:581:LEU:HD13 | 2.35                     | 0.61              |
| 2:H:112:ILE:C    | 2:H:147:ASN:O    | 2.42                     | 0.61              |
| 2:H:144:VAL:HA   | 2:H:153:ILE:HD11 | 1.80                     | 0.61              |
| 1:J:542:PHE:CB   | 4:W:143:TYR:HE1  | 2.13                     | 0.61              |
| 1:J:813:ILE:O    | 1:J:817:GLN:N    | 2.30                     | 0.61              |
| 4:9:190:MET:HE1  | 4:9:206:ARG:HA   | 1.83                     | 0.61              |
| 4:W:190:MET:HE1  | 4:W:206:ARG:HA   | 1.83                     | 0.61              |
| 4:X:291:LYS:HG3  | 4:Z:244:ASP:N    | 1.86                     | 0.61              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:HD22 | 2.35                     | 0.61              |
| 2:B:117:LEU:HD11 | 2:B:147:ASN:HB3  | 1.75                     | 0.61              |
| 1:D:541:MET:SD   | 4:9:346:LEU:O    | 2.48                     | 0.61              |
| 2:E:144:VAL:HA   | 2:E:153:ILE:HD11 | 1.80                     | 0.61              |
| 1:G:274:ARG:HB2  | 1:G:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:G:643:GLY:O    | 1:G:644:SER:CB   | 2.48                     | 0.61              |
| 1:J:274:ARG:HB2  | 1:J:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:J:578:HIS:CB   | 1:J:592:ILE:HD12 | 2.30                     | 0.61              |
| 1:J:579:PHE:CE1  | 1:J:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:HA   | 2.35                     | 0.61              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:CZ    | 2.52                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:361:GLU:HB3  | 4:4:369:ILE:HG12 | 1.82                     | 0.61              |
| 4:5:190:MET:HE1  | 4:5:206:ARG:HA   | 1.83                     | 0.61              |
| 4:8:190:MET:HE1  | 4:8:206:ARG:HA   | 1.83                     | 0.61              |
| 4:V:286:ASP:OD2  | 4:X:203:THR:CG2  | 2.47                     | 0.61              |
| 1:A:542:PHE:CB   | 4:8:143:TYR:HE1  | 2.12                     | 0.61              |
| 2:B:111:SER:OG   | 2:B:148:VAL:CG1  | 2.47                     | 0.61              |
| 1:D:538:GLU:CG   | 4:9:351:THR:C    | 2.73                     | 0.61              |
| 1:D:686:MET:HG3  | 1:D:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:J:95:THR:HA    | 1:J:713:SER:HB3  | 1.82                     | 0.61              |
| 1:J:302:MET:HG2  | 1:J:303:LEU:CD1  | 2.29                     | 0.61              |
| 1:J:553:MLY:HE3  | 4:Y:45:VAL:HG12  | 1.80                     | 0.61              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:HA3  | 2.28                     | 0.61              |
| 4:0:190:MET:HE1  | 4:0:206:ARG:HA   | 1.83                     | 0.61              |
| 4:0:201:VAL:HG23 | 4:Y:287:ILE:HG12 | 1.80                     | 0.61              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:N    | 2.13                     | 0.61              |
| 4:3:190:MET:HE1  | 4:3:206:ARG:HA   | 1.83                     | 0.61              |
| 4:X:190:MET:HE1  | 4:X:206:ARG:HA   | 1.83                     | 0.61              |
| 4:Y:190:MET:HE1  | 4:Y:206:ARG:HA   | 1.83                     | 0.61              |
| 2:B:34:ILE:O     | 2:B:46:ASP:HB3   | 2.01                     | 0.61              |
| 1:D:557:GLU:HG3  | 1:D:557:GLU:O    | 2.00                     | 0.61              |
| 1:D:576:GLU:CG   | 1:D:577:ALA:N    | 2.43                     | 0.61              |
| 2:E:163:ALA:C    | 2:K:22:THR:CB    | 2.74                     | 0.61              |
| 1:G:524:GLU:O    | 1:G:528:MLY:HB3  | 2.01                     | 0.61              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HD13 | 2.19                     | 0.61              |
| 1:J:99:GLU:OE2   | 1:J:696:ARG:NH2  | 2.30                     | 0.61              |
| 1:J:530:MET:HE1  | 4:W:355:MET:SD   | 2.40                     | 0.61              |
| 1:J:643:GLY:O    | 1:J:644:SER:CB   | 2.49                     | 0.61              |
| 4:Z:190:MET:HE1  | 4:Z:206:ARG:HA   | 1.83                     | 0.61              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:CB   | 2.28                     | 0.61              |
| 3:C:63:ILE:HG22  | 3:C:64:THR:O     | 2.01                     | 0.61              |
| 1:D:578:HIS:CD2  | 1:D:591:ASN:HA   | 2.31                     | 0.61              |
| 1:D:579:PHE:CE1  | 1:D:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:D:829:TRP:NE1  | 2:E:67:MET:CG    | 2.41                     | 0.61              |
| 1:G:642:LYS:CA   | 4:V:22:ALA:C     | 2.70                     | 0.61              |
| 1:J:202:SER:HA   | 1:J:207:LYS:HE3  | 1.72                     | 0.61              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:HB   | 2.25                     | 0.61              |
| 1:J:686:MET:HG3  | 1:J:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:J:820:VAL:HG11 | 2:K:136:MET:HE3  | 1.81                     | 0.61              |
| 4:1:190:MET:HE1  | 4:1:206:ARG:HA   | 1.83                     | 0.61              |
| 4:5:223:PHE:HD2  | 4:5:312:ARG:NH2  | 1.99                     | 0.61              |
| 1:A:795:ARG:HG2  | 3:C:118:MET:HE1  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:797:PHE:CD2  | 3:C:126:LEU:HD21 | 2.36                     | 0.61              |
| 2:B:114:LYS:HG3  | 2:B:146:GLY:HA2  | 1.82                     | 0.61              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:D:623:PHE:CG   | 1:D:623:PHE:HA   | 2.35                     | 0.61              |
| 1:D:817:GLN:CG   | 2:E:127:ARG:CD   | 2.77                     | 0.61              |
| 1:D:831:TRP:CH2  | 2:E:50:THR:HB    | 2.35                     | 0.61              |
| 3:F:52:ASN:HB2   | 3:F:53:PRO:CD    | 2.28                     | 0.61              |
| 3:F:52:ASN:N     | 3:F:53:PRO:HD2   | 2.15                     | 0.61              |
| 1:G:567:LYS:HZ3  | 4:X:92:ASN:ND2   | 1.89                     | 0.61              |
| 1:G:686:MET:HG3  | 1:G:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD11 | 0.73                     | 0.61              |
| 1:G:768:MLY:CH2  | 1:G:772:LEU:HD22 | 2.28                     | 0.61              |
| 1:J:154:HIS:CE1  | 1:J:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:J:524:GLU:O    | 1:J:528:MLY:HB3  | 2.01                     | 0.61              |
| 3:L:50:LEU:O     | 3:L:53:PRO:HD2   | 2.00                     | 0.61              |
| 4:2:190:MET:HE1  | 4:2:206:ARG:HA   | 1.83                     | 0.61              |
| 4:4:223:PHE:HD2  | 4:4:312:ARG:NH2  | 1.99                     | 0.61              |
| 4:9:223:PHE:HD2  | 4:9:312:ARG:NH2  | 1.99                     | 0.61              |
| 4:V:190:MET:HE1  | 4:V:206:ARG:HA   | 1.83                     | 0.61              |
| 3:C:52:ASN:N     | 3:C:53:PRO:HD2   | 2.15                     | 0.61              |
| 1:D:530:MET:CG   | 4:9:354:GLN:HG3  | 2.30                     | 0.61              |
| 1:D:643:GLY:O    | 1:D:644:SER:CB   | 2.48                     | 0.61              |
| 3:F:49:ILE:HA    | 3:F:52:ASN:ND2   | 2.05                     | 0.61              |
| 1:G:755:HIS:HA   | 1:G:758:TYR:HE1  | 1.64                     | 0.61              |
| 1:J:543:PRO:HG2  | 4:W:143:TYR:O    | 1.98                     | 0.61              |
| 4:0:167:GLU:OE2  | 4:2:43:VAL:O     | 2.19                     | 0.61              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:OD2  | 2.44                     | 0.61              |
| 1:A:40:VAL:HG22  | 1:A:41:VAL:N     | 2.16                     | 0.60              |
| 1:A:156:PHE:CD1  | 1:A:195:TYR:CD1  | 2.89                     | 0.60              |
| 1:A:524:GLU:O    | 1:A:528:MLY:HB3  | 2.01                     | 0.60              |
| 1:A:553:MLY:NZ   | 4:V:45:VAL:HG13  | 2.16                     | 0.60              |
| 1:D:81:ASN:OD1   | 1:D:96:HIS:HB2   | 2.00                     | 0.60              |
| 1:G:40:VAL:HG22  | 1:G:41:VAL:N     | 2.16                     | 0.60              |
| 1:G:520:ALA:O    | 1:G:524:GLU:HG2  | 2.00                     | 0.60              |
| 1:G:728:ASN:HD22 | 3:I:113:THR:HG1  | 1.45                     | 0.60              |
| 1:G:836:PHE:CE1  | 2:H:159:HIS:CA   | 2.62                     | 0.60              |
| 2:H:114:LYS:HG3  | 2:H:146:GLY:HA2  | 1.82                     | 0.60              |
| 1:J:520:ALA:O    | 1:J:524:GLU:HG2  | 2.00                     | 0.60              |
| 2:K:34:ILE:O     | 2:K:46:ASP:HB3   | 2.01                     | 0.60              |
| 4:8:223:PHE:HD2  | 4:8:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:X:223:PHE:HD2  | 4:X:312:ARG:NH2  | 1.99                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:640:LYS:C    | 1:A:645:SER:OG   | 2.44                     | 0.60              |
| 1:D:837:MLY:O    | 1:D:840:PRO:HD2  | 2.01                     | 0.60              |
| 1:G:124:VAL:CG1  | 1:G:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:G:640:LYS:C    | 1:G:645:SER:OG   | 2.44                     | 0.60              |
| 1:J:837:MLY:O    | 1:J:840:PRO:HD2  | 2.02                     | 0.60              |
| 4:0:361:GLU:HB3  | 4:0:369:ILE:HG12 | 1.82                     | 0.60              |
| 4:1:223:PHE:HD2  | 4:1:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:Y:223:PHE:HD2  | 4:Y:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:A:124:VAL:CG1  | 1:A:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:D:124:VAL:CG1  | 1:D:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:D:640:LYS:C    | 1:D:645:SER:OG   | 2.44                     | 0.60              |
| 1:J:81:ASN:OD1   | 1:J:96:HIS:HB2   | 2.00                     | 0.60              |
| 1:J:95:THR:HG23  | 1:J:96:HIS:ND1   | 2.17                     | 0.60              |
| 1:J:530:MET:CG   | 4:W:354:GLN:HG3  | 2.30                     | 0.60              |
| 1:J:798:LEU:CD2  | 3:L:126:LEU:HG   | 2.18                     | 0.60              |
| 4:4:190:MET:HE1  | 4:4:206:ARG:HA   | 1.83                     | 0.60              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:CG2  | 2.42                     | 0.60              |
| 1:A:831:TRP:NE1  | 2:B:51:PHE:CE2   | 2.63                     | 0.60              |
| 1:D:166:MET:HE2  | 1:D:457:TYR:HB2  | 1.84                     | 0.60              |
| 2:E:34:ILE:O     | 2:E:46:ASP:HB3   | 2.01                     | 0.60              |
| 1:G:508:ILE:CD1  | 1:G:759:ALA:CB   | 2.47                     | 0.60              |
| 1:G:837:MLY:O    | 1:G:840:PRO:HD2  | 2.02                     | 0.60              |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:HD13 | 1.84                     | 0.60              |
| 1:J:202:SER:CA   | 1:J:207:LYS:HE3  | 2.27                     | 0.60              |
| 3:L:63:ILE:HG22  | 3:L:64:THR:O     | 2.01                     | 0.60              |
| 4:1:361:GLU:HB3  | 4:1:369:ILE:HG12 | 1.82                     | 0.60              |
| 1:A:38:VAL:HB    | 1:A:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:A:40:VAL:HG22  | 1:A:41:VAL:H     | 1.67                     | 0.60              |
| 1:A:836:PHE:CE2  | 2:B:160:GLY:C    | 2.80                     | 0.60              |
| 1:D:38:VAL:HB    | 1:D:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:D:40:VAL:HG22  | 1:D:41:VAL:N     | 2.16                     | 0.60              |
| 1:D:542:PHE:N    | 4:9:143:TYR:OH   | 2.32                     | 0.60              |
| 1:G:38:VAL:HB    | 1:G:52:ILE:HD11  | 1.83                     | 0.60              |
| 1:G:538:GLU:CG   | 4:V:351:THR:C    | 2.73                     | 0.60              |
| 1:G:730:SER:OG   | 3:I:109:HIS:CE1  | 2.54                     | 0.60              |
| 1:J:84:MLY:CH1   | 1:J:719:ASP:C    | 2.62                     | 0.60              |
| 1:J:542:PHE:N    | 4:W:143:TYR:OH   | 2.33                     | 0.60              |
| 2:K:130:PRO:HA   | 2:K:133:ILE:HD12 | 1.83                     | 0.60              |
| 4:2:324:THR:CG2  | 4:4:243:PRO:O    | 2.49                     | 0.60              |
| 4:7:223:PHE:HD2  | 4:7:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:V:223:PHE:HD2  | 4:V:312:ARG:NH2  | 1.99                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:553:MLY:NZ   | 4:W:45:VAL:HG13  | 2.16                     | 0.60              |
| 1:G:60:VAL:O     | 1:G:71:THR:HA    | 2.02                     | 0.60              |
| 1:G:93:MET:CB    | 1:G:716:LEU:HD12 | 2.32                     | 0.60              |
| 1:G:542:PHE:CB   | 4:V:143:TYR:HE1  | 2.13                     | 0.60              |
| 1:G:623:PHE:CG   | 1:G:623:PHE:HA   | 2.36                     | 0.60              |
| 1:J:124:VAL:CG1  | 1:J:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:J:578:HIS:CD2  | 1:J:591:ASN:HA   | 2.31                     | 0.60              |
| 1:J:640:LYS:C    | 4:W:23:GLY:CA    | 2.64                     | 0.60              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:HD13 | 2.31                     | 0.60              |
| 1:A:542:PHE:CD1  | 4:8:143:TYR:CE1  | 2.90                     | 0.60              |
| 3:C:52:ASN:N     | 3:C:53:PRO:CD    | 2.65                     | 0.60              |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:HD13 | 1.84                     | 0.60              |
| 1:D:524:GLU:O    | 1:D:528:MLY:HB3  | 2.01                     | 0.60              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:HA2  | 1.66                     | 0.60              |
| 2:E:130:PRO:HA   | 2:E:133:ILE:HD12 | 1.84                     | 0.60              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:HD13 | 2.19                     | 0.60              |
| 1:G:156:PHE:CD1  | 1:G:195:TYR:CD1  | 2.90                     | 0.60              |
| 1:G:795:ARG:HE   | 3:I:118:MET:HE1  | 1.67                     | 0.60              |
| 1:J:38:VAL:HB    | 1:J:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:J:40:VAL:HG22  | 1:J:41:VAL:N     | 2.16                     | 0.60              |
| 1:J:166:MET:HE2  | 1:J:457:TYR:HB2  | 1.84                     | 0.60              |
| 1:J:787:ILE:O    | 1:J:790:THR:N    | 2.35                     | 0.60              |
| 4:9:287:ILE:H    | 4:9:287:ILE:HD12 | 1.67                     | 0.60              |
| 4:Z:223:PHE:HD2  | 4:Z:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:A:505:MLY:HH23 | 1:A:762:HIS:O    | 2.02                     | 0.60              |
| 1:A:550:PHE:CE2  | 1:A:592:ILE:HG23 | 2.37                     | 0.60              |
| 1:A:787:ILE:O    | 1:A:790:THR:N    | 2.35                     | 0.60              |
| 1:A:837:MLY:O    | 1:A:840:PRO:HD2  | 2.02                     | 0.60              |
| 1:D:530:MET:HA   | 4:9:354:GLN:CB   | 2.29                     | 0.60              |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD2  | 2.19                     | 0.60              |
| 1:G:84:MLY:CH1   | 1:G:716:LEU:O    | 2.50                     | 0.60              |
| 1:J:60:VAL:O     | 1:J:71:THR:HA    | 2.02                     | 0.60              |
| 4:0:287:ILE:H    | 4:0:287:ILE:HD12 | 1.67                     | 0.60              |
| 4:7:287:ILE:HD12 | 4:7:287:ILE:H    | 1.67                     | 0.60              |
| 1:A:60:VAL:O     | 1:A:71:THR:HA    | 2.02                     | 0.60              |
| 1:A:95:THR:HG23  | 1:A:96:HIS:ND1   | 2.16                     | 0.60              |
| 1:A:538:GLU:CG   | 4:8:351:THR:C    | 2.74                     | 0.60              |
| 1:D:49:MLY:HH13  | 1:D:108:GLU:OE2  | 2.02                     | 0.60              |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CE1  | 2.37                     | 0.60              |
| 1:D:796:GLY:HA2  | 3:F:35:ARG:HB3   | 1.83                     | 0.60              |
| 1:G:578:HIS:CD2  | 1:G:591:ASN:HA   | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:818:TYR:CG   | 2:H:127:ARG:NH1  | 2.69                     | 0.60              |
| 1:G:838:ILE:HD12 | 2:H:54:MET:HE3   | 1.68                     | 0.60              |
| 3:I:63:ILE:HG22  | 3:I:64:THR:O     | 2.01                     | 0.60              |
| 1:J:640:LYS:C    | 1:J:645:SER:OG   | 2.44                     | 0.60              |
| 1:J:823:PHE:CD1  | 2:K:157:ILE:HA   | 2.37                     | 0.60              |
| 3:L:52:ASN:N     | 3:L:53:PRO:CD    | 2.65                     | 0.60              |
| 4:0:201:VAL:CG2  | 4:Y:287:ILE:CG1  | 2.79                     | 0.60              |
| 1:A:506:GLU:OE2  | 1:A:760:PHE:CD2  | 2.49                     | 0.60              |
| 3:C:46:ILE:O     | 3:C:50:LEU:CG    | 2.47                     | 0.60              |
| 1:D:755:HIS:HA   | 1:D:758:TYR:HE1  | 1.64                     | 0.60              |
| 1:D:789:ALA:C    | 3:F:87:PHE:CZ    | 2.80                     | 0.60              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE3   | 0.62                     | 0.60              |
| 3:I:52:ASN:HB2   | 3:I:53:PRO:CD    | 2.28                     | 0.60              |
| 4:0:243:PRO:CB   | 4:Y:291:LYS:CD   | 2.69                     | 0.60              |
| 4:8:287:ILE:H    | 4:8:287:ILE:HD12 | 1.67                     | 0.60              |
| 1:A:530:MET:CG   | 4:8:354:GLN:HG3  | 2.30                     | 0.59              |
| 1:A:541:MET:SD   | 4:8:346:LEU:O    | 2.48                     | 0.59              |
| 3:C:49:ILE:CA    | 3:C:52:ASN:ND2   | 2.53                     | 0.59              |
| 1:D:95:THR:HG23  | 1:D:96:HIS:ND1   | 2.17                     | 0.59              |
| 1:D:831:TRP:CA   | 2:E:51:PHE:CE1   | 2.85                     | 0.59              |
| 3:F:63:ILE:HG22  | 3:F:64:THR:O     | 2.01                     | 0.59              |
| 2:H:34:ILE:O     | 2:H:46:ASP:HB3   | 2.01                     | 0.59              |
| 1:J:553:MLY:HG3  | 4:Y:45:VAL:O     | 2.02                     | 0.59              |
| 4:5:287:ILE:H    | 4:5:287:ILE:HD12 | 1.67                     | 0.59              |
| 1:A:116:TYR:HB2  | 1:A:153:PRO:O    | 2.03                     | 0.59              |
| 1:A:135:TYR:N    | 1:A:135:TYR:CD1  | 2.69                     | 0.59              |
| 1:D:60:VAL:O     | 1:D:71:THR:HA    | 2.02                     | 0.59              |
| 1:D:783:LEU:O    | 1:D:787:ILE:N    | 2.28                     | 0.59              |
| 1:D:787:ILE:O    | 1:D:790:THR:N    | 2.35                     | 0.59              |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:G:550:PHE:CE2  | 1:G:592:ILE:HG23 | 2.37                     | 0.59              |
| 3:I:52:ASN:N     | 3:I:53:PRO:CD    | 2.65                     | 0.59              |
| 3:L:49:ILE:CA    | 3:L:52:ASN:ND2   | 2.53                     | 0.59              |
| 1:A:195:TYR:O    | 1:A:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:A:546:THR:HG22 | 1:A:547:ASP:N    | 2.17                     | 0.59              |
| 1:A:578:HIS:CD2  | 1:A:591:ASN:HA   | 2.31                     | 0.59              |
| 1:A:776:GLU:O    | 1:A:779:ARG:HB3  | 2.02                     | 0.59              |
| 1:D:549:SER:OG   | 1:D:550:PHE:N    | 2.36                     | 0.59              |
| 1:D:776:GLU:O    | 1:D:779:ARG:HB3  | 2.03                     | 0.59              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:CG   | 2.28                     | 0.59              |
| 1:G:546:THR:HG22 | 1:G:547:ASP:N    | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:140:PHE:O    | 2:H:141:PRO:C    | 2.33                     | 0.59              |
| 1:J:93:MET:SD    | 1:J:764:MLY:HH23 | 2.34                     | 0.59              |
| 1:J:530:MET:HA   | 4:W:354:GLN:CB   | 2.28                     | 0.59              |
| 1:J:549:SER:OG   | 1:J:550:PHE:N    | 2.35                     | 0.59              |
| 1:A:529:PRO:HG3  | 4:8:353:GLN:OE1  | 2.03                     | 0.59              |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:CZ   | 2.69                     | 0.59              |
| 1:D:599:ASN:CB   | 1:D:649:VAL:HB   | 2.32                     | 0.59              |
| 1:G:195:TYR:O    | 1:G:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:G:530:MET:CG   | 4:V:354:GLN:HG3  | 2.30                     | 0.59              |
| 1:G:541:MET:SD   | 4:V:346:LEU:O    | 2.48                     | 0.59              |
| 1:G:728:ASN:HD21 | 3:I:110:VAL:CA   | 2.15                     | 0.59              |
| 1:G:792:ALA:CB   | 3:I:40:ASN:HB3   | 2.32                     | 0.59              |
| 1:G:836:PHE:CE2  | 2:H:160:GLY:CA   | 2.85                     | 0.59              |
| 3:I:52:ASN:N     | 3:I:53:PRO:HD2   | 2.16                     | 0.59              |
| 1:J:156:PHE:CD1  | 1:J:195:TYR:CD1  | 2.90                     | 0.59              |
| 4:2:287:ILE:H    | 4:2:287:ILE:HD12 | 1.67                     | 0.59              |
| 4:V:286:ASP:OD1  | 4:X:202:THR:HB   | 2.01                     | 0.59              |
| 1:A:623:PHE:CG   | 1:A:623:PHE:HA   | 2.36                     | 0.59              |
| 1:A:831:TRP:CZ2  | 2:B:51:PHE:CZ    | 2.87                     | 0.59              |
| 1:D:789:ALA:O    | 3:F:87:PHE:CZ    | 2.55                     | 0.59              |
| 3:F:52:ASN:N     | 3:F:53:PRO:CD    | 2.65                     | 0.59              |
| 1:G:599:ASN:CB   | 1:G:649:VAL:HB   | 2.31                     | 0.59              |
| 1:G:646:PHE:CD2  | 1:G:652:LEU:CD1  | 2.85                     | 0.59              |
| 1:G:787:ILE:O    | 1:G:790:THR:N    | 2.35                     | 0.59              |
| 1:J:49:MLY:HH13  | 1:J:108:GLU:OE2  | 2.02                     | 0.59              |
| 1:J:265:ILE:HG22 | 1:J:266:GLU:N    | 2.18                     | 0.59              |
| 1:J:542:PHE:CD1  | 4:W:143:TYR:CE1  | 2.91                     | 0.59              |
| 1:J:567:LYS:NZ   | 4:Y:92:ASN:ND2   | 2.36                     | 0.59              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:HB3  | 2.01                     | 0.59              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:CB   | 2.32                     | 0.59              |
| 1:A:504:MLY:HB2  | 1:A:762:HIS:CE1  | 2.38                     | 0.59              |
| 1:D:156:PHE:CD1  | 1:D:195:TYR:CD1  | 2.90                     | 0.59              |
| 1:D:464:ILE:HG22 | 1:D:465:ALA:N    | 2.18                     | 0.59              |
| 1:D:822:SER:OG   | 2:E:87:LYS:O     | 2.20                     | 0.59              |
| 1:G:40:VAL:HG22  | 1:G:41:VAL:H     | 1.67                     | 0.59              |
| 1:G:549:SER:OG   | 1:G:550:PHE:N    | 2.35                     | 0.59              |
| 1:J:230:GLU:O    | 1:J:234:ASN:HB2  | 2.03                     | 0.59              |
| 1:J:550:PHE:CE2  | 1:J:592:ILE:HG23 | 2.37                     | 0.59              |
| 1:J:553:MLY:CH1  | 4:Y:45:VAL:HG11  | 2.32                     | 0.59              |
| 1:J:599:ASN:CB   | 1:J:649:VAL:HB   | 2.32                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:287:ILE:O    | 4:Z:205:GLU:OE1  | 2.21                     | 0.59              |
| 1:A:48:VAL:HG22  | 1:A:49:MLY:N     | 2.18                     | 0.59              |
| 1:A:166:MET:HE2  | 1:A:457:TYR:HB2  | 1.84                     | 0.59              |
| 1:A:640:LYS:C    | 4:8:23:GLY:CA    | 2.64                     | 0.59              |
| 1:D:601:ASP:N    | 1:D:602:PRO:HD3  | 2.18                     | 0.59              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:CG   | 2.86                     | 0.59              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:CH2  | 2.80                     | 0.59              |
| 1:D:822:SER:HG   | 2:E:88:LEU:HA    | 1.67                     | 0.59              |
| 1:G:166:MET:HE2  | 1:G:457:TYR:HB2  | 1.84                     | 0.59              |
| 1:G:721:LYS:C    | 1:G:736:GLN:OE1  | 2.46                     | 0.59              |
| 1:J:552:ASN:O    | 4:Y:47:MET:HE1   | 2.03                     | 0.59              |
| 1:J:752:ASP:O    | 1:J:780:ASP:OD2  | 2.21                     | 0.59              |
| 1:J:776:GLU:O    | 1:J:779:ARG:HB3  | 2.02                     | 0.59              |
| 4:1:287:ILE:HB   | 4:3:203:THR:CA   | 2.33                     | 0.59              |
| 1:A:601:ASP:N    | 1:A:602:PRO:HD3  | 2.18                     | 0.59              |
| 1:A:629:GLU:CB   | 1:A:643:GLY:C    | 2.75                     | 0.59              |
| 1:A:735:GLY:O    | 1:A:743:ALA:HA   | 1.94                     | 0.59              |
| 1:D:542:PHE:CD1  | 4:9:143:TYR:CE1  | 2.90                     | 0.59              |
| 1:G:116:TYR:HB2  | 1:G:153:PRO:O    | 2.03                     | 0.59              |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:J:707:CYS:C    | 1:J:714:ARG:HH22 | 2.11                     | 0.59              |
| 4:3:223:PHE:HD2  | 4:3:312:ARG:NH2  | 1.99                     | 0.59              |
| 4:4:287:ILE:H    | 4:4:287:ILE:HD12 | 1.67                     | 0.59              |
| 4:X:291:LYS:CG   | 4:Z:243:PRO:C    | 2.74                     | 0.59              |
| 1:A:230:GLU:O    | 1:A:234:ASN:HB2  | 2.03                     | 0.59              |
| 1:A:599:ASN:CB   | 1:A:649:VAL:HB   | 2.32                     | 0.59              |
| 1:A:642:LYS:HG2  | 4:8:22:ALA:C     | 2.27                     | 0.59              |
| 3:C:127:MET:HE2  | 3:C:137:ILE:HD13 | 1.85                     | 0.59              |
| 1:D:40:VAL:HG22  | 1:D:41:VAL:H     | 1.67                     | 0.59              |
| 1:G:542:PHE:CD1  | 4:V:143:TYR:CE1  | 2.91                     | 0.59              |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:HD1  | 1.68                     | 0.59              |
| 1:J:195:TYR:O    | 1:J:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:J:601:ASP:N    | 1:J:602:PRO:HD3  | 2.18                     | 0.59              |
| 1:J:784:ALA:O    | 1:J:788:THR:HB   | 2.02                     | 0.59              |
| 4:Z:287:ILE:HD12 | 4:Z:287:ILE:H    | 1.67                     | 0.59              |
| 1:A:721:LYS:C    | 1:A:736:GLN:OE1  | 2.46                     | 0.59              |
| 1:A:755:HIS:HA   | 1:A:758:TYR:HE1  | 1.64                     | 0.59              |
| 1:D:135:TYR:N    | 1:D:135:TYR:CD1  | 2.69                     | 0.59              |
| 1:D:141:LEU:O    | 1:D:144:ARG:HB3  | 2.03                     | 0.59              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:HG22 | 1.80                     | 0.59              |
| 1:D:721:LYS:C    | 1:D:736:GLN:OE1  | 2.46                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:817:GLN:NE2  | 2:E:127:ARG:CD   | 2.66                     | 0.59              |
| 1:D:817:GLN:OE1  | 2:E:127:ARG:NH2  | 2.36                     | 0.59              |
| 1:D:818:TYR:HB2  | 2:E:90:GLY:HA3   | 1.85                     | 0.59              |
| 3:F:127:MET:HE2  | 3:F:137:ILE:HD13 | 1.85                     | 0.59              |
| 1:G:95:THR:HG23  | 1:G:96:HIS:ND1   | 2.17                     | 0.59              |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:HD13 | 1.84                     | 0.59              |
| 1:G:730:SER:HB2  | 3:I:109:HIS:NE2  | 2.18                     | 0.59              |
| 1:J:642:LYS:HG2  | 4:W:22:ALA:C     | 2.27                     | 0.59              |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:HD1  | 1.68                     | 0.59              |
| 4:O:247:VAL:N    | 4:Y:324:THR:HB   | 2.18                     | 0.59              |
| 1:A:538:GLU:O    | 1:A:541:MET:HB2  | 2.03                     | 0.58              |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:D:722:GLN:O    | 1:D:782:MLY:HH23 | 2.02                     | 0.58              |
| 1:G:135:TYR:N    | 1:G:135:TYR:CD1  | 2.69                     | 0.58              |
| 1:G:230:GLU:O    | 1:G:234:ASN:HB2  | 2.03                     | 0.58              |
| 1:J:116:TYR:HB2  | 1:J:153:PRO:O    | 2.03                     | 0.58              |
| 1:J:210:GLN:O    | 1:J:211:SER:OG   | 2.15                     | 0.58              |
| 1:J:529:PRO:HG3  | 4:W:353:GLN:OE1  | 2.03                     | 0.58              |
| 1:J:546:THR:HG22 | 1:J:547:ASP:N    | 2.17                     | 0.58              |
| 1:J:646:PHE:CD2  | 1:J:652:LEU:CD1  | 2.85                     | 0.58              |
| 4:3:287:ILE:H    | 4:3:287:ILE:HD12 | 1.67                     | 0.58              |
| 1:A:794:CYS:O    | 1:A:798:LEU:N    | 2.36                     | 0.58              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:HA3   | 1.84                     | 0.58              |
| 1:D:218:LEU:N    | 1:D:221:GLN:HE21 | 2.01                     | 0.58              |
| 1:D:550:PHE:CE2  | 1:D:592:ILE:HG23 | 2.37                     | 0.58              |
| 1:D:629:GLU:CB   | 1:D:643:GLY:C    | 2.75                     | 0.58              |
| 1:D:629:GLU:HB3  | 1:D:645:SER:N    | 2.18                     | 0.58              |
| 1:D:792:ALA:C    | 3:F:40:ASN:CB    | 2.69                     | 0.58              |
| 1:G:629:GLU:CB   | 1:G:643:GLY:C    | 2.75                     | 0.58              |
| 2:H:130:PRO:HA   | 2:H:133:ILE:HD12 | 1.84                     | 0.58              |
| 1:J:629:GLU:CB   | 1:J:643:GLY:C    | 2.76                     | 0.58              |
| 1:J:643:GLY:HA2  | 4:W:24:ASP:OD1   | 2.04                     | 0.58              |
| 4:O:201:VAL:CG2  | 4:Y:287:ILE:HG12 | 2.32                     | 0.58              |
| 4:O:243:PRO:CA   | 4:Y:291:LYS:CE   | 2.81                     | 0.58              |
| 1:A:107:MLY:CB   | 1:A:686:MET:HE2  | 2.32                     | 0.58              |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:HD13 | 1.84                     | 0.58              |
| 1:A:557:GLU:HG3  | 1:A:557:GLU:O    | 2.00                     | 0.58              |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:HD1  | 1.68                     | 0.58              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:CB    | 2.81                     | 0.58              |
| 1:D:220:ASP:O    | 1:D:224:SER:N    | 2.27                     | 0.58              |
| 1:D:529:PRO:HG3  | 4:9:353:GLN:OE1  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:794:CYS:O    | 1:D:798:LEU:N    | 2.36                     | 0.58              |
| 1:D:813:ILE:O    | 1:D:817:GLN:N    | 2.30                     | 0.58              |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:N    | 2.18                     | 0.58              |
| 1:G:642:LYS:CG   | 4:V:22:ALA:CA    | 2.80                     | 0.58              |
| 1:J:629:GLU:HB3  | 1:J:645:SER:N    | 2.18                     | 0.58              |
| 3:L:3:SER:HG     | 3:L:5:ALA:N      | 2.01                     | 0.58              |
| 3:L:52:ASN:HB2   | 3:L:53:PRO:CD    | 2.28                     | 0.58              |
| 4:2:223:PHE:HD2  | 4:2:312:ARG:NH2  | 1.99                     | 0.58              |
| 1:A:549:SER:OG   | 1:A:550:PHE:N    | 2.36                     | 0.58              |
| 1:D:7:MET:HE3    | 1:D:14:ALA:HB1   | 1.85                     | 0.58              |
| 1:D:48:VAL:HG22  | 1:D:49:MLY:N     | 2.18                     | 0.58              |
| 1:D:127:ASN:ND2  | 1:D:128:PRO:HD2  | 2.16                     | 0.58              |
| 1:D:546:THR:HG22 | 1:D:547:ASP:N    | 2.17                     | 0.58              |
| 1:D:642:LYS:CA   | 4:9:22:ALA:C     | 2.71                     | 0.58              |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:HD1  | 1.68                     | 0.58              |
| 1:G:254:PHE:CE2  | 1:G:459:ILE:HD12 | 2.39                     | 0.58              |
| 1:G:601:ASP:N    | 1:G:602:PRO:HD3  | 2.18                     | 0.58              |
| 1:J:649:VAL:HA   | 1:J:649:VAL:HG22 | 1.80                     | 0.58              |
| 4:1:203:THR:HG22 | 4:Z:287:ILE:C    | 2.29                     | 0.58              |
| 1:D:643:GLY:HA2  | 4:9:24:ASP:OD1   | 2.04                     | 0.58              |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:CG1   | 2.25                     | 0.58              |
| 1:G:629:GLU:HB3  | 1:G:645:SER:N    | 2.18                     | 0.58              |
| 3:I:3:SER:HG     | 3:I:5:ALA:N      | 2.01                     | 0.58              |
| 3:I:127:MET:HE2  | 3:I:137:ILE:HD13 | 1.85                     | 0.58              |
| 1:J:7:MET:HE3    | 1:J:14:ALA:HB1   | 1.85                     | 0.58              |
| 1:J:40:VAL:HG22  | 1:J:41:VAL:H     | 1.67                     | 0.58              |
| 1:J:48:VAL:HG22  | 1:J:49:MLY:N     | 2.18                     | 0.58              |
| 1:J:127:ASN:ND2  | 1:J:128:PRO:HD2  | 2.16                     | 0.58              |
| 1:J:135:TYR:N    | 1:J:135:TYR:CD1  | 2.69                     | 0.58              |
| 1:J:218:LEU:N    | 1:J:221:GLN:HE21 | 2.01                     | 0.58              |
| 4:3:324:THR:HG21 | 4:5:244:ASP:N    | 1.80                     | 0.58              |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:D:217:THR:C    | 1:D:221:GLN:NE2  | 2.62                     | 0.58              |
| 1:D:230:GLU:O    | 1:D:234:ASN:HB2  | 2.03                     | 0.58              |
| 1:D:538:GLU:O    | 1:D:541:MET:HB2  | 2.04                     | 0.58              |
| 1:G:64:THR:HG22  | 1:G:65:GLU:N     | 2.19                     | 0.58              |
| 1:G:538:GLU:O    | 1:G:541:MET:HB2  | 2.04                     | 0.58              |
| 1:G:757:GLN:CD   | 1:G:772:LEU:CG   | 2.75                     | 0.58              |
| 1:G:776:GLU:O    | 1:G:779:ARG:HB3  | 2.03                     | 0.58              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:CG    | 2.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:107:MLY:CB   | 1:J:686:MET:HE2  | 2.32                     | 0.58              |
| 1:J:756:THR:HB   | 1:J:776:GLU:CD   | 2.29                     | 0.58              |
| 4:1:287:ILE:H    | 4:1:287:ILE:HD12 | 1.67                     | 0.58              |
| 1:A:64:THR:HG22  | 1:A:65:GLU:N     | 2.19                     | 0.58              |
| 1:A:642:LYS:CG   | 4:8:22:ALA:CA    | 2.81                     | 0.58              |
| 1:J:175:ILE:HA   | 1:J:670:HIS:O    | 2.03                     | 0.58              |
| 1:J:721:LYS:C    | 1:J:736:GLN:OE1  | 2.46                     | 0.58              |
| 1:J:755:HIS:HA   | 1:J:758:TYR:HE1  | 1.64                     | 0.58              |
| 4:W:286:ASP:OD1  | 4:Y:203:THR:HG22 | 2.04                     | 0.58              |
| 4:X:325:MET:CE   | 4:Z:244:ASP:OD2  | 2.51                     | 0.58              |
| 1:A:141:LEU:O    | 1:A:144:ARG:HB3  | 2.03                     | 0.58              |
| 1:A:409:GLY:HA3  | 4:8:333:PRO:CD   | 2.34                     | 0.58              |
| 1:D:254:PHE:CE2  | 1:D:459:ILE:HD12 | 2.39                     | 0.58              |
| 1:D:735:GLY:O    | 1:D:743:ALA:HA   | 1.94                     | 0.58              |
| 1:G:48:VAL:HG22  | 1:G:49:MLY:N     | 2.18                     | 0.58              |
| 1:G:107:MLY:CB   | 1:G:686:MET:HE2  | 2.32                     | 0.58              |
| 1:G:529:PRO:HG3  | 4:V:353:GLN:OE1  | 2.04                     | 0.58              |
| 1:J:279:LEU:HB3  | 1:J:280:PRO:HD2  | 1.86                     | 0.58              |
| 3:L:102:VAL:HG11 | 3:L:107:LEU:HB2  | 1.85                     | 0.58              |
| 4:1:44:MET:HA    | 4:Z:167:GLU:OE1  | 2.03                     | 0.58              |
| 4:2:290:ARG:NE   | 4:4:202:THR:HG21 | 2.15                     | 0.58              |
| 4:W:285:CYS:O    | 4:Y:202:THR:CG2  | 2.52                     | 0.58              |
| 1:A:49:MLY:HH13  | 1:A:108:GLU:OE2  | 2.03                     | 0.58              |
| 1:A:831:TRP:CD2  | 2:B:51:PHE:CZ    | 2.88                     | 0.58              |
| 2:B:130:PRO:HA   | 2:B:133:ILE:HD12 | 1.84                     | 0.58              |
| 3:C:3:SER:HG     | 3:C:5:ALA:N      | 2.01                     | 0.58              |
| 1:D:107:MLY:CB   | 1:D:686:MET:HE2  | 2.32                     | 0.58              |
| 1:D:175:ILE:HA   | 1:D:670:HIS:O    | 2.03                     | 0.58              |
| 1:D:279:LEU:HB3  | 1:D:280:PRO:HD2  | 1.86                     | 0.58              |
| 1:G:141:LEU:O    | 1:G:144:ARG:HB3  | 2.03                     | 0.58              |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:HB2  | 0.73                     | 0.58              |
| 1:G:817:GLN:OE1  | 2:H:127:ARG:CD   | 2.48                     | 0.58              |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:J:464:ILE:HG22 | 1:J:465:ALA:N    | 2.18                     | 0.58              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:CB   | 2.76                     | 0.58              |
| 1:A:175:ILE:HA   | 1:A:670:HIS:O    | 2.04                     | 0.58              |
| 1:A:217:THR:C    | 1:A:221:GLN:NE2  | 2.62                     | 0.58              |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:N    | 2.18                     | 0.58              |
| 1:A:813:ILE:O    | 1:A:817:GLN:N    | 2.30                     | 0.58              |
| 1:D:640:LYS:C    | 4:9:23:GLY:CA    | 2.64                     | 0.58              |
| 1:G:49:MLY:HH13  | 1:G:108:GLU:OE2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:567:LYS:HZ1  | 4:X:92:ASN:HD21  | 1.51                     | 0.58              |
| 1:G:568:PRO:HG3  | 1:G:578:HIS:H    | 1.69                     | 0.58              |
| 1:J:510:TRP:CE2  | 1:J:768:MLY:CH1  | 2.87                     | 0.58              |
| 1:J:538:GLU:O    | 1:J:541:MET:HB2  | 2.03                     | 0.58              |
| 4:O:201:VAL:HG23 | 4:Y:287:ILE:HG13 | 1.85                     | 0.58              |
| 1:A:629:GLU:HB3  | 1:A:645:SER:N    | 2.18                     | 0.57              |
| 3:C:102:VAL:HG11 | 3:C:107:LEU:HB2  | 1.85                     | 0.57              |
| 1:D:642:LYS:HG2  | 4:9:22:ALA:C     | 2.27                     | 0.57              |
| 1:D:724:TYR:CZ   | 1:D:778:MET:HB3  | 2.36                     | 0.57              |
| 1:D:792:ALA:CB   | 3:F:40:ASN:CB    | 2.75                     | 0.57              |
| 1:D:831:TRP:N    | 2:E:51:PHE:HZ    | 2.00                     | 0.57              |
| 1:G:99:GLU:OE2   | 1:G:696:ARG:NH2  | 2.30                     | 0.57              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:HB3   | 2.39                     | 0.57              |
| 3:I:102:VAL:HG11 | 3:I:107:LEU:HB2  | 1.85                     | 0.57              |
| 1:J:541:MET:SD   | 4:W:346:LEU:O    | 2.48                     | 0.57              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:H    | 2.12                     | 0.57              |
| 4:1:244:ASP:HA   | 4:Z:324:THR:HG23 | 1.86                     | 0.57              |
| 1:A:539:GLU:OE2  | 4:V:45:VAL:C     | 2.48                     | 0.57              |
| 1:D:265:ILE:HG22 | 1:D:266:GLU:N    | 2.18                     | 0.57              |
| 1:D:418:THR:HG22 | 1:D:419:VAL:H    | 1.69                     | 0.57              |
| 1:D:676:ILE:HG23 | 1:D:676:ILE:O    | 2.03                     | 0.57              |
| 3:F:102:VAL:HG11 | 3:F:107:LEU:HB2  | 1.84                     | 0.57              |
| 1:G:279:LEU:HB3  | 1:G:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:G:642:LYS:HG2  | 4:V:22:ALA:C     | 2.27                     | 0.57              |
| 1:G:751:GLY:N    | 3:I:114:LEU:HD11 | 2.18                     | 0.57              |
| 1:G:813:ILE:O    | 1:G:816:ILE:N    | 2.37                     | 0.57              |
| 1:G:820:VAL:HG11 | 2:H:136:MET:HE3  | 1.84                     | 0.57              |
| 1:J:676:ILE:HG23 | 1:J:676:ILE:O    | 2.03                     | 0.57              |
| 1:J:827:MLY:HH21 | 2:K:139:ALA:HB3  | 1.85                     | 0.57              |
| 1:A:642:LYS:CA   | 4:8:22:ALA:C     | 2.71                     | 0.57              |
| 1:A:783:LEU:O    | 1:A:787:ILE:N    | 2.28                     | 0.57              |
| 1:D:322:VAL:HG11 | 1:D:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:H    | 2.12                     | 0.57              |
| 1:D:725:ARG:H    | 1:D:782:MLY:HH21 | 1.64                     | 0.57              |
| 1:G:409:GLY:HA3  | 4:V:333:PRO:CD   | 2.35                     | 0.57              |
| 1:G:411:GLU:N    | 4:V:333:PRO:HB2  | 2.11                     | 0.57              |
| 1:J:64:THR:HG22  | 1:J:65:GLU:N     | 2.19                     | 0.57              |
| 1:J:322:VAL:HG11 | 1:J:325:ILE:HD11 | 1.86                     | 0.57              |
| 4:O:203:THR:HG22 | 4:Y:286:ASP:OD2  | 2.04                     | 0.57              |
| 1:A:254:PHE:CE2  | 1:A:459:ILE:HD12 | 2.39                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:LEU:HB3  | 1:A:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:A:418:THR:HG22 | 1:A:419:VAL:H    | 1.69                     | 0.57              |
| 1:A:831:TRP:CZ3  | 2:B:34:ILE:HG12  | 2.40                     | 0.57              |
| 1:D:195:TYR:O    | 1:D:199:ILE:HG23 | 2.03                     | 0.57              |
| 1:G:769:ALA:O    | 1:G:773:GLY:HA2  | 2.04                     | 0.57              |
| 1:J:254:PHE:CE2  | 1:J:459:ILE:HD12 | 2.39                     | 0.57              |
| 1:J:784:ALA:O    | 1:J:788:THR:CB   | 2.52                     | 0.57              |
| 1:J:794:CYS:O    | 1:J:798:LEU:N    | 2.36                     | 0.57              |
| 1:A:218:LEU:N    | 1:A:221:GLN:HE21 | 2.01                     | 0.57              |
| 1:A:220:ASP:O    | 1:A:224:SER:N    | 2.27                     | 0.57              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:CG2  | 2.34                     | 0.57              |
| 1:A:599:ASN:CG   | 1:A:649:VAL:H    | 2.12                     | 0.57              |
| 1:A:635:GLY:HA3  | 4:8:334:GLU:CG   | 2.30                     | 0.57              |
| 1:A:676:ILE:HG23 | 1:A:676:ILE:O    | 2.03                     | 0.57              |
| 1:A:707:CYS:CA   | 1:A:714:ARG:CZ   | 2.78                     | 0.57              |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:CD1  | 2.39                     | 0.57              |
| 1:D:723:ARG:HH21 | 1:D:783:LEU:HD11 | 1.68                     | 0.57              |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:CD1  | 2.39                     | 0.57              |
| 1:G:557:GLU:HG3  | 1:G:557:GLU:O    | 2.00                     | 0.57              |
| 1:G:728:ASN:HA   | 3:I:113:THR:OG1  | 2.05                     | 0.57              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:HD23 | 2.13                     | 0.57              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:CD   | 2.33                     | 0.57              |
| 1:J:82:PRO:HD2   | 1:J:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:J:141:LEU:O    | 1:J:144:ARG:HB3  | 2.03                     | 0.57              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:CG2   | 2.87                     | 0.57              |
| 1:D:22:LYS:O     | 1:D:26:GLU:N     | 2.29                     | 0.57              |
| 1:D:64:THR:HG22  | 1:D:65:GLU:N     | 2.19                     | 0.57              |
| 1:D:409:GLY:HA3  | 4:9:333:PRO:CD   | 2.35                     | 0.57              |
| 1:D:579:PHE:CD2  | 1:D:592:ILE:HD11 | 2.39                     | 0.57              |
| 1:D:813:ILE:O    | 1:D:816:ILE:N    | 2.37                     | 0.57              |
| 1:G:7:MET:HE3    | 1:G:14:ALA:HB1   | 1.85                     | 0.57              |
| 1:G:218:LEU:N    | 1:G:221:GLN:HE21 | 2.01                     | 0.57              |
| 1:G:813:ILE:O    | 1:G:817:GLN:N    | 2.30                     | 0.57              |
| 1:J:409:GLY:HA3  | 4:W:333:PRO:CD   | 2.35                     | 0.57              |
| 4:0:223:PHE:HD2  | 4:0:312:ARG:NH2  | 1.99                     | 0.57              |
| 4:0:246:GLN:N    | 4:Y:324:THR:HB   | 2.19                     | 0.57              |
| 4:X:287:ILE:HG13 | 4:Z:201:VAL:CB   | 2.34                     | 0.57              |
| 1:A:265:ILE:HG22 | 1:A:266:GLU:N    | 2.18                     | 0.57              |
| 1:A:643:GLY:HA2  | 4:8:24:ASP:OD1   | 2.04                     | 0.57              |
| 1:A:839:MLY:CD   | 2:B:159:HIS:HB3  | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:116:TYR:HB2  | 1:D:153:PRO:O    | 2.03                     | 0.57              |
| 1:G:84:MLY:HH11  | 1:G:720:PHE:CA   | 2.34                     | 0.57              |
| 1:G:175:ILE:HA   | 1:G:670:HIS:O    | 2.04                     | 0.57              |
| 1:G:599:ASN:CG   | 1:G:649:VAL:H    | 2.12                     | 0.57              |
| 1:G:751:GLY:CA   | 3:I:114:LEU:CD1  | 2.82                     | 0.57              |
| 1:J:561:LYS:HE3  | 4:Y:48:GLY:CA    | 2.29                     | 0.57              |
| 1:A:109:ARG:O    | 1:A:114:MET:N    | 2.37                     | 0.57              |
| 1:A:322:VAL:HG11 | 1:A:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:411:GLU:N    | 4:8:333:PRO:HB2  | 2.11                     | 0.57              |
| 1:A:839:MLY:HD2  | 2:B:159:HIS:CD2  | 2.38                     | 0.57              |
| 1:D:82:PRO:HD2   | 1:D:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:HA2  | 1.66                     | 0.57              |
| 1:G:642:LYS:CD   | 4:V:340:TRP:CZ3  | 2.80                     | 0.57              |
| 1:G:747:LEU:HD23 | 1:G:747:LEU:O    | 2.05                     | 0.57              |
| 1:G:831:TRP:CZ2  | 2:H:67:MET:HB3   | 2.40                     | 0.57              |
| 1:J:579:PHE:CD2  | 1:J:592:ILE:HD11 | 2.39                     | 0.57              |
| 1:J:783:LEU:O    | 1:J:787:ILE:CB   | 2.52                     | 0.57              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:CG   | 2.17                     | 0.57              |
| 4:3:322:PRO:C    | 4:5:244:ASP:HB2  | 2.30                     | 0.57              |
| 1:A:795:ARG:CG   | 3:C:118:MET:CE   | 2.82                     | 0.57              |
| 1:A:813:ILE:O    | 1:A:816:ILE:N    | 2.37                     | 0.57              |
| 1:A:817:GLN:NE2  | 2:B:127:ARG:CG   | 2.68                     | 0.57              |
| 1:D:646:PHE:CD2  | 1:D:652:LEU:CD1  | 2.85                     | 0.57              |
| 1:G:82:PRO:HD2   | 1:G:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:J:530:MET:CA   | 4:W:354:GLN:HB3  | 2.35                     | 0.57              |
| 4:0:287:ILE:CD1  | 4:2:203:THR:HB   | 2.34                     | 0.57              |
| 1:A:529:PRO:CG   | 4:8:353:GLN:OE1  | 2.53                     | 0.57              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:HG   | 1.86                     | 0.57              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CG   | 2.68                     | 0.57              |
| 1:D:568:PRO:HG3  | 1:D:578:HIS:H    | 1.69                     | 0.57              |
| 1:G:217:THR:C    | 1:G:221:GLN:NE2  | 2.62                     | 0.57              |
| 1:G:676:ILE:HG23 | 1:G:676:ILE:O    | 2.03                     | 0.57              |
| 1:J:642:LYS:CA   | 4:W:22:ALA:C     | 2.70                     | 0.57              |
| 1:J:747:LEU:O    | 1:J:747:LEU:HD23 | 2.05                     | 0.57              |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:CD1  | 2.39                     | 0.57              |
| 4:1:287:ILE:HG22 | 4:3:204:ALA:H    | 1.69                     | 0.57              |
| 1:A:82:PRO:HD2   | 1:A:85:TYR:CD2   | 2.40                     | 0.56              |
| 1:A:634:GLY:N    | 4:8:25:ASP:O     | 2.31                     | 0.56              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:CG    | 2.35                     | 0.56              |
| 1:D:22:LYS:HA    | 1:D:25:ILE:HB    | 1.87                     | 0.56              |
| 1:D:411:GLU:H    | 4:9:333:PRO:HG2  | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:530:MET:CA   | 4:9:354:GLN:HB3  | 2.35                     | 0.56              |
| 1:G:265:ILE:HG22 | 1:G:266:GLU:N    | 2.18                     | 0.56              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:CG2  | 2.35                     | 0.56              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:HH22 | 2.04                     | 0.56              |
| 1:J:95:THR:HA    | 1:J:713:SER:CA   | 2.33                     | 0.56              |
| 1:J:642:LYS:HG2  | 4:W:21:PHE:C     | 2.29                     | 0.56              |
| 1:J:677:PRO:HB2  | 1:J:678:ASN:ND2  | 2.20                     | 0.56              |
| 4:W:223:PHE:HD2  | 4:W:312:ARG:NH2  | 1.99                     | 0.56              |
| 1:A:135:TYR:N    | 1:A:135:TYR:HD1  | 2.03                     | 0.56              |
| 1:A:481:ASN:N    | 1:A:481:ASN:ND2  | 2.51                     | 0.56              |
| 1:A:568:PRO:HG3  | 1:A:578:HIS:H    | 1.69                     | 0.56              |
| 1:A:733:PRO:CA   | 1:A:737:PHE:HE1  | 2.18                     | 0.56              |
| 1:A:753:VAL:CG1  | 1:A:775:LEU:HG   | 2.35                     | 0.56              |
| 1:D:733:PRO:CB   | 1:D:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:G:338:ILE:HG21 | 1:G:348:MLY:HB3  | 1.87                     | 0.56              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:CH2  | 2.78                     | 0.56              |
| 1:J:217:THR:C    | 1:J:221:GLN:NE2  | 2.62                     | 0.56              |
| 3:L:46:ILE:O     | 3:L:50:LEU:CG    | 2.47                     | 0.56              |
| 4:0:243:PRO:C    | 4:Y:291:LYS:CG   | 2.77                     | 0.56              |
| 1:A:7:MET:HE3    | 1:A:14:ALA:HB1   | 1.85                     | 0.56              |
| 1:A:210:GLN:O    | 1:A:211:SER:OG   | 2.15                     | 0.56              |
| 1:A:295:MLY:CG   | 1:A:332:MET:HE2  | 2.36                     | 0.56              |
| 1:A:302:MET:HG2  | 1:A:303:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:411:GLU:H    | 4:8:333:PRO:HG2  | 1.71                     | 0.56              |
| 1:A:630:ALA:CA   | 4:8:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:A:677:PRO:HB2  | 1:A:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:814:PHE:CA   | 2:B:127:ARG:HH22 | 2.18                     | 0.56              |
| 1:D:135:TYR:N    | 1:D:135:TYR:HD1  | 2.03                     | 0.56              |
| 1:D:530:MET:HA   | 4:9:354:GLN:CD   | 2.11                     | 0.56              |
| 1:D:642:LYS:HG2  | 4:9:21:PHE:C     | 2.30                     | 0.56              |
| 1:D:733:PRO:CA   | 1:D:737:PHE:HE1  | 2.19                     | 0.56              |
| 3:F:3:SER:HG     | 3:F:5:ALA:N      | 2.03                     | 0.56              |
| 1:G:677:PRO:HB2  | 1:G:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:G:797:PHE:HE2  | 3:I:126:LEU:HD23 | 1.70                     | 0.56              |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:CD1  | 2.39                     | 0.56              |
| 1:J:418:THR:HG22 | 1:J:419:VAL:H    | 1.69                     | 0.56              |
| 1:J:568:PRO:HG3  | 1:J:578:HIS:H    | 1.69                     | 0.56              |
| 1:J:638:GLY:CA   | 4:W:345:ILE:H    | 2.18                     | 0.56              |
| 1:J:735:GLY:O    | 1:J:743:ALA:HA   | 1.94                     | 0.56              |
| 1:J:813:ILE:O    | 1:J:816:ILE:N    | 2.37                     | 0.56              |
| 3:L:127:MET:HE2  | 3:L:137:ILE:HD13 | 1.85                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:0:205:GLU:CD   | 4:Y:287:ILE:O    | 2.48                     | 0.56              |
| 4:0:299:MET:HE2  | 4:0:331:ALA:HB2  | 1.88                     | 0.56              |
| 4:1:365:ALA:HB3  | 4:1:369:ILE:HB   | 1.88                     | 0.56              |
| 4:2:287:ILE:HB   | 4:4:204:ALA:N    | 2.21                     | 0.56              |
| 4:3:365:ALA:HB3  | 4:3:369:ILE:HB   | 1.88                     | 0.56              |
| 4:X:285:CYS:O    | 4:Z:202:THR:CG2  | 2.48                     | 0.56              |
| 1:A:649:VAL:HA   | 1:A:649:VAL:HG23 | 1.82                     | 0.56              |
| 1:A:733:PRO:CB   | 1:A:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:D:116:TYR:CE2  | 1:D:154:HIS:CD2  | 2.94                     | 0.56              |
| 1:D:677:PRO:HB2  | 1:D:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:D:747:LEU:HD23 | 1:D:747:LEU:O    | 2.04                     | 0.56              |
| 2:E:162:ASP:O    | 2:K:21:GLU:HB2   | 2.06                     | 0.56              |
| 1:G:302:MET:HG2  | 1:G:303:LEU:HD13 | 1.88                     | 0.56              |
| 1:G:322:VAL:HG11 | 1:G:325:ILE:HD11 | 1.86                     | 0.56              |
| 1:G:643:GLY:HA2  | 4:V:24:ASP:OD1   | 2.04                     | 0.56              |
| 1:A:546:THR:HG21 | 1:A:548:THR:HB   | 1.88                     | 0.56              |
| 1:A:649:VAL:HG22 | 1:A:649:VAL:HA   | 1.80                     | 0.56              |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:O    | 2.05                     | 0.56              |
| 1:G:135:TYR:N    | 1:G:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:G:295:MLY:CG   | 1:G:332:MET:HE2  | 2.36                     | 0.56              |
| 1:G:733:PRO:O    | 1:G:737:PHE:CE1  | 2.53                     | 0.56              |
| 1:G:733:PRO:CA   | 1:G:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:J:116:TYR:CE2  | 1:J:154:HIS:CD2  | 2.94                     | 0.56              |
| 1:J:338:ILE:HG21 | 1:J:348:MLY:HB3  | 1.87                     | 0.56              |
| 1:J:768:MLY:NZ   | 1:J:772:LEU:CD2  | 2.40                     | 0.56              |
| 1:J:789:ALA:HB2  | 3:L:81:GLN:HG2   | 1.87                     | 0.56              |
| 4:4:299:MET:HE2  | 4:4:331:ALA:HB2  | 1.88                     | 0.56              |
| 1:A:338:ILE:HG21 | 1:A:348:MLY:HB3  | 1.87                     | 0.56              |
| 1:A:646:PHE:CD2  | 1:A:652:LEU:CD1  | 2.85                     | 0.56              |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:H    | 1.71                     | 0.56              |
| 1:D:435:GLU:O    | 1:D:438:PHE:HB3  | 2.06                     | 0.56              |
| 1:G:559:LEU:HD23 | 1:G:559:LEU:C    | 2.31                     | 0.56              |
| 1:G:820:VAL:CG1  | 2:H:136:MET:CE   | 2.84                     | 0.56              |
| 1:J:135:TYR:N    | 1:J:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:A:116:TYR:CE2  | 1:A:154:HIS:CD2  | 2.94                     | 0.56              |
| 1:A:206:LYS:HB3  | 1:A:217:THR:OG1  | 2.06                     | 0.56              |
| 1:A:217:THR:HG22 | 1:A:218:LEU:O    | 2.05                     | 0.56              |
| 1:A:546:THR:HB   | 1:A:549:SER:H    | 1.71                     | 0.56              |
| 1:D:99:GLU:OE2   | 1:D:696:ARG:NH2  | 2.30                     | 0.56              |
| 1:D:215:GLN:CA   | 1:D:340:ILE:CG2  | 2.63                     | 0.56              |
| 1:G:109:ARG:O    | 1:G:114:MET:N    | 2.37                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:13:ALA:C     | 1:J:15:PRO:HD2   | 2.31                     | 0.56              |
| 1:J:630:ALA:CA   | 4:W:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:J:640:LYS:C    | 4:W:23:GLY:C     | 2.74                     | 0.56              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:HD3  | 2.18                     | 0.56              |
| 4:0:205:GLU:OE1  | 4:Y:287:ILE:C    | 2.49                     | 0.56              |
| 4:0:365:ALA:HB3  | 4:0:369:ILE:HB   | 1.87                     | 0.56              |
| 4:1:287:ILE:HG21 | 4:3:203:THR:N    | 2.19                     | 0.56              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:CB   | 2.53                     | 0.56              |
| 1:A:7:MET:HE3    | 1:A:14:ALA:CB    | 2.36                     | 0.56              |
| 1:A:530:MET:CA   | 4:8:354:GLN:HB3  | 2.35                     | 0.56              |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:C    | 2.31                     | 0.56              |
| 1:D:819:ASN:H    | 2:E:90:GLY:HA3   | 1.71                     | 0.56              |
| 1:G:13:ALA:C     | 1:G:15:PRO:HD2   | 2.31                     | 0.56              |
| 1:G:529:PRO:CG   | 4:V:353:GLN:OE1  | 2.54                     | 0.56              |
| 1:G:557:GLU:HB2  | 4:X:47:MET:O     | 2.04                     | 0.56              |
| 1:G:640:LYS:C    | 1:G:645:SER:HG   | 2.13                     | 0.56              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:HA   | 2.35                     | 0.56              |
| 1:G:649:VAL:HA   | 1:G:649:VAL:HG22 | 1.80                     | 0.56              |
| 1:G:768:MLY:CD   | 1:G:772:LEU:CD2  | 2.70                     | 0.56              |
| 1:J:530:MET:CB   | 4:W:354:GLN:HG3  | 2.36                     | 0.56              |
| 1:J:629:GLU:O    | 1:J:643:GLY:HA3  | 2.06                     | 0.56              |
| 1:J:754:ASP:OD1  | 1:J:779:ARG:HD2  | 2.06                     | 0.56              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:CD1  | 2.82                     | 0.56              |
| 4:1:203:THR:HG23 | 4:Z:288:ASP:CG   | 2.29                     | 0.56              |
| 4:Y:365:ALA:HB3  | 4:Y:369:ILE:HB   | 1.88                     | 0.56              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:CE    | 2.36                     | 0.56              |
| 1:D:529:PRO:CG   | 4:9:353:GLN:OE1  | 2.53                     | 0.56              |
| 1:D:831:TRP:CA   | 2:E:51:PHE:HE1   | 2.18                     | 0.56              |
| 1:G:7:MET:HE3    | 1:G:14:ALA:CB    | 2.36                     | 0.56              |
| 1:G:84:MLY:HH12  | 1:G:716:LEU:O    | 2.05                     | 0.56              |
| 1:G:206:LYS:HB3  | 1:G:217:THR:OG1  | 2.06                     | 0.56              |
| 1:G:418:THR:HG22 | 1:G:419:VAL:H    | 1.69                     | 0.56              |
| 1:G:435:GLU:O    | 1:G:438:PHE:HB3  | 2.06                     | 0.56              |
| 1:G:537:GLU:HB3  | 1:G:648:THR:CB   | 2.36                     | 0.56              |
| 1:G:733:PRO:CB   | 1:G:737:PHE:HE1  | 2.19                     | 0.56              |
| 3:I:46:ILE:O     | 3:I:50:LEU:CG    | 2.47                     | 0.56              |
| 1:A:22:LYS:O     | 1:A:26:GLU:HG3   | 2.06                     | 0.56              |
| 1:A:438:PHE:HA   | 1:A:441:MET:HE3  | 1.88                     | 0.56              |
| 1:A:501:GLU:C    | 1:A:762:HIS:CE1  | 2.84                     | 0.56              |
| 1:A:631:GLU:C    | 4:8:25:ASP:HB2   | 2.31                     | 0.56              |
| 1:D:32:PHE:CG    | 1:D:83:PRO:HD3   | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:290:GLN:HG2  | 1:D:331:LEU:HA   | 1.87                     | 0.56              |
| 1:D:537:GLU:HB3  | 1:D:648:THR:CB   | 2.36                     | 0.56              |
| 1:D:630:ALA:CA   | 4:9:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:D:831:TRP:CD2  | 2:E:51:PHE:CZ    | 2.94                     | 0.56              |
| 1:G:22:LYS:O     | 1:G:26:GLU:HG3   | 2.06                     | 0.56              |
| 1:G:217:THR:HG22 | 1:G:218:LEU:O    | 2.06                     | 0.56              |
| 1:G:631:GLU:C    | 4:V:25:ASP:HB2   | 2.31                     | 0.56              |
| 1:G:794:CYS:O    | 1:G:798:LEU:N    | 2.37                     | 0.56              |
| 1:J:95:THR:HA    | 1:J:713:SER:CB   | 2.36                     | 0.56              |
| 1:J:503:TYR:OH   | 1:J:711:PHE:CD2  | 2.40                     | 0.56              |
| 1:J:733:PRO:CA   | 1:J:737:PHE:HE1  | 2.19                     | 0.56              |
| 4:4:365:ALA:HB3  | 4:4:369:ILE:HB   | 1.88                     | 0.56              |
| 4:W:365:ALA:HB3  | 4:W:369:ILE:HB   | 1.88                     | 0.56              |
| 4:X:365:ALA:HB3  | 4:X:369:ILE:HB   | 1.88                     | 0.56              |
| 1:A:529:PRO:CB   | 4:8:354:GLN:HA   | 2.36                     | 0.55              |
| 1:A:795:ARG:HG2  | 3:C:118:MET:CE   | 2.35                     | 0.55              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:CG   | 2.80                     | 0.55              |
| 1:D:529:PRO:CB   | 4:9:354:GLN:HA   | 2.36                     | 0.55              |
| 1:D:638:GLY:CA   | 4:9:345:ILE:H    | 2.19                     | 0.55              |
| 1:D:640:LYS:C    | 4:9:23:GLY:C     | 2.74                     | 0.55              |
| 1:G:116:TYR:CE2  | 1:G:154:HIS:CD2  | 2.94                     | 0.55              |
| 1:G:411:GLU:H    | 4:V:333:PRO:HG2  | 1.70                     | 0.55              |
| 1:G:530:MET:CA   | 4:V:354:GLN:HB3  | 2.35                     | 0.55              |
| 1:G:757:GLN:NE2  | 1:G:772:LEU:HG   | 2.21                     | 0.55              |
| 4:1:287:ILE:HB   | 4:3:203:THR:CB   | 2.35                     | 0.55              |
| 4:5:299:MET:HE2  | 4:5:331:ALA:HB2  | 1.87                     | 0.55              |
| 4:9:365:ALA:HB3  | 4:9:369:ILE:HB   | 1.88                     | 0.55              |
| 4:V:288:ASP:N    | 4:X:204:ALA:H    | 2.03                     | 0.55              |
| 4:V:291:LYS:HD2  | 4:X:243:PRO:HB2  | 1.87                     | 0.55              |
| 4:X:287:ILE:HG13 | 4:Z:201:VAL:CG2  | 2.32                     | 0.55              |
| 4:Z:365:ALA:HB3  | 4:Z:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:290:GLN:HG2  | 1:A:331:LEU:HA   | 1.87                     | 0.55              |
| 1:A:797:PHE:CG   | 3:C:149:VAL:HG11 | 2.34                     | 0.55              |
| 1:D:13:ALA:C     | 1:D:15:PRO:HD2   | 2.31                     | 0.55              |
| 1:D:629:GLU:O    | 1:D:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:D:724:TYR:C    | 1:D:782:MLY:CH1  | 2.78                     | 0.55              |
| 1:D:786:ILE:HG12 | 3:F:86:ASP:HB3   | 1.88                     | 0.55              |
| 1:G:438:PHE:HA   | 1:G:441:MET:HE3  | 1.88                     | 0.55              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:HD11 | 1.26                     | 0.55              |
| 1:J:217:THR:HG22 | 1:J:218:LEU:O    | 2.05                     | 0.55              |
| 3:L:123:VAL:O    | 3:L:127:MET:HG2  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:287:ILE:CG2  | 4:3:202:THR:CA   | 2.81                     | 0.55              |
| 4:7:365:ALA:HB3  | 4:7:369:ILE:HB   | 1.87                     | 0.55              |
| 1:A:32:PHE:CG    | 1:A:83:PRO:HD3   | 2.42                     | 0.55              |
| 1:A:345:ALA:O    | 1:A:349:THR:N    | 2.40                     | 0.55              |
| 1:A:797:PHE:HD2  | 3:C:126:LEU:CD2  | 2.19                     | 0.55              |
| 1:D:546:THR:HG21 | 1:D:548:THR:HB   | 1.88                     | 0.55              |
| 1:G:629:GLU:O    | 1:G:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:J:634:GLY:N    | 4:W:25:ASP:O     | 2.31                     | 0.55              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:CG   | 2.90                     | 0.55              |
| 1:A:290:GLN:NE2  | 1:A:334:THR:OG1  | 2.40                     | 0.55              |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:H    | 1.71                     | 0.55              |
| 1:A:502:GLU:HA   | 1:A:762:HIS:H    | 1.72                     | 0.55              |
| 1:A:604:ASN:OD1  | 1:A:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:A:629:GLU:O    | 1:A:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:A:640:LYS:C    | 4:8:23:GLY:C     | 2.74                     | 0.55              |
| 1:A:765:VAL:HG12 | 1:A:766:PHE:N    | 2.22                     | 0.55              |
| 1:A:797:PHE:HD2  | 3:C:126:LEU:HD21 | 1.71                     | 0.55              |
| 1:D:217:THR:HG22 | 1:D:218:LEU:O    | 2.06                     | 0.55              |
| 1:D:506:GLU:OE2  | 1:D:764:MLY:HH22 | 2.06                     | 0.55              |
| 1:D:604:ASN:OD1  | 1:D:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:631:GLU:C    | 4:9:25:ASP:HB2   | 2.31                     | 0.55              |
| 1:D:793:ARG:HE   | 3:F:147:MET:HG2  | 1.70                     | 0.55              |
| 1:G:22:LYS:HA    | 1:G:25:ILE:HB    | 1.87                     | 0.55              |
| 1:G:127:ASN:ND2  | 1:G:128:PRO:HD2  | 2.17                     | 0.55              |
| 1:G:836:PHE:CD2  | 2:H:160:GLY:N    | 2.74                     | 0.55              |
| 1:J:7:MET:HE3    | 1:J:14:ALA:CB    | 2.36                     | 0.55              |
| 1:J:206:LYS:HB3  | 1:J:217:THR:OG1  | 2.06                     | 0.55              |
| 1:J:302:MET:HG2  | 1:J:303:LEU:HD13 | 1.87                     | 0.55              |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:H    | 1.71                     | 0.55              |
| 1:J:529:PRO:CB   | 4:W:354:GLN:HA   | 2.36                     | 0.55              |
| 1:J:567:LYS:HZ2  | 4:Y:92:ASN:HA    | 1.69                     | 0.55              |
| 1:J:579:PHE:HE1  | 1:J:581:LEU:HD13 | 1.72                     | 0.55              |
| 1:J:733:PRO:CB   | 1:J:737:PHE:HE1  | 2.19                     | 0.55              |
| 4:2:365:ALA:HB3  | 4:2:369:ILE:HB   | 1.88                     | 0.55              |
| 4:5:365:ALA:HB3  | 4:5:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:537:GLU:HB3  | 1:A:648:THR:CB   | 2.36                     | 0.55              |
| 1:A:768:MLY:C    | 1:A:771:LEU:HB3  | 2.37                     | 0.55              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:CA   | 2.37                     | 0.55              |
| 1:D:438:PHE:HA   | 1:D:441:MET:HE3  | 1.88                     | 0.55              |
| 1:D:559:LEU:HD23 | 1:D:559:LEU:C    | 2.31                     | 0.55              |
| 1:D:723:ARG:C    | 1:D:782:MLY:NZ   | 2.65                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:638:GLY:CA   | 4:V:345:ILE:H    | 2.18                     | 0.55              |
| 1:J:32:PHE:CG    | 1:J:83:PRO:HD3   | 2.41                     | 0.55              |
| 3:L:35:ARG:HA    | 3:L:39:GLN:O     | 2.06                     | 0.55              |
| 4:2:299:MET:HE2  | 4:2:331:ALA:HB2  | 1.88                     | 0.55              |
| 4:3:287:ILE:HG21 | 4:5:204:ALA:H    | 1.67                     | 0.55              |
| 4:3:299:MET:HE2  | 4:3:331:ALA:HB2  | 1.87                     | 0.55              |
| 1:A:725:ARG:HG3  | 1:A:733:PRO:CA   | 2.36                     | 0.55              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CG   | 2.37                     | 0.55              |
| 1:D:338:ILE:HG21 | 1:D:348:MLY:HB3  | 1.87                     | 0.55              |
| 1:D:530:MET:CB   | 4:9:354:GLN:HG3  | 2.36                     | 0.55              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:CG   | 2.90                     | 0.55              |
| 1:G:579:PHE:HE1  | 1:G:581:LEU:HD13 | 1.72                     | 0.55              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CG   | 2.90                     | 0.55              |
| 2:H:156:VAL:HA   | 2:H:159:HIS:O    | 2.07                     | 0.55              |
| 3:I:35:ARG:HA    | 3:I:39:GLN:O     | 2.07                     | 0.55              |
| 1:J:438:PHE:HA   | 1:J:441:MET:HE3  | 1.88                     | 0.55              |
| 1:J:529:PRO:CG   | 4:W:353:GLN:OE1  | 2.54                     | 0.55              |
| 1:J:631:GLU:C    | 4:W:25:ASP:HB2   | 2.31                     | 0.55              |
| 1:J:725:ARG:HG3  | 1:J:733:PRO:CA   | 2.36                     | 0.55              |
| 4:1:287:ILE:CA   | 4:3:202:THR:HB   | 2.35                     | 0.55              |
| 4:W:299:MET:HE2  | 4:W:331:ALA:HB2  | 1.87                     | 0.55              |
| 4:Y:299:MET:HE2  | 4:Y:331:ALA:HB2  | 1.88                     | 0.55              |
| 1:A:530:MET:CB   | 4:8:354:GLN:HG3  | 2.36                     | 0.55              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:HA2  | 1.66                     | 0.55              |
| 3:C:35:ARG:HA    | 3:C:39:GLN:O     | 2.07                     | 0.55              |
| 1:D:7:MET:HE3    | 1:D:14:ALA:CB    | 2.36                     | 0.55              |
| 1:D:206:LYS:HB3  | 1:D:217:THR:OG1  | 2.06                     | 0.55              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:CG   | 2.89                     | 0.55              |
| 2:E:156:VAL:HA   | 2:E:159:HIS:O    | 2.07                     | 0.55              |
| 1:G:546:THR:HB   | 1:G:549:SER:H    | 1.71                     | 0.55              |
| 1:G:604:ASN:OD1  | 1:G:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:G:640:LYS:C    | 4:V:23:GLY:CA    | 2.64                     | 0.55              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:CG   | 2.89                     | 0.55              |
| 1:J:22:LYS:HA    | 1:J:25:ILE:HB    | 1.87                     | 0.55              |
| 1:J:82:PRO:HD2   | 1:J:85:TYR:HD2   | 1.72                     | 0.55              |
| 1:J:345:ALA:O    | 1:J:349:THR:N    | 2.40                     | 0.55              |
| 1:J:411:GLU:H    | 4:W:333:PRO:HG2  | 1.71                     | 0.55              |
| 1:J:435:GLU:O    | 1:J:438:PHE:HB3  | 2.06                     | 0.55              |
| 1:J:635:GLY:HA3  | 4:W:334:GLU:CG   | 2.30                     | 0.55              |
| 1:J:750:GLY:HA2  | 3:L:114:LEU:HD23 | 1.88                     | 0.55              |
| 2:K:156:VAL:HA   | 2:K:159:HIS:O    | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:299:MET:HE2  | 4:1:331:ALA:HB2  | 1.87                     | 0.55              |
| 4:9:299:MET:HE2  | 4:9:331:ALA:HB2  | 1.88                     | 0.55              |
| 1:A:723:ARG:CG   | 1:A:723:ARG:HH11 | 2.20                     | 0.55              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:HG2  | 1.72                     | 0.55              |
| 1:D:302:MET:HG2  | 1:D:303:LEU:HD13 | 1.87                     | 0.55              |
| 1:D:724:TYR:OH   | 1:D:778:MET:HB2  | 2.07                     | 0.55              |
| 1:D:789:ALA:HB2  | 3:F:81:GLN:O     | 2.06                     | 0.55              |
| 1:D:815:CYS:HA   | 2:E:90:GLY:HA2   | 1.88                     | 0.55              |
| 3:F:46:ILE:O     | 3:F:50:LEU:CG    | 2.47                     | 0.55              |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:CG   | 2.20                     | 0.55              |
| 4:1:244:ASP:CG   | 4:Z:322:PRO:HB3  | 2.31                     | 0.55              |
| 1:A:13:ALA:C     | 1:A:15:PRO:HD2   | 2.31                     | 0.55              |
| 1:A:127:ASN:ND2  | 1:A:128:PRO:HD2  | 2.16                     | 0.55              |
| 1:A:630:ALA:HA   | 4:8:25:ASP:OD2   | 2.07                     | 0.55              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CG   | 2.90                     | 0.55              |
| 1:D:295:MLY:CG   | 1:D:332:MET:HE2  | 2.36                     | 0.55              |
| 1:D:629:GLU:CA   | 1:D:643:GLY:C    | 2.73                     | 0.55              |
| 1:D:724:TYR:OH   | 1:D:778:MET:SD   | 2.65                     | 0.55              |
| 1:D:834:LEU:HD22 | 2:E:50:THR:HG22  | 1.89                     | 0.55              |
| 1:G:126:VAL:HG13 | 1:G:675:ILE:HG22 | 1.89                     | 0.55              |
| 1:G:290:GLN:HG2  | 1:G:331:LEU:HA   | 1.87                     | 0.55              |
| 1:G:290:GLN:NE2  | 1:G:334:THR:OG1  | 2.40                     | 0.55              |
| 1:G:649:VAL:HA   | 1:G:649:VAL:HG23 | 1.82                     | 0.55              |
| 1:G:723:ARG:HH11 | 1:G:723:ARG:CG   | 2.20                     | 0.55              |
| 1:J:290:GLN:HG2  | 1:J:331:LEU:HA   | 1.88                     | 0.55              |
| 1:J:561:LYS:CE   | 4:Y:48:GLY:CA    | 2.82                     | 0.55              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HG21  | 2.41                     | 0.55              |
| 4:2:148:THR:HG21 | 4:4:45:VAL:HG21  | 1.89                     | 0.55              |
| 1:A:149:GLN:HB3  | 1:A:719:ASP:CG   | 2.14                     | 0.55              |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CE2  | 2.42                     | 0.55              |
| 1:D:470:PHE:O    | 1:D:473:ASN:ND2  | 2.40                     | 0.55              |
| 1:D:638:GLY:HA2  | 4:9:345:ILE:H    | 1.72                     | 0.55              |
| 3:F:123:VAL:O    | 3:F:127:MET:HG2  | 2.07                     | 0.55              |
| 1:G:638:GLY:HA2  | 4:V:345:ILE:H    | 1.71                     | 0.55              |
| 1:G:783:LEU:HA   | 1:G:786:ILE:HB   | 1.87                     | 0.55              |
| 1:J:295:MLY:CD   | 1:J:332:MET:HE2  | 2.37                     | 0.55              |
| 1:J:295:MLY:CG   | 1:J:332:MET:HE2  | 2.36                     | 0.55              |
| 1:J:503:TYR:HH   | 1:J:711:PHE:HD2  | 0.72                     | 0.55              |
| 1:J:559:LEU:HD23 | 1:J:559:LEU:C    | 2.31                     | 0.55              |
| 1:J:604:ASN:OD1  | 1:J:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:HA   | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:O:202:THR:CA   | 4:Y:286:ASP:OD1  | 2.52                     | 0.55              |
| 4:7:299:MET:HE2  | 4:7:331:ALA:HB2  | 1.88                     | 0.55              |
| 4:X:299:MET:HE2  | 4:X:331:ALA:HB2  | 1.88                     | 0.55              |
| 1:A:22:LYS:HA    | 1:A:25:ILE:HB    | 1.88                     | 0.54              |
| 1:A:97:LEU:HD22  | 1:A:712:PRO:CB   | 2.33                     | 0.54              |
| 1:A:435:GLU:O    | 1:A:438:PHE:HB3  | 2.06                     | 0.54              |
| 1:A:530:MET:HA   | 4:8:354:GLN:CD   | 2.11                     | 0.54              |
| 1:A:638:GLY:CA   | 4:8:345:ILE:H    | 2.19                     | 0.54              |
| 1:A:638:GLY:HA2  | 4:8:345:ILE:H    | 1.72                     | 0.54              |
| 1:A:757:GLN:OE1  | 1:A:771:LEU:HD12 | 2.07                     | 0.54              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:HA   | 2.35                     | 0.54              |
| 1:G:769:ALA:C    | 1:G:773:GLY:HA3  | 2.33                     | 0.54              |
| 1:J:290:GLN:NE2  | 1:J:334:THR:OG1  | 2.40                     | 0.54              |
| 1:J:561:LYS:HE2  | 4:Y:48:GLY:HA3   | 1.88                     | 0.54              |
| 4:1:244:ASP:HB3  | 4:Z:322:PRO:HB2  | 1.89                     | 0.54              |
| 4:V:291:LYS:HD2  | 4:X:243:PRO:CB   | 2.38                     | 0.54              |
| 4:W:286:ASP:OD2  | 4:Y:203:THR:CG2  | 2.47                     | 0.54              |
| 1:A:10:PHE:O     | 1:A:12:GLU:N     | 2.41                     | 0.54              |
| 1:A:78:PHE:HB3   | 1:A:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:A:82:PRO:HD2   | 1:A:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:A:126:VAL:HG13 | 1:A:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CE2  | 2.43                     | 0.54              |
| 3:C:123:VAL:O    | 3:C:127:MET:HG2  | 2.06                     | 0.54              |
| 1:D:295:MLY:CD   | 1:D:332:MET:HE2  | 2.37                     | 0.54              |
| 1:D:539:GLU:OE2  | 4:W:45:VAL:C     | 2.47                     | 0.54              |
| 1:D:635:GLY:HA3  | 4:9:334:GLU:CG   | 2.30                     | 0.54              |
| 1:D:792:ALA:O    | 3:F:40:ASN:HB3   | 2.05                     | 0.54              |
| 1:G:530:MET:CB   | 4:V:354:GLN:HG3  | 2.37                     | 0.54              |
| 1:G:546:THR:HG21 | 1:G:548:THR:HB   | 1.88                     | 0.54              |
| 1:G:735:GLY:O    | 1:G:743:ALA:HA   | 1.94                     | 0.54              |
| 1:J:126:VAL:HG13 | 1:J:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:J:470:PHE:O    | 1:J:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:J:629:GLU:CA   | 1:J:643:GLY:C    | 2.73                     | 0.54              |
| 2:K:146:GLY:O    | 2:K:147:ASN:ND2  | 2.41                     | 0.54              |
| 4:Z:299:MET:HE2  | 4:Z:331:ALA:HB2  | 1.88                     | 0.54              |
| 1:A:51:THR:C     | 1:A:62:VAL:HG13  | 2.32                     | 0.54              |
| 1:D:10:PHE:O     | 1:D:12:GLU:N     | 2.41                     | 0.54              |
| 1:D:22:LYS:O     | 1:D:26:GLU:HG3   | 2.07                     | 0.54              |
| 1:D:788:THR:HG22 | 3:F:81:GLN:NE2   | 2.23                     | 0.54              |
| 1:G:32:PHE:CG    | 1:G:83:PRO:HD3   | 2.41                     | 0.54              |
| 1:G:78:PHE:HB3   | 1:G:98:HIS:NE2   | 2.23                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:82:PRO:HD2   | 1:G:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:G:508:ILE:HG21 | 1:G:711:PHE:CZ   | 2.42                     | 0.54              |
| 1:G:728:ASN:ND2  | 3:I:109:HIS:O    | 2.40                     | 0.54              |
| 3:I:123:VAL:O    | 3:I:127:MET:HG2  | 2.07                     | 0.54              |
| 1:J:503:TYR:CE1  | 1:J:711:PHE:CE2  | 2.94                     | 0.54              |
| 1:J:546:THR:HG21 | 1:J:548:THR:HB   | 1.88                     | 0.54              |
| 4:8:288:ASP:CA   | 4:V:204:ALA:HB2  | 2.31                     | 0.54              |
| 4:V:365:ALA:HB3  | 4:V:369:ILE:HB   | 1.88                     | 0.54              |
| 1:A:579:PHE:HE1  | 1:A:581:LEU:HD13 | 1.72                     | 0.54              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:CB   | 2.20                     | 0.54              |
| 1:D:553:MLY:HG3  | 4:W:44:MET:O     | 2.07                     | 0.54              |
| 1:D:571:ALA:O    | 1:D:572:LYS:CB   | 2.56                     | 0.54              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:CB   | 2.76                     | 0.54              |
| 1:G:38:VAL:CB    | 1:G:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:G:220:ASP:O    | 1:G:224:SER:N    | 2.27                     | 0.54              |
| 1:G:345:ALA:O    | 1:G:349:THR:N    | 2.40                     | 0.54              |
| 1:G:529:PRO:CB   | 4:V:354:GLN:HA   | 2.37                     | 0.54              |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CE2  | 2.43                     | 0.54              |
| 1:J:546:THR:HB   | 1:J:549:SER:H    | 1.71                     | 0.54              |
| 1:J:797:PHE:CD2  | 3:L:126:LEU:CD2  | 2.91                     | 0.54              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:ND2  | 2.35                     | 0.54              |
| 4:V:299:MET:HE2  | 4:V:331:ALA:HB2  | 1.88                     | 0.54              |
| 1:A:295:MLY:CD   | 1:A:332:MET:HE2  | 2.37                     | 0.54              |
| 1:A:768:MLY:HG2  | 1:A:771:LEU:HD13 | 1.89                     | 0.54              |
| 2:B:156:VAL:HA   | 2:B:159:HIS:O    | 2.07                     | 0.54              |
| 1:D:82:PRO:HD2   | 1:D:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:D:126:VAL:HG13 | 1:D:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:D:290:GLN:NE2  | 1:D:334:THR:OG1  | 2.40                     | 0.54              |
| 1:D:345:ALA:O    | 1:D:349:THR:N    | 2.40                     | 0.54              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CE2  | 2.42                     | 0.54              |
| 1:G:707:CYS:C    | 1:G:714:ARG:NH2  | 2.51                     | 0.54              |
| 1:J:10:PHE:O     | 1:J:12:GLU:N     | 2.40                     | 0.54              |
| 1:J:78:PHE:HB3   | 1:J:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:J:537:GLU:HB3  | 1:J:648:THR:CB   | 2.36                     | 0.54              |
| 1:J:642:LYS:HA   | 4:W:22:ALA:C     | 2.33                     | 0.54              |
| 1:J:793:ARG:HG2  | 3:L:147:MET:HG2  | 1.89                     | 0.54              |
| 4:3:324:THR:H    | 4:5:244:ASP:HA   | 1.72                     | 0.54              |
| 4:8:365:ALA:HB3  | 4:8:369:ILE:HB   | 1.88                     | 0.54              |
| 1:A:571:ALA:O    | 1:A:572:LYS:CB   | 2.56                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:78:PHE:HB3   | 1:D:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:D:630:ALA:HA   | 4:9:25:ASP:OD2   | 2.07                     | 0.54              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:HG23 | 1.82                     | 0.54              |
| 1:D:739:ASP:CB   | 1:D:742:LYS:CB   | 2.81                     | 0.54              |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:H    | 1.71                     | 0.54              |
| 1:G:725:ARG:HG3  | 1:G:733:PRO:CA   | 2.36                     | 0.54              |
| 1:G:791:GLN:O    | 1:G:794:CYS:HB2  | 2.08                     | 0.54              |
| 1:J:22:LYS:O     | 1:J:26:GLU:HG3   | 2.07                     | 0.54              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:HA   | 2.35                     | 0.54              |
| 1:D:769:ALA:C    | 1:D:771:LEU:HA   | 2.33                     | 0.54              |
| 1:D:796:GLY:CA   | 3:F:40:ASN:OD1   | 2.51                     | 0.54              |
| 1:G:10:PHE:O     | 1:G:12:GLU:N     | 2.41                     | 0.54              |
| 1:G:51:THR:C     | 1:G:62:VAL:HG13  | 2.32                     | 0.54              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:NH1  | 2.16                     | 0.54              |
| 1:G:818:TYR:CD1  | 2:H:127:ARG:CZ   | 2.79                     | 0.54              |
| 1:J:103:LEU:C    | 1:J:103:LEU:HD12 | 2.33                     | 0.54              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:HG2  | 1.72                     | 0.54              |
| 1:J:493:HIS:ND1  | 1:J:514:ASP:OD2  | 2.41                     | 0.54              |
| 3:L:92:ARG:HA    | 3:L:139:TYR:OH   | 2.08                     | 0.54              |
| 4:1:45:VAL:HG23  | 4:Z:148:THR:OG1  | 2.07                     | 0.54              |
| 1:A:538:GLU:HG3  | 4:8:352:PHE:CA   | 2.38                     | 0.54              |
| 1:A:642:LYS:HG2  | 4:8:21:PHE:C     | 2.30                     | 0.54              |
| 1:D:38:VAL:CB    | 1:D:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:D:218:LEU:CD2  | 1:D:222:ILE:CG1  | 2.86                     | 0.54              |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:D:546:THR:HB   | 1:D:549:SER:H    | 1.71                     | 0.54              |
| 1:D:724:TYR:OH   | 1:D:778:MET:CB   | 2.56                     | 0.54              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:HD11 | 1.26                     | 0.54              |
| 2:E:146:GLY:O    | 2:E:147:ASN:ND2  | 2.41                     | 0.54              |
| 1:G:530:MET:HA   | 4:V:354:GLN:CD   | 2.11                     | 0.54              |
| 1:G:576:GLU:CG   | 1:G:577:ALA:N    | 2.43                     | 0.54              |
| 1:G:640:LYS:C    | 4:V:23:GLY:C     | 2.75                     | 0.54              |
| 1:J:51:THR:C     | 1:J:62:VAL:HG13  | 2.32                     | 0.54              |
| 1:J:638:GLY:HA2  | 4:W:345:ILE:H    | 1.72                     | 0.54              |
| 1:A:38:VAL:CB    | 1:A:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CZ   | 2.43                     | 0.54              |
| 1:A:768:MLY:CG   | 1:A:771:LEU:HD13 | 2.37                     | 0.54              |
| 2:B:146:GLY:O    | 2:B:147:ASN:ND2  | 2.41                     | 0.54              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:HG3  | 1.71                     | 0.54              |
| 1:D:507:GLY:O    | 1:D:761:GLY:C    | 2.50                     | 0.54              |
| 1:D:642:LYS:HA   | 4:9:22:ALA:C     | 2.33                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:839:MLY:HH11 | 2:E:159:HIS:CG   | 2.31                     | 0.54              |
| 1:G:404:PRO:CG   | 1:G:417:GLU:HG3  | 2.38                     | 0.54              |
| 1:G:493:HIS:ND1  | 1:G:514:ASP:OD2  | 2.41                     | 0.54              |
| 1:G:571:ALA:O    | 1:G:572:LYS:CB   | 2.56                     | 0.54              |
| 1:G:642:LYS:HG2  | 4:V:21:PHE:C     | 2.30                     | 0.54              |
| 1:J:791:GLN:O    | 1:J:794:CYS:HB2  | 2.08                     | 0.54              |
| 4:0:243:PRO:O    | 4:Y:291:LYS:HE2  | 2.07                     | 0.54              |
| 4:1:202:THR:HA   | 4:Z:287:ILE:HG13 | 1.90                     | 0.54              |
| 4:3:287:ILE:HB   | 4:5:203:THR:CG2  | 2.35                     | 0.54              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:HG2  | 1.72                     | 0.54              |
| 1:A:218:LEU:N    | 1:A:221:GLN:HG2  | 2.23                     | 0.54              |
| 1:A:470:PHE:O    | 1:A:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:D:51:THR:C     | 1:D:62:VAL:HG13  | 2.32                     | 0.54              |
| 1:D:103:LEU:C    | 1:D:103:LEU:HD12 | 2.33                     | 0.54              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:ND1  | 2.71                     | 0.54              |
| 1:D:765:VAL:HG12 | 1:D:766:PHE:N    | 2.22                     | 0.54              |
| 1:G:93:MET:HB2   | 1:G:764:MLY:NZ   | 2.20                     | 0.54              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:HG2  | 1.72                     | 0.54              |
| 1:G:470:PHE:O    | 1:G:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:G:538:GLU:HG3  | 4:V:352:PHE:CA   | 2.38                     | 0.54              |
| 1:G:642:LYS:HA   | 4:V:22:ALA:C     | 2.33                     | 0.54              |
| 4:8:299:MET:HE2  | 4:8:331:ALA:HB2  | 1.88                     | 0.54              |
| 1:A:553:MLY:O    | 4:V:48:GLY:CA    | 2.56                     | 0.53              |
| 1:A:584:TYR:CD1  | 1:A:585:ALA:N    | 2.77                     | 0.53              |
| 1:D:98:HIS:HB3   | 1:D:100:PRO:CD   | 2.25                     | 0.53              |
| 1:D:723:ARG:CG   | 1:D:723:ARG:HH11 | 2.20                     | 0.53              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:CG    | 2.61                     | 0.53              |
| 2:E:162:ASP:O    | 2:K:21:GLU:HB3   | 2.08                     | 0.53              |
| 1:G:93:MET:CG    | 1:G:716:LEU:HD12 | 2.37                     | 0.53              |
| 1:G:103:LEU:C    | 1:G:103:LEU:HD12 | 2.33                     | 0.53              |
| 1:G:295:MLY:CD   | 1:G:332:MET:HE2  | 2.38                     | 0.53              |
| 1:G:556:ASP:OD2  | 4:X:44:MET:HG3   | 2.08                     | 0.53              |
| 1:G:795:ARG:HH22 | 3:I:43:ASN:HB2   | 1.73                     | 0.53              |
| 2:H:146:GLY:O    | 2:H:147:ASN:ND2  | 2.41                     | 0.53              |
| 3:I:92:ARG:HA    | 3:I:139:TYR:OH   | 2.08                     | 0.53              |
| 1:J:538:GLU:HG3  | 4:W:352:PHE:CA   | 2.38                     | 0.53              |
| 1:J:630:ALA:HA   | 4:W:25:ASP:OD2   | 2.07                     | 0.53              |
| 4:V:324:THR:HG22 | 4:X:247:VAL:HG13 | 1.91                     | 0.53              |
| 1:A:404:PRO:CG   | 1:A:417:GLU:HG3  | 2.38                     | 0.53              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:CG   | 2.89                     | 0.53              |
| 1:D:831:TRP:NE1  | 2:E:67:MET:SD    | 2.80                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:84:MLY:CH1   | 1:G:720:PHE:N    | 2.71                     | 0.53              |
| 1:G:84:MLY:HH11  | 1:G:719:ASP:C    | 2.32                     | 0.53              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:G:765:VAL:HG12 | 1:G:766:PHE:N    | 2.22                     | 0.53              |
| 1:J:38:VAL:CB    | 1:J:52:ILE:HD11  | 2.38                     | 0.53              |
| 4:4:185:LEU:HD23 | 4:4:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:791:GLN:O    | 1:A:794:CYS:HB2  | 2.08                     | 0.53              |
| 1:G:661:MET:O    | 1:G:665:ARG:HG3  | 2.08                     | 0.53              |
| 4:2:322:PRO:C    | 4:4:244:ASP:HB2  | 2.33                     | 0.53              |
| 4:X:287:ILE:HG23 | 4:Z:201:VAL:CG2  | 2.38                     | 0.53              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:A:529:PRO:HB2  | 4:8:354:GLN:HA   | 1.91                     | 0.53              |
| 1:A:818:TYR:HB2  | 2:B:89:LYS:C     | 2.32                     | 0.53              |
| 2:B:130:PRO:O    | 2:B:131:GLU:C    | 2.52                     | 0.53              |
| 1:D:42:HIS:HB3   | 1:D:45:GLN:O     | 2.09                     | 0.53              |
| 1:D:579:PHE:HE1  | 1:D:581:LEU:HD13 | 1.72                     | 0.53              |
| 2:E:114:LYS:O    | 2:E:147:ASN:ND2  | 2.41                     | 0.53              |
| 3:F:35:ARG:HA    | 3:F:39:GLN:O     | 2.07                     | 0.53              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:HB2  | 1.91                     | 0.53              |
| 1:G:277:PHE:CG   | 1:G:278:GLN:N    | 2.76                     | 0.53              |
| 1:G:732:ILE:H    | 1:G:733:PRO:HD2  | 1.74                     | 0.53              |
| 1:J:109:ARG:O    | 1:J:114:MET:N    | 2.37                     | 0.53              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:J:571:ALA:O    | 1:J:572:LYS:CB   | 2.56                     | 0.53              |
| 1:J:765:VAL:HG12 | 1:J:766:PHE:N    | 2.22                     | 0.53              |
| 4:7:185:LEU:HD23 | 4:7:306:TYR:OH   | 2.08                     | 0.53              |
| 4:8:185:LEU:HD23 | 4:8:306:TYR:OH   | 2.08                     | 0.53              |
| 4:W:288:ASP:H    | 4:Y:204:ALA:H    | 1.56                     | 0.53              |
| 1:A:42:HIS:HB3   | 1:A:45:GLN:O     | 2.09                     | 0.53              |
| 1:A:642:LYS:HA   | 4:8:22:ALA:C     | 2.34                     | 0.53              |
| 1:D:277:PHE:CG   | 1:D:278:GLN:N    | 2.76                     | 0.53              |
| 1:D:404:PRO:CG   | 1:D:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:D:529:PRO:HB2  | 4:9:354:GLN:HA   | 1.91                     | 0.53              |
| 1:D:553:MLY:O    | 4:W:48:GLY:CA    | 2.56                     | 0.53              |
| 1:D:584:TYR:CD1  | 1:D:585:ALA:N    | 2.77                     | 0.53              |
| 1:G:32:PHE:CD1   | 1:G:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:J:32:PHE:CD1   | 1:J:83:PRO:HD3   | 2.43                     | 0.53              |
| 1:J:584:TYR:CD1  | 1:J:585:ALA:N    | 2.77                     | 0.53              |
| 1:J:640:LYS:C    | 1:J:645:SER:HG   | 2.09                     | 0.53              |
| 4:Y:185:LEU:HD23 | 4:Y:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:732:ILE:H    | 1:A:733:PRO:HD2  | 1.73                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:661:MET:O    | 1:D:665:ARG:HG3  | 2.09                     | 0.53              |
| 1:D:793:ARG:NE   | 3:F:147:MET:HG2  | 2.22                     | 0.53              |
| 1:D:800:ARG:CG   | 3:F:149:VAL:HG22 | 2.37                     | 0.53              |
| 1:D:831:TRP:HZ3  | 2:E:50:THR:HG21  | 1.74                     | 0.53              |
| 1:D:838:ILE:C    | 1:D:840:PRO:HD2  | 2.34                     | 0.53              |
| 1:J:218:LEU:N    | 1:J:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:J:404:PRO:CG   | 1:J:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:J:642:LYS:CG   | 4:W:22:ALA:CA    | 2.80                     | 0.53              |
| 1:J:661:MET:O    | 1:J:665:ARG:HG3  | 2.09                     | 0.53              |
| 4:2:185:LEU:HD23 | 4:2:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:22:LYS:O     | 1:A:26:GLU:N     | 2.30                     | 0.53              |
| 1:A:156:PHE:HD1  | 1:A:195:TYR:CD1  | 2.27                     | 0.53              |
| 1:D:32:PHE:CD1   | 1:D:83:PRO:HD3   | 2.43                     | 0.53              |
| 1:D:134:VAL:C    | 1:D:136:ASN:H    | 2.16                     | 0.53              |
| 1:D:135:TYR:CD2  | 1:D:191:ARG:HG2  | 2.44                     | 0.53              |
| 1:D:793:ARG:HE   | 3:F:147:MET:CB   | 2.21                     | 0.53              |
| 2:H:114:LYS:O    | 2:H:147:ASN:ND2  | 2.41                     | 0.53              |
| 3:I:53:PRO:HB2   | 3:I:55:LYS:HG3   | 1.91                     | 0.53              |
| 1:J:22:LYS:O     | 1:J:26:GLU:N     | 2.29                     | 0.53              |
| 1:J:84:MLY:HH11  | 1:J:720:PHE:N    | 2.23                     | 0.53              |
| 1:J:757:GLN:OE1  | 1:J:773:GLY:N    | 2.40                     | 0.53              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:HG23 | 1.85                     | 0.53              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:CG   | 2.89                     | 0.53              |
| 4:0:185:LEU:HD23 | 4:0:306:TYR:OH   | 2.08                     | 0.53              |
| 4:0:247:VAL:CG2  | 4:Y:324:THR:HG21 | 2.30                     | 0.53              |
| 4:3:185:LEU:HD23 | 4:3:306:TYR:OH   | 2.08                     | 0.53              |
| 1:A:95:THR:OG1   | 1:A:769:ALA:CA   | 2.55                     | 0.53              |
| 1:A:355:THR:OG1  | 1:A:437:MET:HE1  | 2.09                     | 0.53              |
| 1:A:493:HIS:ND1  | 1:A:514:ASP:OD2  | 2.41                     | 0.53              |
| 1:A:579:PHE:CD2  | 1:A:592:ILE:HD11 | 2.39                     | 0.53              |
| 1:A:640:LYS:C    | 1:A:645:SER:HG   | 2.13                     | 0.53              |
| 1:A:836:PHE:CD2  | 2:B:160:GLY:C    | 2.87                     | 0.53              |
| 2:E:129:THR:O    | 2:E:133:ILE:HG13 | 2.09                     | 0.53              |
| 3:F:92:ARG:HA    | 3:F:139:TYR:OH   | 2.08                     | 0.53              |
| 1:G:218:LEU:N    | 1:G:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:G:355:THR:OG1  | 1:G:437:MET:HE1  | 2.09                     | 0.53              |
| 1:J:510:TRP:CD2  | 1:J:768:MLY:CH1  | 2.92                     | 0.53              |
| 1:J:529:PRO:HB2  | 4:W:354:GLN:HA   | 1.91                     | 0.53              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:HA2  | 1.66                     | 0.53              |
| 2:K:114:LYS:O    | 2:K:147:ASN:ND2  | 2.41                     | 0.53              |
| 2:K:130:PRO:O    | 2:K:131:GLU:C    | 2.52                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:53:PRO:HB2   | 3:L:55:LYS:HG3   | 1.91                     | 0.53              |
| 1:A:661:MET:O    | 1:A:665:ARG:HG3  | 2.08                     | 0.53              |
| 1:A:739:ASP:CB   | 1:A:742:LYS:CB   | 2.81                     | 0.53              |
| 1:A:798:LEU:HD22 | 3:C:126:LEU:HD11 | 1.90                     | 0.53              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:D:494:HIS:O    | 1:D:498:LEU:HB2  | 2.09                     | 0.53              |
| 2:E:114:LYS:N    | 2:E:146:GLY:O    | 2.40                     | 0.53              |
| 1:G:636:LYS:HB2  | 4:V:334:GLU:OE1  | 2.09                     | 0.53              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:HB2  | 1.91                     | 0.53              |
| 1:J:404:PRO:HG3  | 1:J:417:GLU:HG3  | 1.91                     | 0.53              |
| 2:K:129:THR:O    | 2:K:133:ILE:HG13 | 2.09                     | 0.53              |
| 4:5:185:LEU:HD23 | 4:5:306:TYR:OH   | 2.09                     | 0.53              |
| 4:9:185:LEU:HD23 | 4:9:306:TYR:OH   | 2.08                     | 0.53              |
| 4:X:185:LEU:HD23 | 4:X:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:32:PHE:CD1   | 1:A:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:A:103:LEU:C    | 1:A:103:LEU:HD12 | 2.33                     | 0.53              |
| 1:D:218:LEU:N    | 1:D:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:D:404:PRO:HG3  | 1:D:417:GLU:HG3  | 1.91                     | 0.53              |
| 1:D:493:HIS:ND1  | 1:D:514:ASP:OD2  | 2.41                     | 0.53              |
| 1:D:538:GLU:HG3  | 4:9:352:PHE:CA   | 2.38                     | 0.53              |
| 1:D:642:LYS:CG   | 4:9:22:ALA:CA    | 2.80                     | 0.53              |
| 1:D:732:ILE:H    | 1:D:733:PRO:HD2  | 1.74                     | 0.53              |
| 1:D:815:CYS:O    | 2:E:90:GLY:HA3   | 2.09                     | 0.53              |
| 1:G:634:GLY:N    | 4:V:25:ASP:O     | 2.31                     | 0.53              |
| 1:G:727:LEU:O    | 3:I:113:THR:CB   | 2.57                     | 0.53              |
| 2:H:130:PRO:O    | 2:H:131:GLU:C    | 2.52                     | 0.53              |
| 1:J:418:THR:CB   | 1:J:421:GLU:HG3  | 2.37                     | 0.53              |
| 4:0:201:VAL:CB   | 4:Y:287:ILE:CG1  | 2.87                     | 0.53              |
| 4:V:185:LEU:HD23 | 4:V:306:TYR:OH   | 2.09                     | 0.53              |
| 4:X:324:THR:HB   | 4:Z:247:VAL:N    | 2.22                     | 0.53              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CD1  | 1.05                     | 0.52              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:HD2  | 2.27                     | 0.52              |
| 1:D:556:ASP:HB3  | 4:W:43:VAL:HG12  | 1.91                     | 0.52              |
| 1:G:63:MLY:HG3   | 1:G:64:THR:H     | 1.74                     | 0.52              |
| 1:G:584:TYR:CD1  | 1:G:585:ALA:N    | 2.77                     | 0.52              |
| 1:G:642:LYS:CG   | 4:V:22:ALA:HA    | 2.37                     | 0.52              |
| 1:G:838:ILE:C    | 1:G:840:PRO:HD2  | 2.34                     | 0.52              |
| 1:J:197:ALA:O    | 1:J:201:ALA:HB2  | 2.09                     | 0.52              |
| 1:A:135:TYR:CD2  | 1:A:191:ARG:HG2  | 2.44                     | 0.52              |
| 1:A:277:PHE:CG   | 1:A:278:GLN:N    | 2.76                     | 0.52              |
| 1:A:555:TYR:N    | 4:V:48:GLY:N     | 2.58                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:214:MET:C    | 1:D:340:ILE:CD1  | 2.82                     | 0.52              |
| 1:D:510:TRP:CZ3  | 1:D:711:PHE:HE2  | 2.27                     | 0.52              |
| 1:D:636:LYS:HB2  | 4:9:334:GLU:OE1  | 2.09                     | 0.52              |
| 1:D:732:ILE:H    | 1:D:733:PRO:CD   | 2.22                     | 0.52              |
| 1:D:791:GLN:O    | 1:D:794:CYS:HB2  | 2.08                     | 0.52              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:ND2  | 2.35                     | 0.52              |
| 1:G:510:TRP:CH2  | 1:G:768:MLY:HH11 | 2.39                     | 0.52              |
| 1:G:579:PHE:CD2  | 1:G:592:ILE:HD11 | 2.40                     | 0.52              |
| 1:J:98:HIS:HB3   | 1:J:100:PRO:CD   | 2.25                     | 0.52              |
| 1:J:277:PHE:CG   | 1:J:278:GLN:N    | 2.76                     | 0.52              |
| 1:J:795:ARG:HD3  | 3:L:35:ARG:NH2   | 1.90                     | 0.52              |
| 2:K:114:LYS:HA   | 2:K:147:ASN:HD22 | 1.74                     | 0.52              |
| 3:L:104:GLY:HA2  | 3:L:137:ILE:HD11 | 1.92                     | 0.52              |
| 4:7:180:LEU:HD22 | 4:7:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:V:180:LEU:HD22 | 4:V:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:W:185:LEU:HD23 | 4:W:306:TYR:OH   | 2.08                     | 0.52              |
| 1:A:732:ILE:H    | 1:A:733:PRO:CD   | 2.22                     | 0.52              |
| 3:C:104:GLY:HA2  | 3:C:137:ILE:HD11 | 1.91                     | 0.52              |
| 1:D:418:THR:CB   | 1:D:421:GLU:HG3  | 2.36                     | 0.52              |
| 1:D:725:ARG:HG3  | 1:D:733:PRO:CA   | 2.36                     | 0.52              |
| 1:G:42:HIS:HB3   | 1:G:45:GLN:O     | 2.09                     | 0.52              |
| 1:G:404:PRO:HG3  | 1:G:417:GLU:HG3  | 1.91                     | 0.52              |
| 1:G:629:GLU:CA   | 1:G:643:GLY:C    | 2.73                     | 0.52              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:CD2  | 2.92                     | 0.52              |
| 1:J:220:ASP:O    | 1:J:224:SER:N    | 2.27                     | 0.52              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CD1  | 1.05                     | 0.52              |
| 1:J:797:PHE:CG   | 3:L:149:VAL:CG1  | 2.79                     | 0.52              |
| 4:1:203:THR:HG23 | 4:Z:288:ASP:OD1  | 2.09                     | 0.52              |
| 4:3:180:LEU:HD22 | 4:3:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:3:285:CYS:O    | 4:3:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:Z:185:LEU:HD23 | 4:Z:306:TYR:OH   | 2.09                     | 0.52              |
| 4:Z:285:CYS:O    | 4:Z:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:A:502:GLU:OE1  | 1:A:763:THR:CA   | 2.57                     | 0.52              |
| 1:A:636:LYS:HB2  | 4:8:334:GLU:OE1  | 2.08                     | 0.52              |
| 1:A:838:ILE:C    | 1:A:840:PRO:HD2  | 2.34                     | 0.52              |
| 1:G:530:MET:HG2  | 4:V:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CD1  | 1.04                     | 0.52              |
| 2:H:114:LYS:HA   | 2:H:147:ASN:HD22 | 1.75                     | 0.52              |
| 1:J:135:TYR:CD2  | 1:J:191:ARG:HG2  | 2.44                     | 0.52              |
| 1:J:156:PHE:HD1  | 1:J:195:TYR:CD1  | 2.27                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:530:MET:HG2  | 4:W:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:J:759:ALA:O    | 1:J:766:PHE:N    | 2.32                     | 0.52              |
| 3:L:110:VAL:HG13 | 3:L:114:LEU:HD12 | 1.91                     | 0.52              |
| 4:4:180:LEU:HD22 | 4:4:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:5:285:CYS:O    | 4:5:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:8:180:LEU:HD22 | 4:8:267:ILE:HD11 | 1.91                     | 0.52              |
| 4:9:180:LEU:HD22 | 4:9:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:9:285:CYS:O    | 4:9:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:9:287:ILE:HG22 | 4:W:204:ALA:HB3  | 1.91                     | 0.52              |
| 4:W:285:CYS:O    | 4:W:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:Z:180:LEU:HD22 | 4:Z:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:109:ARG:HD3  | 1:A:117:THR:HB   | 1.92                     | 0.52              |
| 1:A:494:HIS:O    | 1:A:498:LEU:HB2  | 2.09                     | 0.52              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:CD2  | 2.44                     | 0.52              |
| 1:G:109:ARG:HD3  | 1:G:117:THR:HB   | 1.91                     | 0.52              |
| 1:J:41:VAL:HG13  | 1:J:42:HIS:N     | 2.25                     | 0.52              |
| 4:0:205:GLU:OE1  | 4:Y:287:ILE:O    | 2.26                     | 0.52              |
| 4:1:180:LEU:HD22 | 4:1:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:1:185:LEU:HD23 | 4:1:306:TYR:OH   | 2.09                     | 0.52              |
| 4:4:285:CYS:O    | 4:4:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:V:285:CYS:O    | 4:V:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:Y:180:LEU:HD22 | 4:Y:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:63:MLY:HG3   | 1:A:64:THR:H     | 1.75                     | 0.52              |
| 1:A:404:PRO:HG3  | 1:A:417:GLU:HG3  | 1.91                     | 0.52              |
| 1:A:491:PHE:HD1  | 1:A:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:A:556:ASP:HB3  | 4:V:43:VAL:HG12  | 1.91                     | 0.52              |
| 3:C:92:ARG:HA    | 3:C:139:TYR:OH   | 2.08                     | 0.52              |
| 1:D:355:THR:OG1  | 1:D:437:MET:HE1  | 2.09                     | 0.52              |
| 1:D:491:PHE:HD1  | 1:D:671:PHE:CE2  | 2.27                     | 0.52              |
| 2:E:130:PRO:O    | 2:E:131:GLU:C    | 2.52                     | 0.52              |
| 3:F:104:GLY:HA2  | 3:F:137:ILE:HD11 | 1.92                     | 0.52              |
| 1:G:40:VAL:HG13  | 1:G:41:VAL:O     | 2.10                     | 0.52              |
| 1:G:128:PRO:O    | 1:G:129:TYR:HB2  | 2.09                     | 0.52              |
| 1:G:135:TYR:CD2  | 1:G:191:ARG:HG2  | 2.44                     | 0.52              |
| 1:J:42:HIS:HB3   | 1:J:45:GLN:O     | 2.09                     | 0.52              |
| 1:J:214:MET:C    | 1:J:340:ILE:CD1  | 2.82                     | 0.52              |
| 1:J:838:ILE:C    | 1:J:840:PRO:HD2  | 2.34                     | 0.52              |
| 4:0:244:ASP:CG   | 4:Y:325:MET:SD   | 2.89                     | 0.52              |
| 4:1:287:ILE:C    | 4:3:203:THR:HG22 | 2.35                     | 0.52              |
| 4:W:180:LEU:HD22 | 4:W:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:X:180:LEU:HD22 | 4:X:267:ILE:HD11 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:214:MET:C    | 1:A:340:ILE:CD1  | 2.82                     | 0.52              |
| 1:A:788:THR:CG2  | 3:C:42:THR:HG21  | 2.40                     | 0.52              |
| 1:A:797:PHE:CD1  | 3:C:149:VAL:HG12 | 2.19                     | 0.52              |
| 2:B:139:ALA:C    | 2:B:141:PRO:HD3  | 2.33                     | 0.52              |
| 1:D:156:PHE:HD1  | 1:D:195:TYR:CD1  | 2.27                     | 0.52              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:CB   | 2.40                     | 0.52              |
| 3:F:53:PRO:HB2   | 3:F:55:LYS:HG3   | 1.91                     | 0.52              |
| 1:G:41:VAL:HG13  | 1:G:42:HIS:N     | 2.25                     | 0.52              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:G:529:PRO:HB2  | 4:V:354:GLN:HA   | 1.92                     | 0.52              |
| 1:G:728:ASN:HD21 | 3:I:109:HIS:C    | 2.18                     | 0.52              |
| 1:G:751:GLY:H    | 3:I:114:LEU:CD1  | 2.23                     | 0.52              |
| 4:0:285:CYS:O    | 4:0:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:5:180:LEU:HD22 | 4:5:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:218:LEU:CD2  | 1:A:222:ILE:CG1  | 2.85                     | 0.52              |
| 1:A:725:ARG:O    | 1:A:729:ALA:HA   | 2.10                     | 0.52              |
| 1:A:795:ARG:CD   | 3:C:43:ASN:OD1   | 2.58                     | 0.52              |
| 3:C:53:PRO:HB2   | 3:C:55:LYS:HG3   | 1.91                     | 0.52              |
| 1:D:733:PRO:O    | 1:D:737:PHE:CE1  | 2.53                     | 0.52              |
| 2:E:139:ALA:C    | 2:E:141:PRO:HD3  | 2.33                     | 0.52              |
| 1:G:156:PHE:HD1  | 1:G:195:TYR:CD1  | 2.27                     | 0.52              |
| 1:G:197:ALA:O    | 1:G:201:ALA:HB2  | 2.09                     | 0.52              |
| 1:G:491:PHE:HD1  | 1:G:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:G:494:HIS:O    | 1:G:498:LEU:HB2  | 2.09                     | 0.52              |
| 3:I:110:VAL:HG13 | 3:I:114:LEU:HD12 | 1.91                     | 0.52              |
| 1:J:40:VAL:HG13  | 1:J:41:VAL:O     | 2.10                     | 0.52              |
| 4:7:287:ILE:HG22 | 4:9:204:ALA:HB3  | 1.91                     | 0.52              |
| 4:X:285:CYS:O    | 4:X:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:40:VAL:HG13  | 1:A:41:VAL:O     | 2.10                     | 0.52              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:HB2  | 1.91                     | 0.52              |
| 3:C:52:ASN:HB2   | 3:C:53:PRO:CD    | 2.28                     | 0.52              |
| 1:D:40:VAL:HG13  | 1:D:41:VAL:O     | 2.10                     | 0.52              |
| 1:D:63:MLY:HG3   | 1:D:64:THR:H     | 1.75                     | 0.52              |
| 1:D:109:ARG:HD3  | 1:D:117:THR:HB   | 1.92                     | 0.52              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:CD1  | 2.93                     | 0.52              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:HB2  | 1.91                     | 0.52              |
| 1:D:818:TYR:HB3  | 2:E:90:GLY:N     | 2.25                     | 0.52              |
| 3:F:110:VAL:HG13 | 3:F:114:LEU:HD12 | 1.91                     | 0.52              |
| 1:G:800:ARG:CZ   | 3:I:149:VAL:HG22 | 2.29                     | 0.52              |
| 1:J:154:HIS:CE1  | 1:J:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:J:221:GLN:HB2  | 1:J:449:LEU:HD11 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:232:PHE:CE1  | 1:J:287:ILE:HD13 | 2.44                     | 0.52              |
| 1:J:355:THR:OG1  | 1:J:437:MET:HE1  | 2.09                     | 0.52              |
| 1:J:795:ARG:CB   | 3:L:35:ARG:NH2   | 2.73                     | 0.52              |
| 4:0:180:LEU:HD22 | 4:0:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:2:180:LEU:HD22 | 4:2:267:ILE:HD11 | 1.91                     | 0.52              |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:A:292:MET:HE2  | 1:A:309:PRO:HD3  | 1.92                     | 0.52              |
| 1:A:408:VAL:CG1  | 4:8:332:PRO:HB3  | 2.40                     | 0.52              |
| 1:A:530:MET:HG2  | 4:8:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:A:642:LYS:CG   | 4:8:22:ALA:HA    | 2.38                     | 0.52              |
| 1:A:757:GLN:HG3  | 1:A:771:LEU:CD1  | 2.28                     | 0.52              |
| 2:B:114:LYS:O    | 2:B:147:ASN:ND2  | 2.41                     | 0.52              |
| 2:B:129:THR:O    | 2:B:133:ILE:HG13 | 2.09                     | 0.52              |
| 1:D:41:VAL:HG21  | 1:D:76:GLN:HG3   | 1.92                     | 0.52              |
| 1:D:634:GLY:N    | 4:9:25:ASP:O     | 2.31                     | 0.52              |
| 1:D:830:PRO:CG   | 2:E:67:MET:HE3   | 1.97                     | 0.52              |
| 1:G:481:ASN:N    | 1:G:481:ASN:ND2  | 2.51                     | 0.52              |
| 1:G:819:ASN:CG   | 2:H:90:GLY:C     | 2.75                     | 0.52              |
| 1:J:128:PRO:O    | 1:J:129:TYR:HB2  | 2.10                     | 0.52              |
| 1:J:491:PHE:HD1  | 1:J:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:J:510:TRP:CE2  | 1:J:768:MLY:HH13 | 2.45                     | 0.52              |
| 1:J:636:LYS:HB2  | 4:W:334:GLU:OE1  | 2.09                     | 0.52              |
| 2:K:139:ALA:C    | 2:K:141:PRO:HD3  | 2.33                     | 0.52              |
| 4:0:243:PRO:CB   | 4:Y:291:LYS:HD2  | 2.37                     | 0.52              |
| 4:1:285:CYS:O    | 4:1:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:2:285:CYS:O    | 4:2:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:8:287:ILE:HG22 | 4:V:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:CD   | 2.23                     | 0.51              |
| 1:A:506:GLU:OE1  | 1:A:761:GLY:N    | 2.40                     | 0.51              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:CB   | 2.39                     | 0.51              |
| 1:A:578:HIS:O    | 1:A:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HG   | 1.90                     | 0.51              |
| 1:D:221:GLN:HB2  | 1:D:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:D:555:TYR:N    | 4:W:48:GLY:N     | 2.58                     | 0.51              |
| 2:E:114:LYS:HA   | 2:E:147:ASN:HD22 | 1.74                     | 0.51              |
| 1:G:798:LEU:HD21 | 3:I:126:LEU:HG   | 1.92                     | 0.51              |
| 1:J:134:VAL:C    | 1:J:136:ASN:H    | 2.16                     | 0.51              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:CD   | 2.23                     | 0.51              |
| 1:J:494:HIS:O    | 1:J:498:LEU:HB2  | 2.09                     | 0.51              |
| 3:L:100:GLY:O    | 3:L:138:ASN:HA   | 2.10                     | 0.51              |
| 1:A:232:PHE:CE1  | 1:A:287:ILE:HD13 | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:100:GLY:O    | 3:F:138:ASN:HA   | 2.10                     | 0.51              |
| 1:G:221:GLN:HB2  | 1:G:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:J:63:MLY:HG3   | 1:J:64:THR:H     | 1.75                     | 0.51              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:J:289:TYR:OH   | 1:J:315:VAL:O    | 2.27                     | 0.51              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:CB   | 2.40                     | 0.51              |
| 1:J:834:LEU:HD11 | 2:K:54:MET:HG3   | 1.92                     | 0.51              |
| 4:7:285:CYS:O    | 4:7:290:ARG:NH1  | 2.43                     | 0.51              |
| 4:Y:285:CYS:O    | 4:Y:290:ARG:NH1  | 2.43                     | 0.51              |
| 1:A:221:GLN:HB2  | 1:A:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:592:ILE:O    | 1:A:592:ILE:HG22 | 2.10                     | 0.51              |
| 1:A:817:GLN:CG   | 2:B:127:ARG:HG2  | 2.40                     | 0.51              |
| 1:D:508:ILE:HG23 | 1:D:766:PHE:CD1  | 2.46                     | 0.51              |
| 1:D:767:PHE:C    | 1:D:771:LEU:HD11 | 2.35                     | 0.51              |
| 1:G:232:PHE:CE1  | 1:G:287:ILE:HD13 | 2.45                     | 0.51              |
| 1:G:546:THR:CG2  | 1:G:548:THR:HB   | 2.41                     | 0.51              |
| 2:H:129:THR:O    | 2:H:133:ILE:HG13 | 2.09                     | 0.51              |
| 1:J:248:MLY:N    | 1:J:463:ASP:O    | 2.44                     | 0.51              |
| 1:A:41:VAL:HG13  | 1:A:42:HIS:N     | 2.25                     | 0.51              |
| 1:A:504:MLY:HB2  | 1:A:762:HIS:NE2  | 2.25                     | 0.51              |
| 1:A:546:THR:CG2  | 1:A:548:THR:HB   | 2.41                     | 0.51              |
| 2:B:114:LYS:HA   | 2:B:147:ASN:HD22 | 1.75                     | 0.51              |
| 1:D:232:PHE:CE1  | 1:D:287:ILE:HD13 | 2.45                     | 0.51              |
| 1:D:248:MLY:N    | 1:D:463:ASP:O    | 2.44                     | 0.51              |
| 1:D:481:ASN:N    | 1:D:481:ASN:ND2  | 2.51                     | 0.51              |
| 1:D:643:GLY:N    | 4:9:23:GLY:C     | 2.55                     | 0.51              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:G:214:MET:C    | 1:G:340:ILE:CD1  | 2.82                     | 0.51              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:CB   | 2.40                     | 0.51              |
| 3:I:100:GLY:O    | 3:I:138:ASN:HA   | 2.11                     | 0.51              |
| 3:I:104:GLY:HA2  | 3:I:137:ILE:HD11 | 1.92                     | 0.51              |
| 1:J:212:GLY:O    | 1:J:213:LYS:HB2  | 2.10                     | 0.51              |
| 1:J:640:LYS:CA   | 1:J:645:SER:OG   | 2.58                     | 0.51              |
| 1:J:820:VAL:CG1  | 2:K:136:MET:CE   | 2.81                     | 0.51              |
| 4:8:285:CYS:O    | 4:8:290:ARG:NH1  | 2.43                     | 0.51              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:A:400:ALA:HB1  | 1:A:606:THR:HG22 | 1.92                     | 0.51              |
| 1:A:836:PHE:CB   | 2:B:161:GLU:CD   | 2.53                     | 0.51              |
| 1:D:197:ALA:O    | 1:D:201:ALA:HB2  | 2.10                     | 0.51              |
| 1:D:809:ARG:NH1  | 2:E:124:GLY:C    | 2.68                     | 0.51              |
| 1:D:813:ILE:CB   | 2:E:127:ARG:NH1  | 2.74                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:121:LEU:HA   | 2:E:128:PHE:CD2  | 2.46                     | 0.51              |
| 1:G:41:VAL:HG21  | 1:G:76:GLN:HG3   | 1.92                     | 0.51              |
| 1:G:292:MET:HE2  | 1:G:309:PRO:HD3  | 1.93                     | 0.51              |
| 1:G:411:GLU:H    | 4:V:333:PRO:CG   | 2.24                     | 0.51              |
| 1:G:418:THR:O    | 1:G:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:G:578:HIS:O    | 1:G:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:G:675:ILE:CG2  | 1:G:676:ILE:N    | 2.74                     | 0.51              |
| 1:J:418:THR:O    | 1:J:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:J:553:MLY:CE   | 4:Y:45:VAL:CG1   | 2.78                     | 0.51              |
| 1:J:687:GLU:O    | 1:J:691:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:38:VAL:CG1   | 1:A:39:PHE:N     | 2.74                     | 0.51              |
| 1:A:248:MLY:N    | 1:A:463:ASP:O    | 2.44                     | 0.51              |
| 1:D:411:GLU:H    | 4:9:333:PRO:CG   | 2.24                     | 0.51              |
| 1:D:592:ILE:O    | 1:D:592:ILE:HG22 | 2.10                     | 0.51              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:HH21 | 2.37                     | 0.51              |
| 1:D:769:ALA:CB   | 1:D:770:GLY:N    | 2.73                     | 0.51              |
| 2:E:112:ILE:HG23 | 2:E:147:ASN:HB3  | 1.93                     | 0.51              |
| 1:G:248:MLY:N    | 1:G:463:ASP:O    | 2.44                     | 0.51              |
| 1:G:725:ARG:O    | 1:G:729:ALA:HA   | 2.10                     | 0.51              |
| 1:J:202:SER:HB2  | 1:J:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:J:592:ILE:HG22 | 1:J:592:ILE:O    | 2.10                     | 0.51              |
| 1:J:629:GLU:HG2  | 1:J:643:GLY:C    | 2.35                     | 0.51              |
| 1:J:768:MLY:HH21 | 1:J:772:LEU:HD13 | 1.93                     | 0.51              |
| 1:J:768:MLY:CE   | 1:J:772:LEU:CD2  | 2.88                     | 0.51              |
| 1:A:134:VAL:C    | 1:A:136:ASN:H    | 2.16                     | 0.51              |
| 1:A:418:THR:O    | 1:A:422:VAL:HG23 | 2.11                     | 0.51              |
| 3:C:110:VAL:HG13 | 3:C:114:LEU:HD12 | 1.91                     | 0.51              |
| 1:D:237:THR:O    | 1:D:240:ASN:O    | 2.29                     | 0.51              |
| 1:D:553:MLY:CE   | 4:W:45:VAL:CA    | 2.49                     | 0.51              |
| 1:D:767:PHE:C    | 1:D:771:LEU:CD1  | 2.84                     | 0.51              |
| 1:G:267:THR:HG21 | 1:G:438:PHE:HE2  | 1.76                     | 0.51              |
| 1:G:311:ASP:HB2  | 1:G:312:TYR:CE1  | 2.46                     | 0.51              |
| 1:G:400:ALA:HB1  | 1:G:606:THR:HG22 | 1.93                     | 0.51              |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:HD21  | 1.93                     | 0.51              |
| 2:H:114:LYS:N    | 2:H:146:GLY:O    | 2.40                     | 0.51              |
| 1:J:742:LYS:O    | 1:J:745:GLU:HB2  | 2.10                     | 0.51              |
| 2:K:114:LYS:N    | 2:K:146:GLY:O    | 2.40                     | 0.51              |
| 4:1:45:VAL:CG2   | 4:Z:148:THR:OG1  | 2.59                     | 0.51              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:HG23 | 1.73                     | 0.51              |
| 1:D:41:VAL:HG13  | 1:D:42:HIS:N     | 2.25                     | 0.51              |
| 1:D:202:SER:HB2  | 1:D:207:LYS:NZ   | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:530:MET:HG2  | 4:9:354:GLN:HB2  | 0.57                     | 0.51              |
| 1:D:629:GLU:HG2  | 1:D:643:GLY:C    | 2.35                     | 0.51              |
| 1:D:632:GLY:HA3  | 1:D:643:GLY:N    | 2.17                     | 0.51              |
| 1:D:822:SER:OG   | 2:E:88:LEU:HA    | 2.11                     | 0.51              |
| 1:G:38:VAL:CG1   | 1:G:39:PHE:N     | 2.74                     | 0.51              |
| 1:G:212:GLY:O    | 1:G:213:LYS:HB2  | 2.10                     | 0.51              |
| 1:J:41:VAL:HG21  | 1:J:76:GLN:HG3   | 1.93                     | 0.51              |
| 1:J:408:VAL:CG1  | 4:W:332:PRO:HB3  | 2.40                     | 0.51              |
| 1:J:553:MLY:CE   | 4:Y:45:VAL:HG11  | 2.32                     | 0.51              |
| 1:J:792:ALA:CB   | 3:L:40:ASN:CB    | 2.51                     | 0.51              |
| 1:A:629:GLU:CA   | 1:A:643:GLY:C    | 2.73                     | 0.51              |
| 1:A:640:LYS:CA   | 1:A:645:SER:OG   | 2.58                     | 0.51              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CD2  | 2.86                     | 0.51              |
| 1:D:218:LEU:N    | 1:D:221:GLN:CG   | 2.74                     | 0.51              |
| 1:D:400:ALA:HB1  | 1:D:606:THR:HG22 | 1.92                     | 0.51              |
| 1:D:818:TYR:CG   | 2:E:89:LYS:CB    | 2.93                     | 0.51              |
| 1:G:218:LEU:N    | 1:G:221:GLN:CG   | 2.74                     | 0.51              |
| 1:G:730:SER:HB2  | 3:I:109:HIS:CE1  | 2.45                     | 0.51              |
| 1:J:578:HIS:O    | 1:J:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:J:733:PRO:O    | 1:J:737:PHE:CE1  | 2.53                     | 0.51              |
| 1:A:128:PRO:O    | 1:A:129:TYR:HB2  | 2.09                     | 0.51              |
| 1:A:197:ALA:O    | 1:A:201:ALA:HB2  | 2.10                     | 0.51              |
| 1:A:311:ASP:HB2  | 1:A:312:TYR:CE1  | 2.46                     | 0.51              |
| 1:A:642:LYS:HA   | 4:8:21:PHE:C     | 2.36                     | 0.51              |
| 1:A:675:ILE:CG2  | 1:A:676:ILE:N    | 2.74                     | 0.51              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:CD   | 2.23                     | 0.51              |
| 1:D:578:HIS:O    | 1:D:579:PHE:HB3  | 2.10                     | 0.51              |
| 1:D:687:GLU:O    | 1:D:691:VAL:HG23 | 2.11                     | 0.51              |
| 1:D:725:ARG:O    | 1:D:729:ALA:HA   | 2.10                     | 0.51              |
| 1:J:632:GLY:HA3  | 1:J:643:GLY:N    | 2.17                     | 0.51              |
| 1:J:642:LYS:HA   | 4:W:21:PHE:C     | 2.36                     | 0.51              |
| 1:J:649:VAL:HA   | 1:J:649:VAL:HG23 | 1.83                     | 0.51              |
| 1:J:707:CYS:C    | 1:J:714:ARG:NH2  | 2.69                     | 0.51              |
| 1:J:818:TYR:CD1  | 2:K:127:ARG:NH1  | 2.79                     | 0.51              |
| 4:X:324:THR:HG21 | 4:Z:247:VAL:HG23 | 1.89                     | 0.51              |
| 1:A:687:GLU:O    | 1:A:691:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:38:VAL:CG1   | 1:D:39:PHE:N     | 2.74                     | 0.50              |
| 1:D:128:PRO:O    | 1:D:129:TYR:HB2  | 2.09                     | 0.50              |
| 1:D:212:GLY:O    | 1:D:213:LYS:HB2  | 2.11                     | 0.50              |
| 1:D:642:LYS:HA   | 4:9:21:PHE:C     | 2.36                     | 0.50              |
| 1:D:742:LYS:O    | 1:D:745:GLU:HB2  | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:815:CYS:O    | 2:E:90:GLY:C     | 2.54                     | 0.50              |
| 1:G:642:LYS:HA   | 4:V:21:PHE:C     | 2.36                     | 0.50              |
| 1:G:732:ILE:H    | 1:G:733:PRO:CD   | 2.23                     | 0.50              |
| 1:J:218:LEU:N    | 1:J:221:GLN:CG   | 2.74                     | 0.50              |
| 1:J:237:THR:O    | 1:J:240:ASN:O    | 2.29                     | 0.50              |
| 1:J:346:ASP:O    | 1:J:349:THR:HB   | 2.11                     | 0.50              |
| 4:1:202:THR:C    | 4:Z:287:ILE:CG2  | 2.79                     | 0.50              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:CA   | 2.21                     | 0.50              |
| 1:D:546:THR:CG2  | 1:D:548:THR:HB   | 2.41                     | 0.50              |
| 1:G:89:GLU:CD    | 1:G:153:PRO:HD2  | 2.36                     | 0.50              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:CD   | 2.23                     | 0.50              |
| 1:G:202:SER:HB2  | 1:G:207:LYS:NZ   | 2.26                     | 0.50              |
| 1:G:429:LEU:O    | 1:G:433:VAL:HG23 | 2.12                     | 0.50              |
| 1:G:538:GLU:OE1  | 4:V:351:THR:HB   | 2.11                     | 0.50              |
| 1:G:557:GLU:CB   | 4:X:47:MET:C     | 2.50                     | 0.50              |
| 1:G:793:ARG:HH11 | 3:I:40:ASN:HD21  | 1.58                     | 0.50              |
| 1:J:109:ARG:HD3  | 1:J:117:THR:HB   | 1.92                     | 0.50              |
| 1:J:411:GLU:H    | 4:W:333:PRO:CG   | 2.24                     | 0.50              |
| 1:J:448:GLN:C    | 1:J:450:ASP:H    | 2.19                     | 0.50              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:CG   | 2.25                     | 0.50              |
| 1:J:732:ILE:H    | 1:J:733:PRO:CD   | 2.23                     | 0.50              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:CD   | 2.40                     | 0.50              |
| 1:A:41:VAL:HG21  | 1:A:76:GLN:HG3   | 1.92                     | 0.50              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:CB   | 2.89                     | 0.50              |
| 1:A:267:THR:HG21 | 1:A:438:PHE:HE2  | 1.76                     | 0.50              |
| 1:A:629:GLU:CB   | 1:A:645:SER:N    | 2.74                     | 0.50              |
| 1:A:814:PHE:CA   | 2:B:127:ARG:NH2  | 2.68                     | 0.50              |
| 3:C:100:GLY:O    | 3:C:138:ASN:HA   | 2.11                     | 0.50              |
| 1:G:149:GLN:OE1  | 1:G:762:HIS:HB3  | 2.11                     | 0.50              |
| 1:G:237:THR:O    | 1:G:240:ASN:O    | 2.29                     | 0.50              |
| 1:G:448:GLN:C    | 1:G:450:ASP:H    | 2.19                     | 0.50              |
| 1:G:797:PHE:CD2  | 3:I:126:LEU:CD2  | 2.93                     | 0.50              |
| 1:J:278:GLN:HG3  | 1:J:318:GLY:H    | 1.75                     | 0.50              |
| 1:J:292:MET:HE2  | 1:J:309:PRO:HD3  | 1.93                     | 0.50              |
| 1:J:629:GLU:CB   | 1:J:645:SER:N    | 2.73                     | 0.50              |
| 1:J:733:PRO:CA   | 1:J:737:PHE:CE1  | 2.94                     | 0.50              |
| 4:W:285:CYS:O    | 4:Y:202:THR:HG22 | 2.11                     | 0.50              |
| 1:A:218:LEU:N    | 1:A:221:GLN:CG   | 2.74                     | 0.50              |
| 1:A:629:GLU:HG2  | 1:A:643:GLY:C    | 2.35                     | 0.50              |
| 1:A:759:ALA:O    | 1:A:766:PHE:N    | 2.32                     | 0.50              |
| 1:D:311:ASP:HB2  | 1:D:312:TYR:CE1  | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:346:ASP:O    | 1:D:349:THR:HB   | 2.11                     | 0.50              |
| 1:D:418:THR:O    | 1:D:422:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:815:CYS:O    | 2:E:90:GLY:CA    | 2.60                     | 0.50              |
| 1:G:742:LYS:O    | 1:G:745:GLU:HB2  | 2.10                     | 0.50              |
| 1:J:154:HIS:CD2  | 1:J:155:ILE:H    | 2.30                     | 0.50              |
| 1:J:311:ASP:HB2  | 1:J:312:TYR:CE1  | 2.46                     | 0.50              |
| 1:J:400:ALA:HB1  | 1:J:606:THR:HG22 | 1.93                     | 0.50              |
| 1:J:725:ARG:O    | 1:J:729:ALA:HA   | 2.10                     | 0.50              |
| 4:0:287:ILE:HB   | 4:2:203:THR:HB   | 1.92                     | 0.50              |
| 4:8:325:MET:HE2  | 4:V:244:ASP:HB3  | 1.94                     | 0.50              |
| 1:A:169:ASP:OD1  | 1:A:169:ASP:N    | 2.44                     | 0.50              |
| 1:D:429:LEU:O    | 1:D:433:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:715:VAL:O    | 1:D:764:MLY:HB3  | 2.12                     | 0.50              |
| 2:E:162:ASP:HB2  | 2:K:20:ASP:HA    | 1.93                     | 0.50              |
| 1:G:592:ILE:HG22 | 1:G:592:ILE:O    | 2.10                     | 0.50              |
| 1:G:640:LYS:CA   | 1:G:645:SER:OG   | 2.58                     | 0.50              |
| 1:G:687:GLU:O    | 1:G:691:VAL:HG23 | 2.11                     | 0.50              |
| 2:K:112:ILE:HG23 | 2:K:147:ASN:HB3  | 1.92                     | 0.50              |
| 1:A:202:SER:HB2  | 1:A:207:LYS:NZ   | 2.26                     | 0.50              |
| 1:A:448:GLN:C    | 1:A:450:ASP:H    | 2.19                     | 0.50              |
| 1:A:601:ASP:N    | 1:A:602:PRO:CD   | 2.75                     | 0.50              |
| 1:A:715:VAL:O    | 1:A:764:MLY:HB3  | 2.12                     | 0.50              |
| 1:A:732:ILE:O    | 1:A:736:GLN:HG3  | 2.11                     | 0.50              |
| 1:A:742:LYS:O    | 1:A:745:GLU:HB2  | 2.10                     | 0.50              |
| 1:A:786:ILE:HD13 | 3:C:90:GLY:HA2   | 1.92                     | 0.50              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:HD2  | 1.24                     | 0.50              |
| 1:D:154:HIS:CD2  | 1:D:155:ILE:H    | 2.30                     | 0.50              |
| 1:D:408:VAL:CG1  | 4:9:332:PRO:HB3  | 2.40                     | 0.50              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:CG   | 2.25                     | 0.50              |
| 1:G:291:ILE:HA   | 1:G:331:LEU:CD1  | 2.39                     | 0.50              |
| 1:G:540:CYS:C    | 4:V:349:LEU:HD21 | 2.36                     | 0.50              |
| 1:G:715:VAL:O    | 1:G:764:MLY:HB3  | 2.12                     | 0.50              |
| 1:J:89:GLU:CD    | 1:J:153:PRO:HD2  | 2.36                     | 0.50              |
| 1:J:795:ARG:NE   | 3:L:35:ARG:HH12  | 2.09                     | 0.50              |
| 1:J:839:MLY:HB2  | 1:J:840:PRO:HD3  | 1.94                     | 0.50              |
| 4:0:287:ILE:HG21 | 4:2:204:ALA:H    | 1.76                     | 0.50              |
| 4:X:287:ILE:CG2  | 4:Z:201:VAL:CG2  | 2.85                     | 0.50              |
| 1:A:212:GLY:O    | 1:A:213:LYS:HB2  | 2.10                     | 0.50              |
| 1:A:237:THR:O    | 1:A:240:ASN:O    | 2.29                     | 0.50              |
| 1:A:471:ASP:HB3  | 1:A:573:GLY:O    | 2.12                     | 0.50              |
| 1:A:733:PRO:CA   | 1:A:737:PHE:CE1  | 2.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:822:SER:HB3  | 2:B:88:LEU:CD2   | 2.41                     | 0.50              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:ND2  | 2.35                     | 0.50              |
| 1:D:109:ARG:O    | 1:D:114:MET:N    | 2.37                     | 0.50              |
| 1:D:278:GLN:HG3  | 1:D:318:GLY:H    | 1.75                     | 0.50              |
| 1:D:292:MET:HE2  | 1:D:309:PRO:HD3  | 1.93                     | 0.50              |
| 1:D:640:LYS:CA   | 1:D:645:SER:OG   | 2.58                     | 0.50              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HD12 | 0.95                     | 0.50              |
| 1:G:218:LEU:CD2  | 1:G:222:ILE:CG1  | 2.85                     | 0.50              |
| 1:G:346:ASP:O    | 1:G:349:THR:HB   | 2.11                     | 0.50              |
| 1:J:169:ASP:N    | 1:J:169:ASP:OD1  | 2.44                     | 0.50              |
| 1:J:429:LEU:O    | 1:J:433:VAL:HG23 | 2.12                     | 0.50              |
| 1:J:546:THR:CG2  | 1:J:548:THR:HB   | 2.41                     | 0.50              |
| 1:J:732:ILE:O    | 1:J:736:GLN:HG3  | 2.12                     | 0.50              |
| 2:K:117:LEU:HG   | 2:K:147:ASN:HB3  | 1.93                     | 0.50              |
| 4:O:287:ILE:CB   | 4:2:203:THR:CB   | 2.85                     | 0.50              |
| 4:8:70:PRO:HG3   | 4:8:81:ASP:HB3   | 1.94                     | 0.50              |
| 4:W:318:THR:HA   | 4:W:327:ILE:HG12 | 1.94                     | 0.50              |
| 1:A:553:MLY:HG3  | 4:V:44:MET:O     | 2.07                     | 0.50              |
| 1:A:576:GLU:CG   | 1:A:577:ALA:N    | 2.43                     | 0.50              |
| 1:D:471:ASP:HB3  | 1:D:573:GLY:O    | 2.12                     | 0.50              |
| 1:D:831:TRP:CZ3  | 2:E:50:THR:CB    | 2.95                     | 0.50              |
| 1:G:471:ASP:HB3  | 1:G:573:GLY:O    | 2.12                     | 0.50              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CD2  | 2.87                     | 0.50              |
| 1:G:733:PRO:CA   | 1:G:737:PHE:CE1  | 2.95                     | 0.50              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:HD23 | 2.45                     | 0.50              |
| 1:G:836:PHE:CE2  | 2:H:160:GLY:HA3  | 2.46                     | 0.50              |
| 1:J:817:GLN:HG3  | 2:K:128:PHE:CZ   | 2.47                     | 0.50              |
| 4:1:288:ASP:CB   | 4:3:203:THR:CG2  | 2.87                     | 0.50              |
| 4:4:70:PRO:HG3   | 4:4:81:ASP:HB3   | 1.93                     | 0.50              |
| 4:V:318:THR:HA   | 4:V:327:ILE:HG12 | 1.94                     | 0.50              |
| 1:A:839:MLY:HD3  | 2:B:159:HIS:CB   | 2.40                     | 0.50              |
| 1:D:89:GLU:CD    | 1:D:153:PRO:HD2  | 2.36                     | 0.50              |
| 1:D:733:PRO:CA   | 1:D:737:PHE:CE1  | 2.94                     | 0.50              |
| 1:G:800:ARG:NH1  | 3:I:149:VAL:CG2  | 2.24                     | 0.50              |
| 1:G:839:MLY:N    | 1:G:840:PRO:CD   | 2.75                     | 0.50              |
| 2:H:137:TRP:CA   | 2:H:145:ALA:CB   | 2.82                     | 0.50              |
| 1:J:38:VAL:CG1   | 1:J:39:PHE:N     | 2.74                     | 0.50              |
| 1:J:192:VAL:O    | 1:J:195:TYR:HB3  | 2.12                     | 0.50              |
| 1:J:214:MET:HA   | 1:J:340:ILE:CD1  | 2.41                     | 0.50              |
| 1:J:251:ARG:O    | 1:J:263:ALA:HA   | 2.12                     | 0.50              |
| 4:1:324:THR:CB   | 4:3:244:ASP:CA   | 2.82                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:287:ILE:CB   | 4:5:204:ALA:H    | 2.24                     | 0.50              |
| 4:9:318:THR:HA   | 4:9:327:ILE:HG12 | 1.94                     | 0.50              |
| 1:A:154:HIS:CD2  | 1:A:155:ILE:H    | 2.30                     | 0.49              |
| 1:A:411:GLU:H    | 4:8:333:PRO:CG   | 2.24                     | 0.49              |
| 1:A:547:ASP:O    | 1:A:550:PHE:HB3  | 2.12                     | 0.49              |
| 1:D:291:ILE:HA   | 1:D:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:D:448:GLN:C    | 1:D:450:ASP:H    | 2.19                     | 0.49              |
| 1:D:507:GLY:C    | 1:D:761:GLY:HA3  | 2.35                     | 0.49              |
| 1:D:538:GLU:OE1  | 4:9:351:THR:HB   | 2.12                     | 0.49              |
| 1:G:93:MET:CE    | 1:G:764:MLY:CG   | 2.89                     | 0.49              |
| 1:G:278:GLN:HG3  | 1:G:318:GLY:H    | 1.75                     | 0.49              |
| 1:G:632:GLY:HA3  | 1:G:643:GLY:N    | 2.17                     | 0.49              |
| 1:G:756:THR:O    | 1:G:758:TYR:N    | 2.45                     | 0.49              |
| 1:G:757:GLN:HE22 | 1:G:772:LEU:CD2  | 2.25                     | 0.49              |
| 1:J:538:GLU:OE1  | 4:W:351:THR:HB   | 2.12                     | 0.49              |
| 1:J:642:LYS:CG   | 4:W:22:ALA:HA    | 2.37                     | 0.49              |
| 1:J:715:VAL:O    | 1:J:764:MLY:HB3  | 2.12                     | 0.49              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:CA   | 2.41                     | 0.49              |
| 4:5:318:THR:HA   | 4:5:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:7:318:THR:HA   | 4:7:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:8:318:THR:HA   | 4:8:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:X:318:THR:HA   | 4:X:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:278:GLN:HG3  | 1:A:318:GLY:H    | 1.75                     | 0.49              |
| 1:A:505:MLY:HB2  | 1:A:761:GLY:CA   | 2.42                     | 0.49              |
| 1:A:715:VAL:HG12 | 1:A:716:LEU:O    | 2.13                     | 0.49              |
| 1:A:756:THR:O    | 1:A:758:TYR:N    | 2.46                     | 0.49              |
| 1:A:839:MLY:HB2  | 1:A:840:PRO:HD3  | 1.94                     | 0.49              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:HG12 | 1.94                     | 0.49              |
| 1:D:169:ASP:OD1  | 1:D:169:ASP:N    | 2.44                     | 0.49              |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:CD   | 2.37                     | 0.49              |
| 2:E:162:ASP:HB3  | 2:K:20:ASP:CB    | 2.36                     | 0.49              |
| 1:G:553:MLY:O    | 4:X:46:GLY:HA3   | 2.12                     | 0.49              |
| 2:H:112:ILE:HG23 | 2:H:147:ASN:HB3  | 1.93                     | 0.49              |
| 1:J:601:ASP:N    | 1:J:602:PRO:CD   | 2.75                     | 0.49              |
| 1:J:739:ASP:OD1  | 1:J:740:SER:N    | 2.45                     | 0.49              |
| 1:J:795:ARG:HH22 | 3:L:116:GLU:CD   | 2.20                     | 0.49              |
| 1:J:823:PHE:HE1  | 2:K:156:VAL:O    | 1.88                     | 0.49              |
| 4:0:318:THR:HA   | 4:0:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:V:322:PRO:HB3  | 4:X:246:GLN:HG2  | 1.92                     | 0.49              |
| 4:Y:318:THR:HA   | 4:Y:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:20:SER:HB3   | 1:A:23:GLU:OE1   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:112:ILE:HG23 | 2:B:147:ASN:HB3  | 1.93                     | 0.49              |
| 2:B:114:LYS:N    | 2:B:146:GLY:O    | 2.40                     | 0.49              |
| 1:D:192:VAL:O    | 1:D:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:D:251:ARG:O    | 1:D:263:ALA:HA   | 2.12                     | 0.49              |
| 1:D:601:ASP:N    | 1:D:602:PRO:CD   | 2.75                     | 0.49              |
| 1:D:732:ILE:O    | 1:D:736:GLN:HG3  | 2.11                     | 0.49              |
| 2:E:140:PHE:HB3  | 2:E:144:VAL:HG12 | 1.94                     | 0.49              |
| 1:G:169:ASP:N    | 1:G:169:ASP:OD1  | 2.44                     | 0.49              |
| 1:G:289:TYR:OH   | 1:G:315:VAL:O    | 2.27                     | 0.49              |
| 1:G:642:LYS:CB   | 4:V:24:ASP:O     | 2.60                     | 0.49              |
| 1:G:728:ASN:ND2  | 3:I:109:HIS:C    | 2.70                     | 0.49              |
| 1:G:747:LEU:C    | 1:G:749:GLY:H    | 2.20                     | 0.49              |
| 2:H:93:PRO:O     | 2:H:97:ILE:HG13  | 2.12                     | 0.49              |
| 1:J:310:TYR:CE2  | 1:J:320:ILE:CD1  | 2.94                     | 0.49              |
| 1:J:543:PRO:CD   | 4:W:146:GLY:O    | 2.61                     | 0.49              |
| 1:J:595:TRP:N    | 1:J:595:TRP:CD1  | 2.80                     | 0.49              |
| 1:J:756:THR:O    | 1:J:758:TYR:N    | 2.45                     | 0.49              |
| 2:K:114:LYS:HG3  | 2:K:137:TRP:CZ2  | 2.48                     | 0.49              |
| 4:3:318:THR:HA   | 4:3:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:Z:318:THR:HA   | 4:Z:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:291:ILE:HA   | 1:A:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:D:173:GLN:OE1  | 1:D:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:HB3  | 1.94                     | 0.49              |
| 1:D:715:VAL:HG12 | 1:D:716:LEU:O    | 2.12                     | 0.49              |
| 1:D:725:ARG:NE   | 1:D:733:PRO:CB   | 1.95                     | 0.49              |
| 2:E:93:PRO:O     | 2:E:97:ILE:HG13  | 2.13                     | 0.49              |
| 1:G:290:GLN:HG2  | 1:G:331:LEU:CA   | 2.43                     | 0.49              |
| 1:G:715:VAL:HG12 | 1:G:716:LEU:O    | 2.12                     | 0.49              |
| 1:J:291:ILE:HA   | 1:J:331:LEU:CD1  | 2.39                     | 0.49              |
| 4:0:201:VAL:HG23 | 4:Y:287:ILE:CB   | 2.42                     | 0.49              |
| 4:2:70:PRO:HG3   | 4:2:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:3:70:PRO:HG3   | 4:3:81:ASP:HB3   | 1.93                     | 0.49              |
| 4:4:318:THR:HA   | 4:4:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:5:70:PRO:HG3   | 4:5:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:8:124:PHE:CZ   | 4:8:132:MET:HG3  | 2.48                     | 0.49              |
| 4:V:70:PRO:HG3   | 4:V:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:X:70:PRO:HG3   | 4:X:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:A:93:MET:HE2   | 1:A:716:LEU:H    | 1.78                     | 0.49              |
| 1:A:543:PRO:CD   | 4:8:146:GLY:O    | 2.61                     | 0.49              |
| 1:D:128:PRO:O    | 1:D:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:D:543:PRO:CD   | 4:9:146:GLY:O    | 2.61                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:642:LYS:CG   | 4:9:22:ALA:HA    | 2.37                     | 0.49              |
| 1:D:747:LEU:C    | 1:D:749:GLY:H    | 2.20                     | 0.49              |
| 1:G:543:PRO:CD   | 4:V:146:GLY:O    | 2.61                     | 0.49              |
| 1:G:601:ASP:N    | 1:G:602:PRO:CD   | 2.75                     | 0.49              |
| 1:G:629:GLU:HG2  | 1:G:643:GLY:C    | 2.35                     | 0.49              |
| 1:J:20:SER:HB3   | 1:J:23:GLU:OE1   | 2.13                     | 0.49              |
| 1:J:128:PRO:O    | 1:J:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:HB3  | 1.94                     | 0.49              |
| 1:J:471:ASP:HB3  | 1:J:573:GLY:O    | 2.12                     | 0.49              |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:CD   | 2.37                     | 0.49              |
| 4:0:243:PRO:O    | 4:Y:291:LYS:HG3  | 2.13                     | 0.49              |
| 4:1:124:PHE:CZ   | 4:1:132:MET:HG3  | 2.48                     | 0.49              |
| 4:2:124:PHE:CZ   | 4:2:132:MET:HG3  | 2.48                     | 0.49              |
| 4:V:124:PHE:CZ   | 4:V:132:MET:HG3  | 2.48                     | 0.49              |
| 1:A:173:GLN:OE1  | 1:A:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:A:295:MLY:HE2  | 1:A:332:MET:HE1  | 1.95                     | 0.49              |
| 1:A:312:TYR:N    | 1:A:312:TYR:CD1  | 2.80                     | 0.49              |
| 1:A:429:LEU:O    | 1:A:433:VAL:HG23 | 2.11                     | 0.49              |
| 1:A:538:GLU:OE1  | 4:8:351:THR:HB   | 2.12                     | 0.49              |
| 1:A:739:ASP:OD1  | 1:A:740:SER:N    | 2.45                     | 0.49              |
| 2:B:121:LEU:HA   | 2:B:128:PHE:CD2  | 2.46                     | 0.49              |
| 1:D:214:MET:HA   | 1:D:340:ILE:CD1  | 2.42                     | 0.49              |
| 1:D:332:MET:O    | 1:D:336:SER:OG   | 2.27                     | 0.49              |
| 1:D:538:GLU:HA   | 4:9:351:THR:H    | 1.77                     | 0.49              |
| 1:D:739:ASP:OD1  | 1:D:740:SER:N    | 2.45                     | 0.49              |
| 2:E:114:LYS:HG3  | 2:E:137:TRP:CZ2  | 2.47                     | 0.49              |
| 2:E:128:PHE:O    | 2:E:133:ILE:HD11 | 2.13                     | 0.49              |
| 1:G:732:ILE:O    | 1:G:736:GLN:HG3  | 2.12                     | 0.49              |
| 3:I:50:LEU:O     | 3:I:55:LYS:HB2   | 2.13                     | 0.49              |
| 1:J:97:LEU:HD13  | 1:J:97:LEU:N     | 2.28                     | 0.49              |
| 1:J:768:MLY:HE2  | 1:J:772:LEU:HD23 | 1.94                     | 0.49              |
| 2:K:121:LEU:O    | 2:K:128:PHE:CG   | 2.61                     | 0.49              |
| 4:1:70:PRO:HG3   | 4:1:81:ASP:HB3   | 1.93                     | 0.49              |
| 4:1:318:THR:HA   | 4:1:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:5:198:TYR:CZ   | 4:5:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:X:124:PHE:CZ   | 4:X:132:MET:HG3  | 2.48                     | 0.49              |
| 4:Z:70:PRO:HG3   | 4:Z:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:A:192:VAL:O    | 1:A:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:D:20:SER:HB3   | 1:D:23:GLU:OE1   | 2.12                     | 0.49              |
| 1:D:290:GLN:HG2  | 1:D:331:LEU:CA   | 2.43                     | 0.49              |
| 1:D:756:THR:O    | 1:D:758:TYR:N    | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:834:LEU:HD13 | 2:E:51:PHE:CD1   | 2.42                     | 0.49              |
| 2:E:117:LEU:HG   | 2:E:147:ASN:HB3  | 1.93                     | 0.49              |
| 1:G:20:SER:HB3   | 1:G:23:GLU:OE1   | 2.12                     | 0.49              |
| 1:G:154:HIS:CD2  | 1:G:155:ILE:H    | 2.30                     | 0.49              |
| 1:J:312:TYR:N    | 1:J:312:TYR:CD1  | 2.81                     | 0.49              |
| 1:J:544:LYS:HD2  | 4:W:147:ARG:CB   | 2.36                     | 0.49              |
| 1:J:715:VAL:HG12 | 1:J:716:LEU:O    | 2.12                     | 0.49              |
| 1:J:747:LEU:C    | 1:J:749:GLY:H    | 2.20                     | 0.49              |
| 1:J:786:ILE:CD1  | 3:L:86:ASP:HB3   | 2.43                     | 0.49              |
| 4:O:124:PHE:CZ   | 4:O:132:MET:HG3  | 2.48                     | 0.49              |
| 4:2:318:THR:HA   | 4:2:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:V:198:TYR:CZ   | 4:V:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:W:124:PHE:CZ   | 4:W:132:MET:HG3  | 2.48                     | 0.49              |
| 4:X:198:TYR:CZ   | 4:X:248:ILE:HG13 | 2.48                     | 0.49              |
| 1:A:89:GLU:CD    | 1:A:153:PRO:HD2  | 2.36                     | 0.49              |
| 1:A:97:LEU:HD13  | 1:A:97:LEU:N     | 2.28                     | 0.49              |
| 1:A:346:ASP:O    | 1:A:349:THR:HB   | 2.11                     | 0.49              |
| 1:A:839:MLY:N    | 1:A:840:PRO:CD   | 2.75                     | 0.49              |
| 1:D:310:TYR:CE2  | 1:D:320:ILE:CD1  | 2.94                     | 0.49              |
| 1:G:168:THR:HG22 | 1:G:169:ASP:OD1  | 2.12                     | 0.49              |
| 1:G:237:THR:HG22 | 1:G:238:VAL:N    | 2.28                     | 0.49              |
| 1:G:707:CYS:CB   | 1:G:714:ARG:NH1  | 2.44                     | 0.49              |
| 2:H:114:LYS:HG3  | 2:H:137:TRP:CZ2  | 2.48                     | 0.49              |
| 1:J:64:THR:CG2   | 1:J:65:GLU:N     | 2.75                     | 0.49              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:HG3  | 1.71                     | 0.49              |
| 1:J:540:CYS:C    | 4:W:349:LEU:HD21 | 2.36                     | 0.49              |
| 3:L:50:LEU:O     | 3:L:55:LYS:HB2   | 2.13                     | 0.49              |
| 4:O:173:HIS:CD2  | 4:1:268:GLY:HA3  | 2.48                     | 0.49              |
| 4:4:213:LYS:O    | 4:4:217:CYS:HB2  | 2.13                     | 0.49              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:HB3  | 2.43                     | 0.49              |
| 1:A:128:PRO:O    | 1:A:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:A:168:THR:HG22 | 1:A:169:ASP:OD1  | 2.12                     | 0.49              |
| 1:A:720:PHE:CD2  | 1:A:744:SER:HB3  | 2.48                     | 0.49              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD12 | 0.95                     | 0.49              |
| 2:B:114:LYS:HG3  | 2:B:137:TRP:CZ2  | 2.48                     | 0.49              |
| 3:C:50:LEU:O     | 3:C:55:LYS:HB2   | 2.13                     | 0.49              |
| 1:D:267:THR:HG21 | 1:D:438:PHE:HE2  | 1.76                     | 0.49              |
| 1:D:547:ASP:O    | 1:D:550:PHE:HB3  | 2.12                     | 0.49              |
| 1:D:790:THR:HA   | 3:F:87:PHE:CZ    | 2.46                     | 0.49              |
| 1:D:793:ARG:O    | 1:D:797:PHE:N    | 2.39                     | 0.49              |
| 1:D:839:MLY:N    | 1:D:840:PRO:CD   | 2.75                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:839:MLY:HB2  | 1:D:840:PRO:HD3  | 1.94                     | 0.49              |
| 3:F:50:LEU:O     | 3:F:55:LYS:HB2   | 2.13                     | 0.49              |
| 1:G:192:VAL:O    | 1:G:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:J:173:GLN:OE1  | 1:J:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:J:290:GLN:HG2  | 1:J:331:LEU:CA   | 2.43                     | 0.49              |
| 1:J:768:MLY:CE   | 1:J:772:LEU:HD23 | 2.43                     | 0.49              |
| 4:0:198:TYR:CZ   | 4:0:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:1:148:THR:OG1  | 4:3:45:VAL:CG2   | 2.61                     | 0.49              |
| 4:7:124:PHE:CZ   | 4:7:132:MET:HG3  | 2.48                     | 0.49              |
| 4:7:198:TYR:CZ   | 4:7:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:9:70:PRO:HG3   | 4:9:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:9:124:PHE:CZ   | 4:9:132:MET:HG3  | 2.48                     | 0.49              |
| 4:W:70:PRO:HG3   | 4:W:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:Z:124:PHE:CZ   | 4:Z:132:MET:HG3  | 2.48                     | 0.49              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG13 | 1.95                     | 0.49              |
| 1:A:251:ARG:O    | 1:A:263:ALA:HA   | 2.12                     | 0.49              |
| 1:D:289:TYR:OH   | 1:D:315:VAL:O    | 2.27                     | 0.49              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:CD1  | 0.64                     | 0.49              |
| 1:D:818:TYR:CD2  | 2:E:89:LYS:O     | 2.62                     | 0.49              |
| 1:D:831:TRP:CE3  | 2:E:34:ILE:HD13  | 2.47                     | 0.49              |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:HB3  | 1.90                     | 0.49              |
| 1:G:175:ILE:C    | 1:G:176:LEU:HD12 | 2.38                     | 0.49              |
| 1:G:248:MLY:HE2  | 1:G:250:ILE:HD11 | 1.95                     | 0.49              |
| 1:G:547:ASP:O    | 1:G:550:PHE:HB3  | 2.12                     | 0.49              |
| 1:G:797:PHE:HB2  | 3:I:149:VAL:CG1  | 2.43                     | 0.49              |
| 1:G:839:MLY:HB2  | 1:G:840:PRO:HD3  | 1.94                     | 0.49              |
| 1:J:237:THR:HG22 | 1:J:238:VAL:N    | 2.28                     | 0.49              |
| 1:J:476:GLU:CD   | 1:J:476:GLU:H    | 2.21                     | 0.49              |
| 1:J:720:PHE:CD2  | 1:J:744:SER:HB3  | 2.48                     | 0.49              |
| 1:J:798:LEU:HD21 | 3:L:122:GLU:O    | 2.12                     | 0.49              |
| 1:J:818:TYR:OH   | 2:K:127:ARG:NH2  | 2.37                     | 0.49              |
| 2:K:93:PRO:O     | 2:K:97:ILE:HG13  | 2.12                     | 0.49              |
| 4:0:70:PRO:HG3   | 4:0:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:7:70:PRO:HG3   | 4:7:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:7:325:MET:HE2  | 4:9:244:ASP:HB3  | 1.94                     | 0.49              |
| 4:9:198:TYR:CZ   | 4:9:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:9:325:MET:HE2  | 4:W:244:ASP:HB3  | 1.94                     | 0.49              |
| 1:A:237:THR:HG22 | 1:A:238:VAL:N    | 2.28                     | 0.48              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:CZ    | 2.77                     | 0.48              |
| 2:B:93:PRO:O     | 2:B:97:ILE:HG13  | 2.12                     | 0.48              |
| 1:D:64:THR:CG2   | 1:D:65:GLU:N     | 2.75                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:806:MET:SD   | 3:F:17:PHE:HE2   | 2.36                     | 0.48              |
| 1:G:128:PRO:O    | 1:G:683:PRO:HB3  | 2.12                     | 0.48              |
| 1:G:295:MLY:HE2  | 1:G:332:MET:HE1  | 1.95                     | 0.48              |
| 1:G:405:ARG:HB2  | 1:G:414:THR:OG1  | 2.13                     | 0.48              |
| 1:G:556:ASP:OD1  | 4:X:47:MET:CE    | 2.27                     | 0.48              |
| 1:G:730:SER:CB   | 3:I:109:HIS:CE1  | 2.95                     | 0.48              |
| 1:G:739:ASP:OD1  | 1:G:740:SER:N    | 2.45                     | 0.48              |
| 2:H:139:ALA:C    | 2:H:141:PRO:HD3  | 2.33                     | 0.48              |
| 1:J:215:GLN:H    | 1:J:340:ILE:CD1  | 2.20                     | 0.48              |
| 1:J:405:ARG:HB2  | 1:J:414:THR:OG1  | 2.13                     | 0.48              |
| 1:J:739:ASP:CB   | 1:J:742:LYS:CB   | 2.81                     | 0.48              |
| 1:J:753:VAL:CA   | 1:J:780:ASP:OD2  | 2.54                     | 0.48              |
| 2:K:128:PHE:O    | 2:K:133:ILE:HD11 | 2.13                     | 0.48              |
| 4:0:112:PRO:HG3  | 4:1:195:GLU:C    | 2.38                     | 0.48              |
| 4:1:213:LYS:O    | 4:1:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:4:198:TYR:CZ   | 4:4:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:8:198:TYR:CZ   | 4:8:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:X:324:THR:O    | 4:Z:245:GLY:C    | 2.56                     | 0.48              |
| 1:A:290:GLN:HG2  | 1:A:331:LEU:CA   | 2.43                     | 0.48              |
| 1:A:310:TYR:CE2  | 1:A:320:ILE:CD1  | 2.94                     | 0.48              |
| 1:A:499:GLU:OE1  | 1:A:499:GLU:HA   | 2.13                     | 0.48              |
| 1:A:502:GLU:CD   | 1:A:763:THR:N    | 2.56                     | 0.48              |
| 1:A:747:LEU:C    | 1:A:749:GLY:H    | 2.20                     | 0.48              |
| 1:D:168:THR:HG22 | 1:D:169:ASP:OD1  | 2.12                     | 0.48              |
| 1:D:404:PRO:HD2  | 1:D:415:MLY:O    | 2.13                     | 0.48              |
| 1:D:540:CYS:C    | 4:9:349:LEU:HD21 | 2.36                     | 0.48              |
| 1:D:541:MET:SD   | 4:9:345:ILE:C    | 2.95                     | 0.48              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:CH1  | 2.89                     | 0.48              |
| 1:D:747:LEU:C    | 1:D:749:GLY:N    | 2.71                     | 0.48              |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HB3  | 1.78                     | 0.48              |
| 1:G:93:MET:CE    | 1:G:763:THR:O    | 2.60                     | 0.48              |
| 1:G:95:THR:OG1   | 1:G:713:SER:CB   | 2.56                     | 0.48              |
| 1:G:309:PRO:C    | 1:G:311:ASP:H    | 2.22                     | 0.48              |
| 1:G:759:ALA:O    | 1:G:766:PHE:N    | 2.32                     | 0.48              |
| 1:J:168:THR:HG22 | 1:J:169:ASP:OD1  | 2.12                     | 0.48              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:CB   | 2.80                     | 0.48              |
| 1:J:839:MLY:N    | 1:J:840:PRO:CD   | 2.75                     | 0.48              |
| 4:1:198:TYR:CZ   | 4:1:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:1:243:PRO:C    | 4:Z:324:THR:OG1  | 2.53                     | 0.48              |
| 4:3:120:THR:HG21 | 4:3:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:3:124:PHE:CZ   | 4:3:132:MET:HG3  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:198:TYR:CZ   | 4:3:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:Y:124:PHE:CZ   | 4:Y:132:MET:HG3  | 2.48                     | 0.48              |
| 1:A:175:ILE:C    | 1:A:176:LEU:HD12 | 2.38                     | 0.48              |
| 1:A:542:PHE:CD2  | 4:8:143:TYR:CD1  | 3.02                     | 0.48              |
| 2:B:128:PHE:O    | 2:B:133:ILE:HD11 | 2.13                     | 0.48              |
| 1:D:237:THR:HG22 | 1:D:238:VAL:N    | 2.28                     | 0.48              |
| 1:D:405:ARG:HB2  | 1:D:414:THR:OG1  | 2.13                     | 0.48              |
| 1:G:538:GLU:HA   | 4:V:351:THR:H    | 1.76                     | 0.48              |
| 1:G:617:MLY:O    | 1:G:620:ALA:HB3  | 2.14                     | 0.48              |
| 2:H:117:LEU:HG   | 2:H:147:ASN:HB3  | 1.93                     | 0.48              |
| 1:J:136:ASN:O    | 1:J:139:VAL:N    | 2.46                     | 0.48              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:CD1  | 0.63                     | 0.48              |
| 2:K:149:ASP:CG   | 2:K:150:TYR:N    | 2.49                     | 0.48              |
| 4:0:287:ILE:HG21 | 4:2:203:THR:HG22 | 1.78                     | 0.48              |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:H    | 1.74                     | 0.48              |
| 4:4:120:THR:HG21 | 4:4:370:VAL:HG11 | 1.95                     | 0.48              |
| 1:A:405:ARG:HB2  | 1:A:414:THR:OG1  | 2.13                     | 0.48              |
| 1:A:549:SER:C    | 4:V:45:VAL:O     | 2.56                     | 0.48              |
| 1:A:834:LEU:HD13 | 2:B:54:MET:HG3   | 1.86                     | 0.48              |
| 2:B:117:LEU:HG   | 2:B:147:ASN:HB3  | 1.93                     | 0.48              |
| 1:D:295:MLY:HE2  | 1:D:332:MET:HE1  | 1.95                     | 0.48              |
| 1:D:544:LYS:HD2  | 4:9:147:ARG:CB   | 2.36                     | 0.48              |
| 1:G:251:ARG:O    | 1:G:263:ALA:HA   | 2.12                     | 0.48              |
| 1:G:310:TYR:CE2  | 1:G:320:ILE:CD1  | 2.94                     | 0.48              |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:CD   | 2.37                     | 0.48              |
| 1:G:720:PHE:CD2  | 1:G:744:SER:HB3  | 2.48                     | 0.48              |
| 1:G:739:ASP:CB   | 1:G:742:LYS:CB   | 2.81                     | 0.48              |
| 2:H:128:PHE:O    | 2:H:133:ILE:HD11 | 2.13                     | 0.48              |
| 1:J:41:VAL:CG1   | 1:J:42:HIS:N     | 2.75                     | 0.48              |
| 1:J:84:MLY:HH11  | 1:J:719:ASP:C    | 2.38                     | 0.48              |
| 1:J:267:THR:HG21 | 1:J:438:PHE:HE2  | 1.76                     | 0.48              |
| 1:J:404:PRO:HD2  | 1:J:415:MLY:O    | 2.13                     | 0.48              |
| 1:J:410:ASN:HD22 | 4:W:336:LYS:HE2  | 1.78                     | 0.48              |
| 1:J:538:GLU:HA   | 4:W:351:THR:H    | 1.77                     | 0.48              |
| 1:J:707:CYS:CB   | 1:J:714:ARG:NH2  | 2.73                     | 0.48              |
| 4:5:213:LYS:O    | 4:5:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:7:213:LYS:O    | 4:7:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:X:324:THR:CB   | 4:Z:247:VAL:H    | 2.23                     | 0.48              |
| 4:Z:198:TYR:CZ   | 4:Z:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:Z:213:LYS:O    | 4:Z:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:A:406:VAL:CG1  | 1:A:407:GLY:N    | 2.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:544:LYS:HD2  | 4:8:147:ARG:CB   | 2.36                     | 0.48              |
| 1:A:769:ALA:N    | 1:A:771:LEU:CB   | 2.76                     | 0.48              |
| 1:D:314:TYR:CZ   | 1:D:362:GLY:HA2  | 2.48                     | 0.48              |
| 1:D:617:MLY:O    | 1:D:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:D:642:LYS:CB   | 4:9:24:ASP:O     | 2.59                     | 0.48              |
| 1:D:720:PHE:CD2  | 1:D:744:SER:HB3  | 2.48                     | 0.48              |
| 1:G:64:THR:CG2   | 1:G:65:GLU:N     | 2.75                     | 0.48              |
| 1:G:173:GLN:OE1  | 1:G:668:HIS:HB3  | 2.13                     | 0.48              |
| 1:G:312:TYR:N    | 1:G:312:TYR:CD1  | 2.80                     | 0.48              |
| 1:G:499:GLU:OE1  | 1:G:499:GLU:HA   | 2.13                     | 0.48              |
| 1:G:553:MLY:CB   | 4:X:45:VAL:O     | 2.57                     | 0.48              |
| 1:G:723:ARG:HH11 | 1:G:723:ARG:HG3  | 1.78                     | 0.48              |
| 1:J:314:TYR:CZ   | 1:J:362:GLY:HA2  | 2.48                     | 0.48              |
| 1:J:547:ASP:O    | 1:J:550:PHE:HB3  | 2.12                     | 0.48              |
| 4:0:120:THR:HG21 | 4:0:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:5:250:ILE:HG23 | 4:5:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:V:120:THR:HG21 | 4:V:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:W:198:TYR:CZ   | 4:W:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:W:213:LYS:O    | 4:W:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:W:250:ILE:HG23 | 4:W:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:Y:250:ILE:HG23 | 4:Y:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:A:10:PHE:CD2   | 1:A:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:CD   | 2.37                     | 0.48              |
| 2:B:112:ILE:CG2  | 2:B:147:ASN:O    | 2.62                     | 0.48              |
| 1:D:436:MLY:HE3  | 1:D:626:TYR:HE1  | 1.77                     | 0.48              |
| 1:D:476:GLU:H    | 1:D:476:GLU:CD   | 2.21                     | 0.48              |
| 1:D:550:PHE:CE2  | 1:D:592:ILE:CG2  | 2.97                     | 0.48              |
| 1:D:689:GLU:O    | 1:D:689:GLU:HG2  | 2.14                     | 0.48              |
| 1:D:792:ALA:HB2  | 3:F:40:ASN:O     | 2.10                     | 0.48              |
| 1:G:84:MLY:HH11  | 1:G:715:VAL:HG12 | 1.77                     | 0.48              |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:CD2   | 2.43                     | 0.48              |
| 1:J:10:PHE:CD2   | 1:J:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:J:295:MLY:HE2  | 1:J:332:MET:HE1  | 1.95                     | 0.48              |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:HG3  | 1.78                     | 0.48              |
| 1:J:831:TRP:HH2  | 2:K:34:ILE:CG2   | 2.25                     | 0.48              |
| 4:0:287:ILE:HG21 | 4:2:203:THR:CA   | 2.43                     | 0.48              |
| 4:4:250:ILE:HG23 | 4:4:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:5:124:PHE:CZ   | 4:5:132:MET:HG3  | 2.48                     | 0.48              |
| 4:Y:70:PRO:HG3   | 4:Y:81:ASP:HB3   | 1.94                     | 0.48              |
| 1:A:64:THR:CG2   | 1:A:65:GLU:N     | 2.75                     | 0.48              |
| 1:A:248:MLY:HE2  | 1:A:250:ILE:HD11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:617:MLY:O    | 1:A:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:A:747:LEU:C    | 1:A:749:GLY:N    | 2.71                     | 0.48              |
| 1:A:795:ARG:NE   | 3:C:43:ASN:OD1   | 2.10                     | 0.48              |
| 1:D:106:LEU:HD12 | 1:D:117:THR:HG21 | 1.96                     | 0.48              |
| 1:D:789:ALA:C    | 3:F:87:PHE:HE2   | 2.11                     | 0.48              |
| 1:G:10:PHE:CD2   | 1:G:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:G:635:GLY:HA3  | 4:V:334:GLU:CG   | 2.30                     | 0.48              |
| 1:J:84:MLY:HH12  | 1:J:715:VAL:HG12 | 1.84                     | 0.48              |
| 1:J:617:MLY:O    | 1:J:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:J:664:LEU:HD12 | 1:J:664:LEU:HA   | 1.52                     | 0.48              |
| 2:K:137:TRP:CA   | 2:K:145:ALA:CB   | 2.82                     | 0.48              |
| 4:O:213:LYS:O    | 4:O:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:O:250:ILE:HG23 | 4:O:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:3:250:ILE:HG23 | 4:3:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:3:253:GLU:HA   | 4:3:256:ARG:CG   | 2.42                     | 0.48              |
| 4:4:124:PHE:CZ   | 4:4:132:MET:HG3  | 2.48                     | 0.48              |
| 4:7:250:ILE:HG23 | 4:7:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:8:250:ILE:HG23 | 4:8:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:X:213:LYS:O    | 4:X:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:X:324:THR:CG2  | 4:Z:247:VAL:H    | 2.27                     | 0.48              |
| 1:A:505:MLY:HB2  | 1:A:761:GLY:HA2  | 1.95                     | 0.48              |
| 1:A:765:VAL:CG1  | 1:A:766:PHE:N    | 2.77                     | 0.48              |
| 1:D:723:ARG:HH11 | 1:D:723:ARG:HG3  | 1.79                     | 0.48              |
| 1:G:97:LEU:HD13  | 1:G:97:LEU:N     | 2.27                     | 0.48              |
| 1:G:476:GLU:H    | 1:G:476:GLU:CD   | 2.21                     | 0.48              |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:HB3  | 1.79                     | 0.48              |
| 2:H:140:PHE:HB3  | 2:H:144:VAL:HG12 | 1.95                     | 0.48              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:HE3   | 2.42                     | 0.48              |
| 2:K:112:ILE:CG2  | 2:K:147:ASN:O    | 2.62                     | 0.48              |
| 4:1:253:GLU:HA   | 4:1:256:ARG:CG   | 2.42                     | 0.48              |
| 4:2:198:TYR:CZ   | 4:2:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:V:213:LYS:O    | 4:V:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:V:285:CYS:O    | 4:X:202:THR:HG22 | 2.14                     | 0.48              |
| 4:X:250:ILE:HG23 | 4:X:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:A:540:CYS:C    | 4:8:349:LEU:HD21 | 2.36                     | 0.48              |
| 1:A:556:ASP:CA   | 4:V:49:GLN:O     | 2.52                     | 0.48              |
| 1:A:664:LEU:HD12 | 1:A:664:LEU:HA   | 1.53                     | 0.48              |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:HG3  | 1.78                     | 0.48              |
| 1:D:546:THR:CG2  | 1:D:547:ASP:N    | 2.77                     | 0.48              |
| 1:J:510:TRP:CD2  | 1:J:768:MLY:HH13 | 2.49                     | 0.48              |
| 1:J:769:ALA:HB2  | 1:J:770:GLY:N    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:213:LYS:O    | 4:2:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:2:250:ILE:HG23 | 4:2:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:8:120:THR:HG21 | 4:8:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:9:250:ILE:HG23 | 4:9:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:Y:213:LYS:O    | 4:Y:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:A:410:ASN:HD22 | 4:8:336:LYS:HE2  | 1.78                     | 0.48              |
| 1:A:506:GLU:OE2  | 1:A:760:PHE:HD2  | 1.97                     | 0.48              |
| 1:A:546:THR:CG2  | 1:A:547:ASP:N    | 2.77                     | 0.48              |
| 1:A:550:PHE:CE2  | 1:A:592:ILE:CG2  | 2.97                     | 0.48              |
| 1:A:640:LYS:HD2  | 1:A:646:PHE:O    | 2.14                     | 0.48              |
| 1:A:689:GLU:HG2  | 1:A:689:GLU:O    | 2.14                     | 0.48              |
| 1:D:10:PHE:CD2   | 1:D:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:D:312:TYR:N    | 1:D:312:TYR:CD1  | 2.80                     | 0.48              |
| 1:D:542:PHE:CD2  | 4:9:143:TYR:CD1  | 3.02                     | 0.48              |
| 1:D:602:PRO:O    | 1:D:603:LEU:HD12 | 2.14                     | 0.48              |
| 2:E:160:GLY:O    | 2:E:161:GLU:HG2  | 2.14                     | 0.48              |
| 1:G:544:LYS:HD2  | 4:V:147:ARG:CB   | 2.36                     | 0.48              |
| 1:G:550:PHE:CE2  | 1:G:592:ILE:CG2  | 2.96                     | 0.48              |
| 1:G:701:LEU:HA   | 1:G:701:LEU:HD12 | 1.55                     | 0.48              |
| 2:H:121:LEU:O    | 2:H:128:PHE:CG   | 2.61                     | 0.48              |
| 1:J:636:LYS:O    | 4:W:144:ALA:HB1  | 2.14                     | 0.48              |
| 1:J:643:GLY:N    | 4:W:23:GLY:C     | 2.55                     | 0.48              |
| 1:J:747:LEU:C    | 1:J:749:GLY:N    | 2.71                     | 0.48              |
| 2:K:121:LEU:HA   | 2:K:128:PHE:CD2  | 2.46                     | 0.48              |
| 4:4:217:CYS:C    | 4:4:218:TYR:HD1  | 2.22                     | 0.48              |
| 4:7:120:THR:HG21 | 4:7:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:V:250:ILE:HG23 | 4:V:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:X:120:THR:HG21 | 4:X:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:Y:198:TYR:CZ   | 4:Y:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:Z:120:THR:HG21 | 4:Z:370:VAL:HG11 | 1.95                     | 0.48              |
| 1:A:166:MET:HE3  | 1:A:459:ILE:HG13 | 1.96                     | 0.47              |
| 1:A:476:GLU:H    | 1:A:476:GLU:CD   | 2.21                     | 0.47              |
| 1:A:538:GLU:HA   | 4:8:351:THR:H    | 1.77                     | 0.47              |
| 1:A:817:GLN:NE2  | 2:B:127:ARG:HG2  | 2.28                     | 0.47              |
| 1:D:97:LEU:HD13  | 1:D:97:LEU:N     | 2.27                     | 0.47              |
| 1:D:578:HIS:HB3  | 1:D:592:ILE:CD1  | 2.38                     | 0.47              |
| 1:D:797:PHE:CE2  | 3:F:126:LEU:HD22 | 2.48                     | 0.47              |
| 1:D:809:ARG:CZ   | 2:E:124:GLY:HA2  | 2.33                     | 0.47              |
| 2:E:137:TRP:CA   | 2:E:145:ALA:CB   | 2.82                     | 0.47              |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:HD13 | 1.92                     | 0.47              |
| 1:G:166:MET:HE3  | 1:G:459:ILE:HG13 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:564:ASN:HD22 | 1:G:582:VAL:HB   | 1.79                     | 0.47              |
| 1:G:640:LYS:HD2  | 1:G:646:PHE:O    | 2.14                     | 0.47              |
| 1:J:436:MLY:HE3  | 1:J:626:TYR:HE1  | 1.77                     | 0.47              |
| 1:J:481:ASN:N    | 1:J:481:ASN:ND2  | 2.51                     | 0.47              |
| 1:J:542:PHE:CD2  | 4:W:143:TYR:CD1  | 3.02                     | 0.47              |
| 1:J:550:PHE:CE2  | 1:J:592:ILE:CG2  | 2.97                     | 0.47              |
| 1:J:765:VAL:CG1  | 1:J:766:PHE:N    | 2.77                     | 0.47              |
| 4:1:250:ILE:HG23 | 4:1:253:GLU:HG2  | 1.96                     | 0.47              |
| 1:A:402:CYS:C    | 1:A:404:PRO:HD3  | 2.40                     | 0.47              |
| 1:A:602:PRO:O    | 1:A:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:A:783:LEU:HA   | 1:A:786:ILE:HB   | 1.96                     | 0.47              |
| 1:A:836:PHE:CB   | 2:B:161:GLU:HG2  | 2.35                     | 0.47              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:D:175:ILE:C    | 1:D:176:LEU:HD12 | 2.38                     | 0.47              |
| 1:D:550:PHE:C    | 4:W:46:GLY:CA    | 2.87                     | 0.47              |
| 1:D:564:ASN:HD22 | 1:D:582:VAL:HB   | 1.79                     | 0.47              |
| 1:D:568:PRO:HD3  | 1:D:579:PHE:HA   | 1.96                     | 0.47              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:CB   | 2.80                     | 0.47              |
| 1:G:149:GLN:OE1  | 1:G:762:HIS:CB   | 2.61                     | 0.47              |
| 1:G:314:TYR:CZ   | 1:G:362:GLY:HA2  | 2.48                     | 0.47              |
| 1:G:410:ASN:HD22 | 4:V:336:LYS:HE2  | 1.79                     | 0.47              |
| 1:G:546:THR:CG2  | 1:G:547:ASP:N    | 2.77                     | 0.47              |
| 1:G:793:ARG:O    | 1:G:797:PHE:N    | 2.39                     | 0.47              |
| 1:J:84:MLY:HH11  | 1:J:720:PHE:CA   | 2.44                     | 0.47              |
| 1:J:218:LEU:CD2  | 1:J:222:ILE:CG1  | 2.86                     | 0.47              |
| 1:J:546:THR:CG2  | 1:J:547:ASP:N    | 2.77                     | 0.47              |
| 1:J:675:ILE:CG2  | 1:J:676:ILE:N    | 2.74                     | 0.47              |
| 3:L:53:PRO:O     | 3:L:55:LYS:HG3   | 2.14                     | 0.47              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:H    | 2.27                     | 0.47              |
| 4:5:253:GLU:HA   | 4:5:256:ARG:CG   | 2.42                     | 0.47              |
| 4:9:120:THR:HG21 | 4:9:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:9:217:CYS:C    | 4:9:218:TYR:HD1  | 2.22                     | 0.47              |
| 4:Z:250:ILE:HG23 | 4:Z:253:GLU:HG2  | 1.96                     | 0.47              |
| 1:A:314:TYR:CZ   | 1:A:362:GLY:HA2  | 2.48                     | 0.47              |
| 1:A:595:TRP:N    | 1:A:595:TRP:CD1  | 2.80                     | 0.47              |
| 1:A:768:MLY:O    | 1:A:771:LEU:HB3  | 2.14                     | 0.47              |
| 2:B:160:GLY:O    | 2:B:161:GLU:HG2  | 2.14                     | 0.47              |
| 1:D:541:MET:HE2  | 4:9:346:LEU:HD12 | 1.96                     | 0.47              |
| 1:G:22:LYS:O     | 1:G:26:GLU:N     | 2.29                     | 0.47              |
| 1:G:106:LEU:HD12 | 1:G:117:THR:HG21 | 1.96                     | 0.47              |
| 1:G:602:PRO:O    | 1:G:603:LEU:HD12 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:160:GLY:O    | 2:H:161:GLU:HG2  | 2.14                     | 0.47              |
| 1:J:541:MET:HE2  | 4:W:346:LEU:HD12 | 1.96                     | 0.47              |
| 1:J:564:ASN:HD22 | 1:J:582:VAL:HB   | 1.79                     | 0.47              |
| 2:K:140:PHE:HB3  | 2:K:144:VAL:HG12 | 1.94                     | 0.47              |
| 4:2:120:THR:HG21 | 4:2:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:2:253:GLU:HA   | 4:2:256:ARG:CG   | 2.42                     | 0.47              |
| 4:7:217:CYS:C    | 4:7:218:TYR:HD1  | 2.22                     | 0.47              |
| 4:9:213:LYS:O    | 4:9:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:V:285:CYS:O    | 4:X:202:THR:CG2  | 2.62                     | 0.47              |
| 4:W:162:ASN:OD1  | 4:W:277:THR:HG22 | 2.15                     | 0.47              |
| 4:W:217:CYS:C    | 4:W:218:TYR:HD1  | 2.22                     | 0.47              |
| 4:Y:162:ASN:OD1  | 4:Y:277:THR:HG22 | 2.15                     | 0.47              |
| 1:A:122:PHE:CE2  | 1:A:700:VAL:HA   | 2.49                     | 0.47              |
| 1:A:136:ASN:O    | 1:A:139:VAL:N    | 2.47                     | 0.47              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:H    | 1.79                     | 0.47              |
| 1:A:404:PRO:HD2  | 1:A:415:MLY:O    | 2.13                     | 0.47              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:CG   | 2.24                     | 0.47              |
| 1:D:188:ASN:ND2  | 1:D:674:CYS:SG   | 2.88                     | 0.47              |
| 1:D:248:MLY:HE2  | 1:D:250:ILE:HD11 | 1.95                     | 0.47              |
| 1:D:410:ASN:HD22 | 4:9:336:LYS:HE2  | 1.78                     | 0.47              |
| 1:D:549:SER:C    | 4:W:45:VAL:O     | 2.56                     | 0.47              |
| 1:D:640:LYS:HD2  | 1:D:646:PHE:O    | 2.14                     | 0.47              |
| 1:D:675:ILE:CG2  | 1:D:676:ILE:N    | 2.74                     | 0.47              |
| 2:E:163:ALA:O    | 2:K:21:GLU:N     | 2.46                     | 0.47              |
| 1:G:134:VAL:C    | 1:G:136:ASN:H    | 2.16                     | 0.47              |
| 1:G:402:CYS:C    | 1:G:404:PRO:HD3  | 2.40                     | 0.47              |
| 1:G:408:VAL:HG22 | 1:G:636:LYS:HG2  | 1.51                     | 0.47              |
| 1:G:725:ARG:CG   | 1:G:733:PRO:HA   | 2.43                     | 0.47              |
| 2:H:112:ILE:CG2  | 2:H:147:ASN:O    | 2.62                     | 0.47              |
| 1:J:175:ILE:C    | 1:J:176:LEU:HD12 | 2.38                     | 0.47              |
| 1:J:188:ASN:ND2  | 1:J:674:CYS:SG   | 2.88                     | 0.47              |
| 4:1:120:THR:HG21 | 4:1:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:3:217:CYS:C    | 4:3:218:TYR:HD1  | 2.22                     | 0.47              |
| 4:5:120:THR:HG21 | 4:5:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:7:162:ASN:OD1  | 4:7:277:THR:HG22 | 2.15                     | 0.47              |
| 4:X:162:ASN:OD1  | 4:X:277:THR:HG22 | 2.15                     | 0.47              |
| 4:X:217:CYS:C    | 4:X:218:TYR:HD1  | 2.22                     | 0.47              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:A:176:LEU:N    | 1:A:176:LEU:CD1  | 2.74                     | 0.47              |
| 1:D:640:LYS:C    | 1:D:645:SER:HG   | 2.10                     | 0.47              |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:CD1  | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:765:VAL:CG1  | 1:D:766:PHE:N    | 2.77                     | 0.47              |
| 1:G:122:PHE:CE2  | 1:G:700:VAL:HA   | 2.50                     | 0.47              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:G:747:LEU:C    | 1:G:749:GLY:N    | 2.71                     | 0.47              |
| 1:G:795:ARG:HB2  | 3:I:35:ARG:CZ    | 2.44                     | 0.47              |
| 1:J:166:MET:HE3  | 1:J:459:ILE:HG13 | 1.96                     | 0.47              |
| 1:J:689:GLU:O    | 1:J:689:GLU:HG2  | 2.14                     | 0.47              |
| 4:0:162:ASN:OD1  | 4:0:277:THR:HG22 | 2.15                     | 0.47              |
| 4:1:162:ASN:OD1  | 4:1:277:THR:HG22 | 2.15                     | 0.47              |
| 4:3:213:LYS:O    | 4:3:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:8:213:LYS:O    | 4:8:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:9:162:ASN:OD1  | 4:9:277:THR:HG22 | 2.15                     | 0.47              |
| 4:9:288:ASP:CA   | 4:W:204:ALA:HB2  | 2.31                     | 0.47              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:OD2  | 2.73                     | 0.47              |
| 1:A:501:GLU:CA   | 1:A:762:HIS:CE1  | 2.98                     | 0.47              |
| 1:A:564:ASN:HD22 | 1:A:582:VAL:HB   | 1.79                     | 0.47              |
| 1:D:499:GLU:OE1  | 1:D:499:GLU:HA   | 2.13                     | 0.47              |
| 1:D:636:LYS:O    | 4:9:144:ALA:HB1  | 2.14                     | 0.47              |
| 1:D:642:LYS:HB2  | 4:9:24:ASP:O     | 1.88                     | 0.47              |
| 3:F:53:PRO:O     | 3:F:55:LYS:HG3   | 2.14                     | 0.47              |
| 1:G:404:PRO:HD2  | 1:G:415:MLY:O    | 2.13                     | 0.47              |
| 1:G:418:THR:CB   | 1:G:421:GLU:HG3  | 2.36                     | 0.47              |
| 1:G:542:PHE:CD2  | 4:V:143:TYR:CD1  | 3.03                     | 0.47              |
| 1:G:819:ASN:CB   | 2:H:92:ASP:HB2   | 2.41                     | 0.47              |
| 1:J:154:HIS:CE1  | 1:J:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:J:406:VAL:CG1  | 1:J:407:GLY:N    | 2.77                     | 0.47              |
| 1:J:554:LEU:HD12 | 1:J:554:LEU:HA   | 1.77                     | 0.47              |
| 1:J:568:PRO:HD3  | 1:J:579:PHE:HA   | 1.96                     | 0.47              |
| 4:2:162:ASN:OD1  | 4:2:277:THR:HG22 | 2.15                     | 0.47              |
| 4:8:217:CYS:C    | 4:8:218:TYR:HD1  | 2.22                     | 0.47              |
| 4:V:217:CYS:C    | 4:V:218:TYR:HD1  | 2.22                     | 0.47              |
| 4:Y:120:THR:HG21 | 4:Y:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:Z:162:ASN:OD1  | 4:Z:277:THR:HG22 | 2.15                     | 0.47              |
| 4:Z:253:GLU:HA   | 4:Z:256:ARG:CG   | 2.42                     | 0.47              |
| 1:A:309:PRO:C    | 1:A:311:ASP:H    | 2.22                     | 0.47              |
| 1:A:400:ALA:HB1  | 1:A:606:THR:CG2  | 2.45                     | 0.47              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:CD1  | 0.65                     | 0.47              |
| 1:D:309:PRO:C    | 1:D:311:ASP:H    | 2.22                     | 0.47              |
| 1:D:311:ASP:CB   | 1:D:312:TYR:CE1  | 2.98                     | 0.47              |
| 1:D:402:CYS:C    | 1:D:404:PRO:HD3  | 2.40                     | 0.47              |
| 1:D:524:GLU:HB3  | 1:D:528:MLY:HG2  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:629:GLU:CB   | 1:D:645:SER:N    | 2.74                     | 0.47              |
| 1:D:724:TYR:HD1  | 1:D:727:LEU:CD1  | 2.27                     | 0.47              |
| 1:D:783:LEU:HA   | 1:D:786:ILE:HB   | 1.97                     | 0.47              |
| 1:D:809:ARG:NH1  | 2:E:124:GLY:O    | 2.47                     | 0.47              |
| 1:D:818:TYR:HB3  | 2:E:89:LYS:C     | 2.39                     | 0.47              |
| 1:D:822:SER:HB3  | 2:E:88:LEU:CD2   | 2.38                     | 0.47              |
| 1:G:214:MET:HA   | 1:G:340:ILE:CD1  | 2.41                     | 0.47              |
| 1:G:215:GLN:H    | 1:G:340:ILE:CD1  | 2.20                     | 0.47              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:HB3  | 1.95                     | 0.47              |
| 1:G:595:TRP:N    | 1:G:595:TRP:CD1  | 2.80                     | 0.47              |
| 1:G:689:GLU:O    | 1:G:689:GLU:HG2  | 2.14                     | 0.47              |
| 1:G:695:LEU:HB3  | 1:G:701:LEU:HD22 | 1.97                     | 0.47              |
| 2:H:121:LEU:HA   | 2:H:128:PHE:CD2  | 2.47                     | 0.47              |
| 1:J:400:ALA:HB1  | 1:J:606:THR:CG2  | 2.45                     | 0.47              |
| 1:J:406:VAL:CG1  | 1:J:407:GLY:H    | 2.28                     | 0.47              |
| 1:J:499:GLU:OE1  | 1:J:499:GLU:HA   | 2.13                     | 0.47              |
| 1:J:519:LEU:N    | 1:J:519:LEU:CD1  | 2.77                     | 0.47              |
| 1:J:524:GLU:HB3  | 1:J:528:MLY:HG2  | 1.97                     | 0.47              |
| 1:J:530:MET:HA   | 4:W:354:GLN:CD   | 2.11                     | 0.47              |
| 1:J:602:PRO:O    | 1:J:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:J:640:LYS:HD2  | 1:J:646:PHE:O    | 2.14                     | 0.47              |
| 1:J:725:ARG:NE   | 1:J:733:PRO:CB   | 1.95                     | 0.47              |
| 1:J:839:MLY:HH21 | 2:K:158:THR:HG22 | 1.96                     | 0.47              |
| 2:K:137:TRP:CZ3  | 2:K:145:ALA:N    | 2.81                     | 0.47              |
| 4:O:166:TYR:OH   | 4:2:64:ILE:HD13  | 2.15                     | 0.47              |
| 4:1:203:THR:CA   | 4:Z:287:ILE:HB   | 2.44                     | 0.47              |
| 4:1:217:CYS:C    | 4:1:218:TYR:HD1  | 2.22                     | 0.47              |
| 4:3:162:ASN:OD1  | 4:3:277:THR:HG22 | 2.15                     | 0.47              |
| 4:3:287:ILE:HG21 | 4:5:204:ALA:N    | 2.28                     | 0.47              |
| 4:V:253:GLU:HA   | 4:V:256:ARG:CG   | 2.42                     | 0.47              |
| 4:W:120:THR:HG21 | 4:W:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:Y:217:CYS:C    | 4:Y:218:TYR:HD1  | 2.22                     | 0.47              |
| 1:A:406:VAL:CG1  | 1:A:407:GLY:H    | 2.28                     | 0.47              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:CD1  | 0.63                     | 0.47              |
| 1:D:543:PRO:HD2  | 4:9:146:GLY:O    | 2.15                     | 0.47              |
| 1:D:695:LEU:HB3  | 1:D:701:LEU:HD22 | 1.97                     | 0.47              |
| 1:D:739:ASP:OD1  | 1:D:739:ASP:C    | 2.58                     | 0.47              |
| 1:G:406:VAL:CG1  | 1:G:407:GLY:N    | 2.77                     | 0.47              |
| 1:G:765:VAL:CG1  | 1:G:766:PHE:N    | 2.77                     | 0.47              |
| 1:G:831:TRP:CZ2  | 2:H:67:MET:CB    | 2.98                     | 0.47              |
| 4:7:253:GLU:HA   | 4:7:256:ARG:CG   | 2.42                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:88:LEU:HB3   | 2:B:91:ALA:HB2   | 1.97                     | 0.47              |
| 1:D:30:MLY:HB3   | 1:D:31:PRO:HD2   | 1.97                     | 0.47              |
| 1:D:221:GLN:HG2  | 1:D:221:GLN:H    | 1.47                     | 0.47              |
| 1:D:400:ALA:HB1  | 1:D:606:THR:CG2  | 2.45                     | 0.47              |
| 1:D:406:VAL:CG1  | 1:D:407:GLY:N    | 2.77                     | 0.47              |
| 1:D:496:PHE:CE2  | 1:D:514:ASP:HA   | 2.50                     | 0.47              |
| 1:D:769:ALA:HB1  | 1:D:771:LEU:N    | 2.22                     | 0.47              |
| 1:D:822:SER:HG   | 2:E:87:LYS:C     | 2.20                     | 0.47              |
| 2:E:112:ILE:CG2  | 2:E:147:ASN:O    | 2.62                     | 0.47              |
| 1:G:406:VAL:CG1  | 1:G:407:GLY:H    | 2.28                     | 0.47              |
| 1:G:559:LEU:HD23 | 1:G:560:GLY:N    | 2.30                     | 0.47              |
| 1:G:793:ARG:HB2  | 3:I:40:ASN:ND2   | 2.30                     | 0.47              |
| 1:J:122:PHE:CE2  | 1:J:700:VAL:HA   | 2.50                     | 0.47              |
| 1:J:311:ASP:CB   | 1:J:312:TYR:CE1  | 2.98                     | 0.47              |
| 1:J:714:ARG:HD3  | 1:J:766:PHE:CE2  | 2.50                     | 0.47              |
| 1:J:836:PHE:CD2  | 2:K:160:GLY:C    | 2.88                     | 0.47              |
| 3:L:50:LEU:O     | 3:L:53:PRO:CD    | 2.63                     | 0.47              |
| 1:A:202:SER:HA   | 1:A:207:LYS:NZ   | 2.22                     | 0.47              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:HB3  | 1.95                     | 0.47              |
| 1:A:636:LYS:O    | 4:8:144:ALA:HB1  | 2.15                     | 0.47              |
| 2:B:121:LEU:O    | 2:B:128:PHE:CG   | 2.61                     | 0.47              |
| 3:C:53:PRO:O     | 3:C:55:LYS:HG3   | 2.14                     | 0.47              |
| 1:D:122:PHE:CE2  | 1:D:700:VAL:HA   | 2.50                     | 0.47              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:H    | 1.79                     | 0.47              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:CD1  | 0.65                     | 0.47              |
| 1:G:188:ASN:ND2  | 1:G:674:CYS:SG   | 2.88                     | 0.47              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:HB2  | 1.96                     | 0.47              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:CD   | 2.73                     | 0.47              |
| 1:J:106:LEU:HD12 | 1:J:117:THR:HG21 | 1.96                     | 0.47              |
| 1:J:248:MLY:HE2  | 1:J:250:ILE:HD11 | 1.95                     | 0.47              |
| 1:J:402:CYS:C    | 1:J:404:PRO:HD3  | 2.39                     | 0.47              |
| 1:J:578:HIS:HB3  | 1:J:592:ILE:CD1  | 2.38                     | 0.47              |
| 1:J:715:VAL:CG1  | 1:J:720:PHE:HB2  | 2.45                     | 0.47              |
| 2:K:160:GLY:O    | 2:K:161:GLU:HG2  | 2.14                     | 0.47              |
| 4:4:162:ASN:OD1  | 4:4:277:THR:HG22 | 2.15                     | 0.47              |
| 4:8:162:ASN:OD1  | 4:8:277:THR:HG22 | 2.15                     | 0.47              |
| 4:V:162:ASN:OD1  | 4:V:277:THR:HG22 | 2.15                     | 0.47              |
| 1:A:106:LEU:HD12 | 1:A:117:THR:HG21 | 1.96                     | 0.46              |
| 1:A:188:ASN:ND2  | 1:A:674:CYS:SG   | 2.88                     | 0.46              |
| 1:A:265:ILE:CG2  | 1:A:266:GLU:N    | 2.78                     | 0.46              |
| 1:A:524:GLU:HB3  | 1:A:528:MLY:HG2  | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:640:LYS:HB3  | 1:A:645:SER:CB   | 2.42                     | 0.46              |
| 1:A:724:TYR:HD1  | 1:A:727:LEU:CD1  | 2.27                     | 0.46              |
| 1:A:757:GLN:CD   | 1:A:771:LEU:CD1  | 2.86                     | 0.46              |
| 1:D:42:HIS:O     | 1:D:45:GLN:O     | 2.33                     | 0.46              |
| 1:D:541:MET:CG   | 4:9:345:ILE:C    | 2.87                     | 0.46              |
| 1:D:556:ASP:CA   | 4:W:49:GLN:O     | 2.52                     | 0.46              |
| 1:D:723:ARG:O    | 1:D:782:MLY:HD2  | 1.97                     | 0.46              |
| 1:D:822:SER:HB3  | 2:E:88:LEU:HD21  | 1.97                     | 0.46              |
| 1:G:202:SER:HA   | 1:G:207:LYS:NZ   | 2.22                     | 0.46              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:H    | 1.79                     | 0.46              |
| 1:G:543:PRO:HD2  | 4:V:146:GLY:O    | 2.16                     | 0.46              |
| 1:G:640:LYS:HB3  | 1:G:645:SER:CB   | 2.42                     | 0.46              |
| 1:G:646:PHE:HE2  | 1:G:652:LEU:CG   | 2.24                     | 0.46              |
| 1:G:823:PHE:CD1  | 2:H:157:ILE:HA   | 2.50                     | 0.46              |
| 1:G:823:PHE:CZ   | 2:H:156:VAL:HG12 | 2.50                     | 0.46              |
| 3:I:53:PRO:O     | 3:I:55:LYS:HG3   | 2.14                     | 0.46              |
| 1:J:206:LYS:HD2  | 1:J:217:THR:CG2  | 2.17                     | 0.46              |
| 1:J:374:GLN:NE2  | 1:J:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:J:496:PHE:CE2  | 1:J:514:ASP:HA   | 2.50                     | 0.46              |
| 4:W:6:THR:HG22   | 4:W:101:HIS:HA   | 1.97                     | 0.46              |
| 1:A:144:ARG:HA   | 1:A:144:ARG:HD2  | 1.79                     | 0.46              |
| 1:A:332:MET:O    | 1:A:336:SER:OG   | 2.27                     | 0.46              |
| 1:A:541:MET:SD   | 4:8:345:ILE:C    | 2.95                     | 0.46              |
| 1:A:559:LEU:HD23 | 1:A:560:GLY:N    | 2.30                     | 0.46              |
| 1:A:810:ARG:HG2  | 1:A:810:ARG:NH1  | 2.29                     | 0.46              |
| 1:D:406:VAL:CG1  | 1:D:407:GLY:H    | 2.28                     | 0.46              |
| 1:D:709:LYS:C    | 1:D:710:GLY:HA2  | 2.39                     | 0.46              |
| 1:D:714:ARG:HD3  | 1:D:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:D:715:VAL:CG1  | 1:D:720:PHE:HB2  | 2.46                     | 0.46              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CD1  | 1.04                     | 0.46              |
| 1:G:139:VAL:HG12 | 1:G:143:TYR:HD2  | 1.81                     | 0.46              |
| 1:G:541:MET:HE2  | 4:V:346:LEU:HD12 | 1.96                     | 0.46              |
| 1:G:568:PRO:HD3  | 1:G:579:PHE:HA   | 1.97                     | 0.46              |
| 1:G:784:ALA:O    | 1:G:788:THR:CA   | 2.61                     | 0.46              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:H    | 1.79                     | 0.46              |
| 1:J:503:TYR:CZ   | 1:J:711:PHE:CD2  | 3.03                     | 0.46              |
| 1:J:529:PRO:HB2  | 4:W:354:GLN:HB3  | 1.98                     | 0.46              |
| 1:J:559:LEU:HD23 | 1:J:560:GLY:N    | 2.30                     | 0.46              |
| 4:0:217:CYS:C    | 4:0:218:TYR:HD1  | 2.22                     | 0.46              |
| 4:2:217:CYS:C    | 4:2:218:TYR:HD1  | 2.22                     | 0.46              |
| 4:9:6:THR:HG22   | 4:9:101:HIS:HA   | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:6:THR:HG22   | 4:Y:101:HIS:HA   | 1.97                     | 0.46              |
| 1:A:42:HIS:O     | 1:A:45:GLN:O     | 2.33                     | 0.46              |
| 1:A:136:ASN:HA   | 1:A:137:PRO:HD3  | 1.49                     | 0.46              |
| 1:A:541:MET:HE2  | 4:8:346:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:568:PRO:HD3  | 1:A:579:PHE:HA   | 1.96                     | 0.46              |
| 1:A:714:ARG:HD3  | 1:A:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:839:MLY:NZ   | 2:B:159:HIS:CB   | 2.63                     | 0.46              |
| 1:D:166:MET:HE3  | 1:D:459:ILE:HG13 | 1.96                     | 0.46              |
| 1:D:529:PRO:HB2  | 4:9:354:GLN:HB3  | 1.98                     | 0.46              |
| 1:D:540:CYS:N    | 4:9:349:LEU:HD11 | 2.31                     | 0.46              |
| 1:D:543:PRO:CD   | 4:9:143:TYR:O    | 2.64                     | 0.46              |
| 1:D:595:TRP:N    | 1:D:595:TRP:CD1  | 2.80                     | 0.46              |
| 1:G:715:VAL:CG1  | 1:G:720:PHE:HB2  | 2.45                     | 0.46              |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:CD1  | 2.50                     | 0.46              |
| 1:J:42:HIS:O     | 1:J:45:GLN:O     | 2.33                     | 0.46              |
| 1:J:540:CYS:N    | 4:W:349:LEU:HD11 | 2.30                     | 0.46              |
| 1:J:749:GLY:O    | 3:L:114:LEU:HD22 | 2.13                     | 0.46              |
| 1:J:757:GLN:OE1  | 1:J:773:GLY:HA2  | 2.16                     | 0.46              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:CA   | 2.45                     | 0.46              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:OD1  | 2.64                     | 0.46              |
| 4:Z:217:CYS:C    | 4:Z:218:TYR:HD1  | 2.22                     | 0.46              |
| 1:A:87:MLY:HH12  | 1:A:87:MLY:HD3   | 1.61                     | 0.46              |
| 1:A:715:VAL:CG1  | 1:A:720:PHE:HB2  | 2.45                     | 0.46              |
| 1:A:795:ARG:HG3  | 3:C:118:MET:HE1  | 1.95                     | 0.46              |
| 1:D:374:GLN:NE2  | 1:D:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:D:640:LYS:HB3  | 1:D:645:SER:CB   | 2.42                     | 0.46              |
| 1:G:311:ASP:CB   | 1:G:312:TYR:CE1  | 2.98                     | 0.46              |
| 1:G:400:ALA:HB1  | 1:G:606:THR:CG2  | 2.45                     | 0.46              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG1   | 2.29                     | 0.46              |
| 1:G:659:MLY:HD2  | 1:G:659:MLY:HH22 | 1.42                     | 0.46              |
| 1:G:724:TYR:HD1  | 1:G:727:LEU:CD1  | 2.27                     | 0.46              |
| 1:J:82:PRO:HG2   | 1:J:85:TYR:CE2   | 2.50                     | 0.46              |
| 1:J:793:ARG:O    | 1:J:797:PHE:N    | 2.39                     | 0.46              |
| 4:8:287:ILE:CB   | 4:V:204:ALA:H    | 2.13                     | 0.46              |
| 4:8:288:ASP:CG   | 4:V:203:THR:C    | 2.83                     | 0.46              |
| 4:Y:366:GLY:O    | 4:Y:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:A:361:TYR:O    | 1:A:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:A:543:PRO:HD2  | 4:8:146:GLY:O    | 2.15                     | 0.46              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:HG13 | 1.97                     | 0.46              |
| 1:D:332:MET:H    | 1:D:332:MET:HG2  | 1.52                     | 0.46              |
| 1:D:726:VAL:H    | 1:D:782:MLY:HH21 | 1.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:210:GLN:C    | 1:G:211:SER:HG   | 2.16                     | 0.46              |
| 1:G:374:GLN:NE2  | 1:G:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:G:524:GLU:HB3  | 1:G:528:MLY:HG2  | 1.96                     | 0.46              |
| 1:G:636:LYS:O    | 4:V:144:ALA:HB1  | 2.14                     | 0.46              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:OG1  | 2.16                     | 0.46              |
| 1:J:541:MET:CG   | 4:W:345:ILE:C    | 2.87                     | 0.46              |
| 4:0:6:THR:HG22   | 4:0:101:HIS:HA   | 1.97                     | 0.46              |
| 4:0:246:GLN:HA   | 4:Y:324:THR:HG1  | 1.76                     | 0.46              |
| 4:5:162:ASN:OD1  | 4:5:277:THR:HG22 | 2.15                     | 0.46              |
| 4:5:217:CYS:C    | 4:5:218:TYR:HD1  | 2.22                     | 0.46              |
| 4:7:47:MET:HE2   | 4:7:47:MET:HB2   | 1.79                     | 0.46              |
| 4:W:286:ASP:HA   | 4:Y:202:THR:HG22 | 1.32                     | 0.46              |
| 1:A:311:ASP:CB   | 1:A:312:TYR:CE1  | 2.98                     | 0.46              |
| 1:A:326:ASP:O    | 1:A:330:GLU:HG2  | 2.16                     | 0.46              |
| 1:A:335:ASP:OD1  | 1:A:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:A:374:GLN:NE2  | 1:A:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:A:543:PRO:CD   | 4:8:143:TYR:O    | 2.63                     | 0.46              |
| 1:A:695:LEU:HB3  | 1:A:701:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:783:LEU:N    | 1:A:783:LEU:CD1  | 2.78                     | 0.46              |
| 1:D:82:PRO:HG2   | 1:D:85:TYR:CE2   | 2.51                     | 0.46              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:OG1  | 2.16                     | 0.46              |
| 1:D:265:ILE:CG2  | 1:D:266:GLU:N    | 2.78                     | 0.46              |
| 1:D:724:TYR:N    | 1:D:782:MLY:CH2  | 2.79                     | 0.46              |
| 1:D:818:TYR:HB3  | 2:E:89:LYS:HB2   | 1.98                     | 0.46              |
| 1:G:354:LEU:HD12 | 1:G:354:LEU:HA   | 1.56                     | 0.46              |
| 1:G:714:ARG:HD3  | 1:G:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:G:835:PHE:O    | 1:G:839:MLY:N    | 2.49                     | 0.46              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:HH21 | 2.06                     | 0.46              |
| 1:J:194:GLN:HE21 | 1:J:194:GLN:HB3  | 1.43                     | 0.46              |
| 1:J:309:PRO:C    | 1:J:311:ASP:H    | 2.22                     | 0.46              |
| 1:J:754:ASP:CB   | 1:J:776:GLU:HB3  | 2.03                     | 0.46              |
| 4:0:253:GLU:HA   | 4:0:256:ARG:CG   | 2.42                     | 0.46              |
| 4:7:6:THR:HG22   | 4:7:101:HIS:HA   | 1.98                     | 0.46              |
| 4:7:288:ASP:CG   | 4:9:203:THR:C    | 2.83                     | 0.46              |
| 4:W:366:GLY:O    | 4:W:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:X:324:THR:O    | 4:Z:245:GLY:CA   | 2.64                     | 0.46              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:OG1  | 2.16                     | 0.46              |
| 1:A:214:MET:HA   | 1:A:340:ILE:CD1  | 2.41                     | 0.46              |
| 1:A:411:GLU:H    | 4:8:333:PRO:HB2  | 1.80                     | 0.46              |
| 1:A:502:GLU:OE2  | 1:A:764:MLY:O    | 2.33                     | 0.46              |
| 1:A:642:LYS:CB   | 4:8:24:ASP:O     | 2.59                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:665:ARG:C    | 1:A:667:THR:N    | 2.74                     | 0.46              |
| 1:A:725:ARG:NE   | 1:A:733:PRO:CB   | 1.95                     | 0.46              |
| 1:D:335:ASP:OD1  | 1:D:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:D:629:GLU:HB3  | 1:D:643:GLY:C    | 2.41                     | 0.46              |
| 2:E:114:LYS:CG   | 2:E:146:GLY:HA2  | 2.46                     | 0.46              |
| 1:G:42:HIS:O     | 1:G:45:GLN:O     | 2.33                     | 0.46              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:OG1  | 2.16                     | 0.46              |
| 1:G:326:ASP:O    | 1:G:330:GLU:HG2  | 2.16                     | 0.46              |
| 1:G:335:ASP:OD1  | 1:G:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:G:757:GLN:NE2  | 1:G:772:LEU:CD2  | 2.79                     | 0.46              |
| 2:H:88:LEU:HB3   | 2:H:91:ALA:HB2   | 1.98                     | 0.46              |
| 2:H:149:ASP:CG   | 2:H:150:TYR:N    | 2.49                     | 0.46              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:HG13 | 1.98                     | 0.46              |
| 1:J:543:PRO:HD2  | 4:W:146:GLY:O    | 2.15                     | 0.46              |
| 4:2:6:THR:HG22   | 4:2:101:HIS:HA   | 1.97                     | 0.46              |
| 1:A:418:THR:CB   | 1:A:421:GLU:HG3  | 2.36                     | 0.46              |
| 1:A:464:ILE:CG2  | 1:A:465:ALA:N    | 2.79                     | 0.46              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:CE1  | 2.44                     | 0.46              |
| 3:C:50:LEU:O     | 3:C:53:PRO:CD    | 2.63                     | 0.46              |
| 1:D:559:LEU:HD23 | 1:D:560:GLY:N    | 2.30                     | 0.46              |
| 2:E:149:ASP:CG   | 2:E:150:TYR:N    | 2.49                     | 0.46              |
| 1:G:136:ASN:HA   | 1:G:137:PRO:HD3  | 1.49                     | 0.46              |
| 1:G:278:GLN:HE21 | 1:G:278:GLN:HB3  | 1.42                     | 0.46              |
| 1:G:361:TYR:O    | 1:G:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:G:725:ARG:NE   | 1:G:733:PRO:CB   | 1.95                     | 0.46              |
| 2:H:137:TRP:CZ3  | 2:H:145:ALA:N    | 2.81                     | 0.46              |
| 1:J:30:MLY:HB3   | 1:J:31:PRO:HD2   | 1.97                     | 0.46              |
| 1:J:361:TYR:O    | 1:J:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:J:695:LEU:HB3  | 1:J:701:LEU:HD22 | 1.97                     | 0.46              |
| 1:J:815:CYS:SG   | 2:K:92:ASP:OD1   | 2.73                     | 0.46              |
| 4:1:223:PHE:CD2  | 4:1:259:GLU:HG3  | 2.51                     | 0.46              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:HB3  | 2.16                     | 0.46              |
| 4:2:366:GLY:O    | 4:2:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:4:6:THR:HG22   | 4:4:101:HIS:HA   | 1.97                     | 0.46              |
| 4:7:324:THR:N    | 4:9:245:GLY:CA   | 2.69                     | 0.46              |
| 4:7:366:GLY:O    | 4:7:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:9:366:GLY:O    | 4:9:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:A:418:THR:CG2  | 1:A:419:VAL:N    | 2.79                     | 0.46              |
| 1:D:99:GLU:N     | 1:D:100:PRO:CD   | 2.79                     | 0.46              |
| 1:D:664:LEU:HD12 | 1:D:664:LEU:HA   | 1.53                     | 0.46              |
| 3:F:50:LEU:O     | 3:F:53:PRO:CD    | 2.63                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:55:MLY:HH23  | 1:G:60:VAL:HG22  | 1.98                     | 0.46              |
| 1:G:82:PRO:HG2   | 1:G:85:TYR:CE2   | 2.51                     | 0.46              |
| 1:G:665:ARG:C    | 1:G:667:THR:N    | 2.74                     | 0.46              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG13 | 1.95                     | 0.46              |
| 2:K:88:LEU:HB3   | 2:K:91:ALA:HB2   | 1.98                     | 0.46              |
| 2:K:112:ILE:O    | 2:K:148:VAL:HA   | 2.16                     | 0.46              |
| 3:L:52:ASN:CB    | 3:L:53:PRO:CD    | 2.92                     | 0.46              |
| 4:O:247:VAL:N    | 4:Y:324:THR:CB   | 2.77                     | 0.46              |
| 4:4:190:MET:O    | 4:4:194:THR:HG23 | 2.16                     | 0.46              |
| 1:A:332:MET:H    | 1:A:332:MET:HG2  | 1.52                     | 0.46              |
| 1:A:793:ARG:HE   | 3:C:147:MET:CB   | 2.29                     | 0.46              |
| 1:A:793:ARG:O    | 1:A:797:PHE:N    | 2.40                     | 0.46              |
| 2:B:137:TRP:CA   | 2:B:145:ALA:HB2  | 2.37                     | 0.46              |
| 1:D:136:ASN:O    | 1:D:139:VAL:N    | 2.47                     | 0.46              |
| 1:D:136:ASN:HA   | 1:D:137:PRO:HD3  | 1.49                     | 0.46              |
| 1:D:476:GLU:OE2  | 1:D:598:MLY:HH13 | 2.16                     | 0.46              |
| 1:D:665:ARG:C    | 1:D:667:THR:N    | 2.74                     | 0.46              |
| 1:D:810:ARG:HG2  | 1:D:810:ARG:NH1  | 2.29                     | 0.46              |
| 1:G:206:LYS:HD2  | 1:G:217:THR:CG2  | 2.17                     | 0.46              |
| 1:G:411:GLU:H    | 4:V:333:PRO:HB2  | 1.80                     | 0.46              |
| 1:G:436:MLY:HE3  | 1:G:626:TYR:HE1  | 1.77                     | 0.46              |
| 1:G:543:PRO:CD   | 4:V:143:TYR:O    | 2.64                     | 0.46              |
| 1:G:664:LEU:HD12 | 1:G:664:LEU:HA   | 1.52                     | 0.46              |
| 1:J:265:ILE:CG2  | 1:J:266:GLU:N    | 2.78                     | 0.46              |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:CD1  | 2.49                     | 0.46              |
| 1:J:783:LEU:N    | 1:J:783:LEU:CD1  | 2.78                     | 0.46              |
| 1:J:797:PHE:CD2  | 3:L:126:LEU:HD22 | 2.50                     | 0.46              |
| 1:J:797:PHE:CE2  | 3:L:126:LEU:CD2  | 2.99                     | 0.46              |
| 1:J:800:ARG:CB   | 3:L:149:VAL:HG23 | 2.26                     | 0.46              |
| 4:O:190:MET:O    | 4:O:194:THR:HG23 | 2.16                     | 0.46              |
| 4:5:190:MET:O    | 4:5:194:THR:HG23 | 2.16                     | 0.46              |
| 4:W:223:PHE:CD2  | 4:W:259:GLU:HG3  | 2.51                     | 0.46              |
| 4:W:253:GLU:HA   | 4:W:256:ARG:CG   | 2.42                     | 0.46              |
| 1:A:17:LEU:HD12  | 1:A:17:LEU:HA    | 1.68                     | 0.45              |
| 1:A:82:PRO:HG2   | 1:A:85:TYR:CE2   | 2.50                     | 0.45              |
| 1:A:322:VAL:HB   | 1:A:325:ILE:HG13 | 1.98                     | 0.45              |
| 1:A:476:GLU:OE2  | 1:A:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:G:322:VAL:HB   | 1:G:325:ILE:HG13 | 1.98                     | 0.45              |
| 1:G:332:MET:O    | 1:G:336:SER:OG   | 2.27                     | 0.45              |
| 1:G:464:ILE:CG2  | 1:G:465:ALA:N    | 2.79                     | 0.45              |
| 1:J:202:SER:HA   | 1:J:207:LYS:NZ   | 2.22                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:335:ASP:OD1  | 1:J:348:MLY:NZ   | 2.49                     | 0.45              |
| 1:J:642:LYS:NZ   | 4:W:340:TRP:O    | 2.50                     | 0.45              |
| 1:J:817:GLN:CB   | 2:K:127:ARG:HD2  | 2.46                     | 0.45              |
| 4:3:190:MET:O    | 4:3:194:THR:HG23 | 2.16                     | 0.45              |
| 4:3:223:PHE:CD2  | 4:3:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:3:366:GLY:O    | 4:3:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:5:6:THR:HG22   | 4:5:101:HIS:HA   | 1.97                     | 0.45              |
| 4:W:287:ILE:HG13 | 4:Y:202:THR:HG23 | 1.72                     | 0.45              |
| 4:X:223:PHE:CD2  | 4:X:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:Z:223:PHE:CD2  | 4:Z:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:A:139:VAL:HG12 | 1:A:143:TYR:HD2  | 1.81                     | 0.45              |
| 1:A:296:MLY:O    | 1:A:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:A:637:LYS:HD2  | 4:8:144:ALA:HB3  | 1.21                     | 0.45              |
| 1:A:723:ARG:CG   | 1:A:723:ARG:NH1  | 2.79                     | 0.45              |
| 1:D:410:ASN:HA   | 4:9:334:GLU:HB3  | 1.29                     | 0.45              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:CB    | 2.95                     | 0.45              |
| 1:G:30:MLY:HB3   | 1:G:31:PRO:HD2   | 1.97                     | 0.45              |
| 1:G:186:THR:O    | 1:G:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:G:540:CYS:N    | 4:V:349:LEU:HD11 | 2.31                     | 0.45              |
| 2:H:112:ILE:O    | 2:H:148:VAL:HA   | 2.16                     | 0.45              |
| 1:J:56:GLU:HB2   | 1:J:59:MLY:CB    | 2.30                     | 0.45              |
| 1:J:330:GLU:O    | 1:J:333:ALA:HB3  | 2.16                     | 0.45              |
| 1:J:541:MET:SD   | 4:W:345:ILE:C    | 2.95                     | 0.45              |
| 1:J:798:LEU:HA   | 1:J:798:LEU:HD12 | 1.36                     | 0.45              |
| 4:1:366:GLY:O    | 4:1:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:2:190:MET:O    | 4:2:194:THR:HG23 | 2.16                     | 0.45              |
| 4:4:223:PHE:CD2  | 4:4:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:8:253:GLU:HA   | 4:8:256:ARG:CG   | 2.42                     | 0.45              |
| 4:9:288:ASP:CG   | 4:W:203:THR:C    | 2.83                     | 0.45              |
| 4:V:32:PRO:HB2   | 4:V:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:W:190:MET:O    | 4:W:194:THR:HG23 | 2.16                     | 0.45              |
| 1:A:55:MLY:HH23  | 1:A:60:VAL:HG22  | 1.99                     | 0.45              |
| 1:A:206:LYS:CE   | 1:A:217:THR:HG23 | 2.29                     | 0.45              |
| 1:A:496:PHE:CE2  | 1:A:514:ASP:HA   | 2.50                     | 0.45              |
| 1:A:529:PRO:HB2  | 4:8:354:GLN:HB3  | 1.97                     | 0.45              |
| 1:A:642:LYS:HB2  | 4:8:24:ASP:O     | 1.88                     | 0.45              |
| 1:A:667:THR:O    | 1:A:669:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:733:PRO:O    | 1:A:737:PHE:CE1  | 2.53                     | 0.45              |
| 1:D:330:GLU:O    | 1:D:333:ALA:HB3  | 2.17                     | 0.45              |
| 1:D:464:ILE:CG2  | 1:D:465:ALA:N    | 2.79                     | 0.45              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:H    | 2.14                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:112:ILE:O    | 2:E:148:VAL:HA   | 2.16                     | 0.45              |
| 1:G:17:LEU:HA    | 1:G:17:LEU:HD12  | 1.67                     | 0.45              |
| 1:G:41:VAL:CG1   | 1:G:42:HIS:N     | 2.75                     | 0.45              |
| 1:G:93:MET:SD    | 1:G:763:THR:CG2  | 2.95                     | 0.45              |
| 1:G:144:ARG:HA   | 1:G:144:ARG:HD2  | 1.78                     | 0.45              |
| 1:G:265:ILE:CG2  | 1:G:266:GLU:N    | 2.78                     | 0.45              |
| 1:G:795:ARG:NE   | 3:I:118:MET:HE1  | 2.31                     | 0.45              |
| 1:J:84:MLY:HH23  | 1:J:716:LEU:O    | 2.12                     | 0.45              |
| 1:J:186:THR:O    | 1:J:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:J:332:MET:O    | 1:J:336:SER:OG   | 2.27                     | 0.45              |
| 1:J:723:ARG:CG   | 1:J:723:ARG:NH1  | 2.79                     | 0.45              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:CD1  | 0.65                     | 0.45              |
| 1:J:797:PHE:HE2  | 3:L:126:LEU:HD23 | 1.81                     | 0.45              |
| 4:0:47:MET:HE2   | 4:0:47:MET:HB2   | 1.79                     | 0.45              |
| 4:0:366:GLY:O    | 4:0:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:3:6:THR:HG22   | 4:3:101:HIS:HA   | 1.97                     | 0.45              |
| 4:4:366:GLY:O    | 4:4:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:5:32:PRO:HB2   | 4:5:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:9:223:PHE:CD2  | 4:9:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:9:290:ARG:HH22 | 4:W:202:THR:CG2  | 2.17                     | 0.45              |
| 4:X:6:THR:HG22   | 4:X:101:HIS:HA   | 1.97                     | 0.45              |
| 1:A:30:MLY:HB3   | 1:A:31:PRO:HD2   | 1.97                     | 0.45              |
| 1:A:179:GLY:O    | 1:A:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:A:210:GLN:C    | 1:A:211:SER:HG   | 2.10                     | 0.45              |
| 1:D:97:LEU:HD12  | 1:D:97:LEU:HA    | 1.67                     | 0.45              |
| 1:D:411:GLU:H    | 4:9:333:PRO:CB   | 2.29                     | 0.45              |
| 1:D:449:LEU:HD12 | 1:D:449:LEU:HA   | 1.60                     | 0.45              |
| 1:D:510:TRP:CZ3  | 1:D:711:PHE:CE2  | 3.04                     | 0.45              |
| 1:D:723:ARG:C    | 1:D:782:MLY:CH2  | 2.89                     | 0.45              |
| 1:D:725:ARG:HH21 | 1:D:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:D:818:TYR:CD2  | 2:E:89:LYS:HB3   | 2.52                     | 0.45              |
| 1:G:541:MET:SD   | 4:V:345:ILE:C    | 2.96                     | 0.45              |
| 1:G:629:GLU:CB   | 1:G:645:SER:N    | 2.74                     | 0.45              |
| 1:G:637:LYS:HD2  | 4:V:144:ALA:HB3  | 1.20                     | 0.45              |
| 1:G:639:GLY:CA   | 4:V:344:SER:O    | 2.40                     | 0.45              |
| 2:H:114:LYS:CG   | 2:H:146:GLY:HA2  | 2.46                     | 0.45              |
| 3:I:50:LEU:O     | 3:I:53:PRO:CD    | 2.63                     | 0.45              |
| 1:J:84:MLY:HG2   | 1:J:719:ASP:OD2  | 2.16                     | 0.45              |
| 1:J:88:ILE:HG22  | 1:J:90:ASP:C     | 2.42                     | 0.45              |
| 1:J:476:GLU:OE2  | 1:J:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:J:534:SER:HB2  | 4:W:354:GLN:HE22 | 1.56                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:724:TYR:HD1  | 1:J:727:LEU:CD1  | 2.27                     | 0.45              |
| 1:J:725:ARG:HA   | 1:J:732:ILE:HG22 | 1.99                     | 0.45              |
| 4:8:366:GLY:O    | 4:8:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:X:32:PRO:HB2   | 4:X:34:ILE:HD11  | 1.98                     | 0.45              |
| 2:B:112:ILE:O    | 2:B:148:VAL:HA   | 2.16                     | 0.45              |
| 1:D:179:GLY:O    | 1:D:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:D:830:PRO:CB   | 2:E:51:PHE:CE2   | 2.94                     | 0.45              |
| 1:G:476:GLU:OE2  | 1:G:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:G:642:LYS:NZ   | 4:V:340:TRP:O    | 2.50                     | 0.45              |
| 1:G:725:ARG:HH21 | 1:G:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:J:17:LEU:HA    | 1:J:17:LEU:HD12  | 1.68                     | 0.45              |
| 1:J:640:LYS:HB3  | 1:J:645:SER:CB   | 2.42                     | 0.45              |
| 1:J:732:ILE:H    | 1:J:733:PRO:HD2  | 1.74                     | 0.45              |
| 4:V:6:THR:HG22   | 4:V:101:HIS:HA   | 1.97                     | 0.45              |
| 4:X:190:MET:O    | 4:X:194:THR:HG23 | 2.16                     | 0.45              |
| 4:Z:32:PRO:HB2   | 4:Z:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:411:GLU:H    | 4:8:333:PRO:CB   | 2.30                     | 0.45              |
| 1:A:768:MLY:CA   | 1:A:771:LEU:HB2  | 2.45                     | 0.45              |
| 1:D:103:LEU:HD22 | 1:D:692:LEU:HG   | 1.98                     | 0.45              |
| 1:D:229:LEU:HD12 | 1:D:229:LEU:HA   | 1.75                     | 0.45              |
| 1:D:296:MLY:O    | 1:D:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:D:326:ASP:O    | 1:D:330:GLU:HG2  | 2.16                     | 0.45              |
| 1:D:361:TYR:O    | 1:D:364:LEU:HB2  | 2.16                     | 0.45              |
| 1:D:642:LYS:NZ   | 4:9:340:TRP:O    | 2.50                     | 0.45              |
| 1:D:725:ARG:CG   | 1:D:733:PRO:HA   | 2.43                     | 0.45              |
| 1:D:783:LEU:N    | 1:D:783:LEU:CD1  | 2.78                     | 0.45              |
| 1:D:818:TYR:CD2  | 2:E:89:LYS:CB    | 2.99                     | 0.45              |
| 1:D:834:LEU:CD2  | 2:E:50:THR:HG22  | 2.46                     | 0.45              |
| 1:D:835:PHE:O    | 1:D:839:MLY:N    | 2.49                     | 0.45              |
| 1:G:173:GLN:HG3  | 1:G:670:HIS:HD2  | 1.82                     | 0.45              |
| 1:G:418:THR:CG2  | 1:G:419:VAL:N    | 2.79                     | 0.45              |
| 1:G:529:PRO:HB2  | 4:V:354:GLN:HB3  | 1.98                     | 0.45              |
| 1:G:728:ASN:ND2  | 3:I:110:VAL:HA   | 2.20                     | 0.45              |
| 1:J:173:GLN:HG3  | 1:J:670:HIS:HD2  | 1.82                     | 0.45              |
| 1:J:179:GLY:O    | 1:J:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:J:326:ASP:O    | 1:J:330:GLU:HG2  | 2.16                     | 0.45              |
| 1:J:797:PHE:HD2  | 3:L:126:LEU:CD2  | 2.27                     | 0.45              |
| 4:0:201:VAL:CB   | 4:Y:287:ILE:HG13 | 2.46                     | 0.45              |
| 4:1:190:MET:O    | 4:1:194:THR:HG23 | 2.16                     | 0.45              |
| 4:5:366:GLY:O    | 4:5:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:7:32:PRO:HB2   | 4:7:34:ILE:HD11  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:190:MET:O    | 4:7:194:THR:HG23 | 2.16                     | 0.45              |
| 4:Y:190:MET:O    | 4:Y:194:THR:HG23 | 2.16                     | 0.45              |
| 1:A:37:SER:O     | 1:A:38:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:206:LYS:HD2  | 1:A:217:THR:CG2  | 2.17                     | 0.45              |
| 1:A:278:GLN:HE21 | 1:A:278:GLN:HB3  | 1.41                     | 0.45              |
| 1:A:540:CYS:N    | 4:8:349:LEU:HD11 | 2.31                     | 0.45              |
| 1:A:643:GLY:N    | 4:8:23:GLY:C     | 2.55                     | 0.45              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CD1  | 2.46                     | 0.45              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:HD11 | 1.99                     | 0.45              |
| 1:D:708:ARG:O    | 1:D:710:GLY:N    | 2.50                     | 0.45              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:HD3   | 1.92                     | 0.45              |
| 2:E:163:ALA:C    | 2:K:22:THR:HG1   | 2.22                     | 0.45              |
| 1:G:410:ASN:HA   | 4:V:334:GLU:HB3  | 1.28                     | 0.45              |
| 1:G:485:GLU:OE1  | 1:G:583:HIS:ND1  | 2.49                     | 0.45              |
| 1:G:496:PHE:CE2  | 1:G:514:ASP:HA   | 2.50                     | 0.45              |
| 1:G:597:GLU:O    | 1:G:600:MLY:N    | 2.50                     | 0.45              |
| 1:G:823:PHE:CE2  | 2:H:140:PHE:CZ   | 3.05                     | 0.45              |
| 4:2:32:PRO:HB2   | 4:2:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:5:47:MET:HE2   | 4:5:47:MET:HB2   | 1.79                     | 0.45              |
| 4:5:223:PHE:CD2  | 4:5:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:8:6:THR:HG22   | 4:8:101:HIS:HA   | 1.97                     | 0.45              |
| 4:8:190:MET:O    | 4:8:194:THR:HG23 | 2.16                     | 0.45              |
| 4:Y:253:GLU:HA   | 4:Y:256:ARG:CG   | 2.42                     | 0.45              |
| 1:A:41:VAL:CG1   | 1:A:42:HIS:N     | 2.75                     | 0.45              |
| 1:A:322:VAL:CG1  | 1:A:325:ILE:HD11 | 2.47                     | 0.45              |
| 1:A:550:PHE:C    | 4:V:46:GLY:CA    | 2.87                     | 0.45              |
| 1:D:14:ALA:N     | 1:D:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:D:37:SER:O     | 1:D:38:VAL:HG23  | 2.17                     | 0.45              |
| 1:D:88:ILE:HG22  | 1:D:90:ASP:C     | 2.42                     | 0.45              |
| 1:D:202:SER:HA   | 1:D:207:LYS:NZ   | 2.22                     | 0.45              |
| 1:D:226:ASN:N    | 1:D:227:PRO:HD2  | 2.32                     | 0.45              |
| 1:D:597:GLU:O    | 1:D:600:MLY:N    | 2.50                     | 0.45              |
| 1:G:14:ALA:N     | 1:G:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:G:92:ALA:HB3   | 1:G:764:MLY:HH13 | 1.31                     | 0.45              |
| 1:G:99:GLU:N     | 1:G:100:PRO:CD   | 2.80                     | 0.45              |
| 1:G:176:LEU:N    | 1:G:176:LEU:CD1  | 2.74                     | 0.45              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:H    | 2.14                     | 0.45              |
| 1:G:643:GLY:N    | 4:V:23:GLY:C     | 2.55                     | 0.45              |
| 1:G:725:ARG:CG   | 1:G:733:PRO:CA   | 2.95                     | 0.45              |
| 1:G:794:CYS:O    | 1:G:797:PHE:HB3  | 2.17                     | 0.45              |
| 1:J:642:LYS:CB   | 4:W:24:ASP:O     | 2.60                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:794:CYS:O    | 1:J:797:PHE:HB3  | 2.17                     | 0.45              |
| 2:K:137:TRP:CA   | 2:K:145:ALA:HB2  | 2.37                     | 0.45              |
| 4:0:32:PRO:HB2   | 4:0:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:1:322:PRO:CA   | 4:3:244:ASP:HB2  | 2.47                     | 0.45              |
| 1:A:106:LEU:HD12 | 1:A:106:LEU:HA   | 1.79                     | 0.45              |
| 1:A:519:LEU:N    | 1:A:519:LEU:CD1  | 2.77                     | 0.45              |
| 1:A:642:LYS:NZ   | 4:8:340:TRP:O    | 2.50                     | 0.45              |
| 1:D:139:VAL:HG12 | 1:D:143:TYR:HD2  | 1.81                     | 0.45              |
| 1:D:186:THR:O    | 1:D:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:D:568:PRO:CG   | 1:D:578:HIS:H    | 2.30                     | 0.45              |
| 1:D:724:TYR:CZ   | 1:D:778:MET:CB   | 2.96                     | 0.45              |
| 1:G:93:MET:HE2   | 1:G:763:THR:CB   | 2.21                     | 0.45              |
| 1:G:296:MLY:O    | 1:G:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:G:567:LYS:HZ2  | 4:X:92:ASN:ND2   | 1.80                     | 0.45              |
| 1:G:757:GLN:HE22 | 1:G:772:LEU:HG   | 1.81                     | 0.45              |
| 2:H:137:TRP:CA   | 2:H:145:ALA:HB2  | 2.37                     | 0.45              |
| 1:J:226:ASN:N    | 1:J:227:PRO:HD2  | 2.32                     | 0.45              |
| 1:J:541:MET:CE   | 4:W:346:LEU:HD12 | 2.47                     | 0.45              |
| 1:J:597:GLU:O    | 1:J:600:MLY:N    | 2.50                     | 0.45              |
| 4:0:223:PHE:CD2  | 4:0:259:GLU:HG3  | 2.52                     | 0.45              |
| 4:3:32:PRO:HB2   | 4:3:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:8:32:PRO:HB2   | 4:8:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:V:223:PHE:CD2  | 4:V:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:Z:299:MET:HE2  | 4:Z:299:MET:HB2  | 1.82                     | 0.45              |
| 4:Z:366:GLY:O    | 4:Z:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:163:TYR:O    | 1:A:166:MET:HB3  | 2.16                     | 0.45              |
| 1:A:224:SER:O    | 1:A:227:PRO:HD2  | 2.17                     | 0.45              |
| 1:A:488:GLN:O    | 1:A:491:PHE:HB3  | 2.17                     | 0.45              |
| 1:D:64:THR:HB    | 1:D:68:GLU:N     | 2.32                     | 0.45              |
| 1:D:106:LEU:HD12 | 1:D:106:LEU:HA   | 1.79                     | 0.45              |
| 1:G:519:LEU:N    | 1:G:519:LEU:CD1  | 2.77                     | 0.45              |
| 1:J:14:ALA:N     | 1:J:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:J:37:SER:O     | 1:J:38:VAL:HG23  | 2.17                     | 0.45              |
| 1:J:93:MET:HG2   | 1:J:764:MLY:HD3  | 0.93                     | 0.45              |
| 1:J:408:VAL:HG22 | 1:J:636:LYS:HG2  | 1.52                     | 0.45              |
| 1:J:464:ILE:CG2  | 1:J:465:ALA:N    | 2.79                     | 0.45              |
| 1:J:629:GLU:HB3  | 1:J:643:GLY:C    | 2.41                     | 0.45              |
| 1:J:667:THR:O    | 1:J:669:PRO:HD3  | 2.16                     | 0.45              |
| 1:J:725:ARG:HH21 | 1:J:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HD12 | 0.95                     | 0.45              |
| 4:1:32:PRO:HB2   | 4:1:34:ILE:HD11  | 1.98                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:7:288:ASP:CA  | 4:9:204:ALA:HB2  | 2.31                     | 0.45              |
| 4:8:223:PHE:CD2 | 4:8:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:8:324:THR:N   | 4:V:245:GLY:CA   | 2.69                     | 0.45              |
| 4:9:32:PRO:HB2  | 4:9:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:X:253:GLU:HA  | 4:X:256:ARG:CG   | 2.42                     | 0.45              |
| 4:X:366:GLY:O   | 4:X:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:Y:223:PHE:CD2 | 4:Y:259:GLU:HG3  | 2.52                     | 0.45              |
| 1:A:186:THR:O   | 1:A:190:MLY:HG2  | 2.17                     | 0.44              |
| 1:A:195:TYR:CE2 | 1:A:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:A:346:ASP:O   | 1:A:350:ALA:N    | 2.46                     | 0.44              |
| 1:A:597:GLU:O   | 1:A:600:MLY:N    | 2.50                     | 0.44              |
| 1:A:629:GLU:HB3 | 1:A:643:GLY:C    | 2.41                     | 0.44              |
| 1:A:711:PHE:HB3 | 1:A:766:PHE:HB3  | 1.99                     | 0.44              |
| 1:A:794:CYS:O   | 1:A:797:PHE:HB3  | 2.17                     | 0.44              |
| 1:A:831:TRP:CZ2 | 2:B:51:PHE:CE1   | 3.04                     | 0.44              |
| 2:B:144:VAL:C   | 2:B:153:ILE:HD11 | 2.42                     | 0.44              |
| 1:D:41:VAL:CG1  | 1:D:42:HIS:N     | 2.75                     | 0.44              |
| 1:D:163:TYR:O   | 1:D:166:MET:HB3  | 2.17                     | 0.44              |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:C    | 2.60                     | 0.44              |
| 1:D:689:GLU:HA  | 1:D:692:LEU:HB2  | 1.99                     | 0.44              |
| 2:E:137:TRP:CZ3 | 2:E:145:ALA:N    | 2.81                     | 0.44              |
| 1:G:64:THR:HB   | 1:G:68:GLU:N     | 2.32                     | 0.44              |
| 1:G:408:VAL:CG1 | 4:V:332:PRO:HB3  | 2.41                     | 0.44              |
| 1:G:485:GLU:HA  | 1:G:584:TYR:HE2  | 1.82                     | 0.44              |
| 1:G:488:GLN:O   | 1:G:491:PHE:HB3  | 2.17                     | 0.44              |
| 1:G:629:GLU:HB3 | 1:G:643:GLY:C    | 2.41                     | 0.44              |
| 1:G:667:THR:O   | 1:G:669:PRO:HD3  | 2.16                     | 0.44              |
| 1:J:296:MLY:O   | 1:J:299:LEU:HB2  | 2.17                     | 0.44              |
| 1:J:322:VAL:CG1 | 1:J:325:ILE:HD11 | 2.47                     | 0.44              |
| 1:J:543:PRO:CD  | 4:W:143:TYR:O    | 2.64                     | 0.44              |
| 1:J:639:GLY:H   | 4:W:344:SER:HB3  | 1.82                     | 0.44              |
| 1:J:689:GLU:HA  | 1:J:692:LEU:HB2  | 2.00                     | 0.44              |
| 1:J:829:TRP:HA  | 1:J:830:PRO:HD2  | 1.86                     | 0.44              |
| 4:0:223:PHE:HB3 | 4:0:259:GLU:OE2  | 2.17                     | 0.44              |
| 4:0:287:ILE:CB  | 4:2:203:THR:HB   | 2.47                     | 0.44              |
| 4:2:223:PHE:HB3 | 4:2:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:4:32:PRO:HB2  | 4:4:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:4:253:GLU:HA  | 4:4:256:ARG:CG   | 2.42                     | 0.44              |
| 4:5:223:PHE:HB3 | 4:5:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:7:223:PHE:HB3 | 4:7:259:GLU:OE2  | 2.17                     | 0.44              |
| 4:9:190:MET:O   | 4:9:194:THR:HG23 | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:W:32:PRO:HB2   | 4:W:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:W:223:PHE:HB3  | 4:W:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:48:VAL:HA    | 1:A:104:TYR:OH   | 2.18                     | 0.44              |
| 1:A:64:THR:HB    | 1:A:68:GLU:N     | 2.33                     | 0.44              |
| 1:A:97:LEU:HD12  | 1:A:97:LEU:HA    | 1.67                     | 0.44              |
| 1:A:99:GLU:N     | 1:A:100:PRO:CD   | 2.80                     | 0.44              |
| 1:A:229:LEU:HD12 | 1:A:229:LEU:HA   | 1.75                     | 0.44              |
| 1:D:278:GLN:HE21 | 1:D:278:GLN:HB3  | 1.42                     | 0.44              |
| 1:D:488:GLN:O    | 1:D:491:PHE:HB3  | 2.17                     | 0.44              |
| 1:G:37:SER:O     | 1:G:38:VAL:HG23  | 2.17                     | 0.44              |
| 1:G:155:ILE:HG22 | 1:G:156:PHE:N    | 2.33                     | 0.44              |
| 1:J:64:THR:HB    | 1:J:68:GLU:N     | 2.33                     | 0.44              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:C    | 2.60                     | 0.44              |
| 1:J:673:ARG:HA   | 1:J:673:ARG:HD2  | 1.79                     | 0.44              |
| 4:2:223:PHE:CD2  | 4:2:259:GLU:HG3  | 2.51                     | 0.44              |
| 4:7:223:PHE:CD2  | 4:7:259:GLU:HG3  | 2.51                     | 0.44              |
| 4:9:223:PHE:HB3  | 4:9:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:Z:6:THR:HG22   | 4:Z:101:HIS:HA   | 1.97                     | 0.44              |
| 1:A:725:ARG:HH21 | 1:A:733:PRO:HB2  | 1.81                     | 0.44              |
| 1:A:800:ARG:NE   | 3:C:149:VAL:C    | 2.75                     | 0.44              |
| 1:D:725:ARG:CG   | 1:D:733:PRO:CA   | 2.95                     | 0.44              |
| 1:D:794:CYS:O    | 1:D:797:PHE:HB3  | 2.16                     | 0.44              |
| 2:E:121:LEU:O    | 2:E:128:PHE:CG   | 2.61                     | 0.44              |
| 2:E:163:ALA:CA   | 2:K:21:GLU:HB3   | 2.36                     | 0.44              |
| 1:G:136:ASN:O    | 1:G:139:VAL:N    | 2.47                     | 0.44              |
| 1:G:179:GLY:O    | 1:G:185:LYS:HE2  | 2.17                     | 0.44              |
| 1:G:411:GLU:H    | 4:V:333:PRO:CB   | 2.29                     | 0.44              |
| 2:H:144:VAL:C    | 2:H:153:ILE:HD11 | 2.42                     | 0.44              |
| 1:J:99:GLU:N     | 1:J:100:PRO:CD   | 2.80                     | 0.44              |
| 1:J:408:VAL:HA   | 1:J:636:LYS:HG3  | 1.03                     | 0.44              |
| 1:J:410:ASN:HA   | 4:W:334:GLU:HB3  | 1.29                     | 0.44              |
| 1:J:488:GLN:O    | 1:J:491:PHE:HB3  | 2.17                     | 0.44              |
| 1:J:797:PHE:CE2  | 3:L:126:LEU:HD23 | 2.52                     | 0.44              |
| 4:8:223:PHE:HB3  | 4:8:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:9:47:MET:HE2   | 4:9:47:MET:HB2   | 1.79                     | 0.44              |
| 4:Y:223:PHE:HB3  | 4:Y:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:289:TYR:OH   | 1:A:315:VAL:O    | 2.27                     | 0.44              |
| 1:A:835:PHE:O    | 1:A:839:MLY:N    | 2.49                     | 0.44              |
| 1:D:136:ASN:C    | 1:D:138:MLY:N    | 2.75                     | 0.44              |
| 1:D:642:LYS:HG3  | 4:9:23:GLY:CA    | 2.31                     | 0.44              |
| 1:D:675:ILE:HG23 | 1:D:676:ILE:N    | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:692:LEU:O    | 1:D:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:D:809:ARG:NH2  | 2:E:124:GLY:HA3  | 2.33                     | 0.44              |
| 1:D:813:ILE:CG2  | 2:E:127:ARG:NH1  | 2.76                     | 0.44              |
| 2:E:129:THR:HG23 | 2:E:132:GLU:OE1  | 2.18                     | 0.44              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:N    | 2.31                     | 0.44              |
| 1:G:103:LEU:HD22 | 1:G:692:LEU:HG   | 1.98                     | 0.44              |
| 1:G:530:MET:CE   | 4:V:354:GLN:CB   | 2.95                     | 0.44              |
| 1:G:723:ARG:CG   | 1:G:723:ARG:NH1  | 2.79                     | 0.44              |
| 2:H:129:THR:HG23 | 2:H:132:GLU:OE1  | 2.17                     | 0.44              |
| 1:J:163:TYR:O    | 1:J:166:MET:HB3  | 2.17                     | 0.44              |
| 1:J:443:ILE:HG22 | 1:J:444:ARG:N    | 2.29                     | 0.44              |
| 1:J:692:LEU:O    | 1:J:696:ARG:HG3  | 2.18                     | 0.44              |
| 2:K:113:LYS:C    | 2:K:147:ASN:HB2  | 2.43                     | 0.44              |
| 2:K:114:LYS:CG   | 2:K:146:GLY:HA2  | 2.46                     | 0.44              |
| 4:1:6:THR:HG22   | 4:1:101:HIS:HA   | 1.97                     | 0.44              |
| 4:3:288:ASP:OD2  | 4:5:203:THR:OG1  | 2.32                     | 0.44              |
| 4:4:253:GLU:H    | 4:4:253:GLU:CD   | 2.25                     | 0.44              |
| 4:V:190:MET:O    | 4:V:194:THR:HG23 | 2.16                     | 0.44              |
| 4:V:223:PHE:HB3  | 4:V:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:V:287:ILE:HG13 | 4:X:202:THR:HG23 | 1.65                     | 0.44              |
| 4:W:253:GLU:H    | 4:W:253:GLU:CD   | 2.25                     | 0.44              |
| 4:X:220:ALA:HB3  | 4:X:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:X:253:GLU:CD   | 4:X:253:GLU:H    | 2.25                     | 0.44              |
| 4:Y:32:PRO:HB2   | 4:Y:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:Z:190:MET:O    | 4:Z:194:THR:HG23 | 2.16                     | 0.44              |
| 1:A:103:LEU:HD22 | 1:A:692:LEU:HG   | 1.98                     | 0.44              |
| 1:A:123:CYS:CB   | 1:A:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:516:GLY:O    | 1:A:518:ASP:N    | 2.51                     | 0.44              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CB   | 2.74                     | 0.44              |
| 1:A:655:GLU:CD   | 4:8:1:ASP:HB2    | 2.43                     | 0.44              |
| 1:A:701:LEU:HA   | 1:A:701:LEU:HD12 | 1.54                     | 0.44              |
| 1:A:709:LYS:C    | 1:A:710:GLY:CA   | 2.75                     | 0.44              |
| 1:A:725:ARG:CG   | 1:A:733:PRO:CA   | 2.95                     | 0.44              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CG   | 2.46                     | 0.44              |
| 1:D:166:MET:CE   | 1:D:254:PHE:HB2  | 2.46                     | 0.44              |
| 1:D:322:VAL:CG1  | 1:D:325:ILE:HD11 | 2.47                     | 0.44              |
| 1:D:418:THR:CG2  | 1:D:419:VAL:N    | 2.79                     | 0.44              |
| 1:D:725:ARG:CZ   | 1:D:733:PRO:CB   | 2.83                     | 0.44              |
| 1:G:88:ILE:HG22  | 1:G:90:ASP:C     | 2.42                     | 0.44              |
| 1:G:214:MET:CA   | 1:G:340:ILE:HD11 | 2.45                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:493:HIS:O    | 1:G:496:PHE:HB3  | 2.18                     | 0.44              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:C    | 2.60                     | 0.44              |
| 1:G:692:LEU:O    | 1:G:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:G:725:ARG:CZ   | 1:G:733:PRO:CB   | 2.83                     | 0.44              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:CD1  | 0.64                     | 0.44              |
| 1:G:823:PHE:HE1  | 2:H:156:VAL:O    | 1.90                     | 0.44              |
| 1:J:139:VAL:HG12 | 1:J:143:TYR:HD2  | 1.81                     | 0.44              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:J:411:GLU:H    | 4:W:333:PRO:CB   | 2.30                     | 0.44              |
| 1:J:485:GLU:OE1  | 1:J:583:HIS:ND1  | 2.49                     | 0.44              |
| 1:J:516:GLY:O    | 1:J:518:ASP:N    | 2.51                     | 0.44              |
| 1:J:568:PRO:CG   | 1:J:578:HIS:H    | 2.30                     | 0.44              |
| 1:J:725:ARG:CG   | 1:J:733:PRO:CA   | 2.95                     | 0.44              |
| 2:K:129:THR:HG23 | 2:K:132:GLU:OE1  | 2.17                     | 0.44              |
| 3:L:122:GLU:HA   | 3:L:125:GLU:OE1  | 2.18                     | 0.44              |
| 4:3:287:ILE:HG13 | 4:5:202:THR:HA   | 1.40                     | 0.44              |
| 4:8:193:LEU:O    | 4:8:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:8:287:ILE:HA   | 4:V:202:THR:HG21 | 1.59                     | 0.44              |
| 4:9:253:GLU:H    | 4:9:253:GLU:CD   | 2.25                     | 0.44              |
| 4:V:366:GLY:O    | 4:V:369:ILE:HG22 | 2.16                     | 0.44              |
| 1:A:14:ALA:N     | 1:A:15:PRO:HD2   | 2.32                     | 0.44              |
| 1:A:173:GLN:HG3  | 1:A:670:HIS:HD2  | 1.82                     | 0.44              |
| 1:A:226:ASN:N    | 1:A:227:PRO:HD2  | 2.32                     | 0.44              |
| 1:A:439:LEU:N    | 1:A:439:LEU:CD1  | 2.81                     | 0.44              |
| 1:A:485:GLU:HA   | 1:A:584:TYR:HE2  | 1.83                     | 0.44              |
| 1:A:485:GLU:OE2  | 1:A:584:TYR:N    | 2.50                     | 0.44              |
| 1:A:632:GLY:HA3  | 1:A:643:GLY:N    | 2.17                     | 0.44              |
| 1:A:675:ILE:HG23 | 1:A:676:ILE:N    | 2.32                     | 0.44              |
| 1:A:692:LEU:O    | 1:A:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:A:831:TRP:CG   | 2:B:51:PHE:CZ    | 3.03                     | 0.44              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:NE2  | 2.32                     | 0.44              |
| 1:D:723:ARG:HH21 | 1:D:783:LEU:CD1  | 2.30                     | 0.44              |
| 1:D:726:VAL:CA   | 1:D:782:MLY:HH13 | 2.44                     | 0.44              |
| 1:D:798:LEU:HA   | 1:D:798:LEU:HD12 | 1.36                     | 0.44              |
| 1:G:163:TYR:O    | 1:G:166:MET:HB3  | 2.17                     | 0.44              |
| 1:G:330:GLU:O    | 1:G:333:ALA:HB3  | 2.17                     | 0.44              |
| 1:G:675:ILE:HG23 | 1:G:676:ILE:N    | 2.32                     | 0.44              |
| 3:I:119:THR:O    | 3:I:123:VAL:HG23 | 2.18                     | 0.44              |
| 1:J:103:LEU:HD22 | 1:J:692:LEU:HG   | 1.98                     | 0.44              |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:CD1  | 2.47                     | 0.44              |
| 4:1:220:ALA:HB3  | 4:1:223:PHE:CD1  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:5:171:LEU:HA   | 4:5:172:PRO:HD2  | 1.84                     | 0.44              |
| 4:5:253:GLU:CD   | 4:5:253:GLU:H    | 2.26                     | 0.44              |
| 1:A:88:ILE:HG22  | 1:A:90:ASP:C     | 2.42                     | 0.44              |
| 1:A:530:MET:CE   | 4:8:354:GLN:CB   | 2.96                     | 0.44              |
| 1:D:206:LYS:CE   | 1:D:217:THR:HG23 | 2.29                     | 0.44              |
| 1:D:266:GLU:OE1  | 1:D:659:MLY:NZ   | 2.51                     | 0.44              |
| 1:D:439:LEU:N    | 1:D:439:LEU:CD1  | 2.81                     | 0.44              |
| 1:D:485:GLU:OE1  | 1:D:583:HIS:ND1  | 2.49                     | 0.44              |
| 1:D:541:MET:HB3  | 4:9:345:ILE:HG22 | 2.00                     | 0.44              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:HG22 | 2.00                     | 0.44              |
| 2:E:113:LYS:C    | 2:E:147:ASN:HB2  | 2.43                     | 0.44              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:G:226:ASN:HB2  | 1:G:227:PRO:CD   | 2.47                     | 0.44              |
| 1:G:322:VAL:CG1  | 1:G:325:ILE:HD11 | 2.47                     | 0.44              |
| 1:G:708:ARG:HA   | 1:G:714:ARG:NH2  | 2.33                     | 0.44              |
| 1:G:751:GLY:C    | 1:G:753:VAL:HG22 | 2.43                     | 0.44              |
| 3:I:122:GLU:HA   | 3:I:125:GLU:OE1  | 2.18                     | 0.44              |
| 1:J:55:MLY:HH23  | 1:J:60:VAL:HG22  | 1.99                     | 0.44              |
| 1:J:136:ASN:HA   | 1:J:137:PRO:HD3  | 1.49                     | 0.44              |
| 1:J:174:SER:OG   | 1:J:669:PRO:HA   | 2.18                     | 0.44              |
| 1:J:439:LEU:N    | 1:J:439:LEU:CD1  | 2.81                     | 0.44              |
| 1:J:642:LYS:HB2  | 4:W:24:ASP:O     | 1.88                     | 0.44              |
| 1:J:675:ILE:HG23 | 1:J:676:ILE:N    | 2.32                     | 0.44              |
| 1:J:725:ARG:CG   | 1:J:733:PRO:HA   | 2.43                     | 0.44              |
| 1:J:790:THR:N    | 3:L:87:PHE:HE2   | 2.12                     | 0.44              |
| 3:L:50:LEU:O     | 3:L:53:PRO:HG2   | 2.18                     | 0.44              |
| 4:O:205:GLU:O    | 4:O:208:ILE:HG22 | 2.18                     | 0.44              |
| 4:V:220:ALA:HB3  | 4:V:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:W:205:GLU:O    | 4:W:208:ILE:HG22 | 2.18                     | 0.44              |
| 4:Z:220:ALA:HB3  | 4:Z:223:PHE:CD1  | 2.53                     | 0.44              |
| 1:A:530:MET:CB   | 4:8:354:GLN:CB   | 2.95                     | 0.44              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:C    | 2.60                     | 0.44              |
| 1:A:639:GLY:H    | 4:8:344:SER:HB3  | 1.82                     | 0.44              |
| 1:D:123:CYS:CB   | 1:D:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:D:667:THR:O    | 1:D:669:PRO:HD3  | 2.16                     | 0.44              |
| 1:D:711:PHE:HB3  | 1:D:766:PHE:HB3  | 1.99                     | 0.44              |
| 2:E:137:TRP:CA   | 2:E:145:ALA:HB2  | 2.37                     | 0.44              |
| 3:F:122:GLU:HA   | 3:F:125:GLU:OE1  | 2.18                     | 0.44              |
| 1:G:14:ALA:N     | 1:G:15:PRO:CD    | 2.81                     | 0.44              |
| 1:G:136:ASN:C    | 1:G:138:MLY:N    | 2.75                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:193:ILE:HD11 | 1:G:250:ILE:CD1  | 2.48                     | 0.44              |
| 1:G:224:SER:O    | 1:G:227:PRO:HD2  | 2.17                     | 0.44              |
| 1:G:661:MET:HE3  | 1:G:661:MET:HB3  | 1.74                     | 0.44              |
| 3:I:50:LEU:O     | 3:I:53:PRO:HG2   | 2.18                     | 0.44              |
| 3:I:69:LEU:HB3   | 3:I:70:PRO:HD3   | 1.99                     | 0.44              |
| 3:I:101:THR:HA   | 3:I:137:ILE:O    | 2.18                     | 0.44              |
| 1:J:123:CYS:CB   | 1:J:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:J:129:TYR:HD1  | 1:J:129:TYR:HA   | 1.65                     | 0.44              |
| 1:J:136:ASN:C    | 1:J:138:MLY:N    | 2.75                     | 0.44              |
| 1:J:144:ARG:HA   | 1:J:144:ARG:HD2  | 1.78                     | 0.44              |
| 1:J:210:GLN:C    | 1:J:211:SER:HG   | 2.18                     | 0.44              |
| 1:J:308:ASN:HA   | 1:J:309:PRO:HD2  | 1.88                     | 0.44              |
| 1:J:493:HIS:O    | 1:J:496:PHE:HB3  | 2.18                     | 0.44              |
| 1:J:810:ARG:HG2  | 1:J:810:ARG:NH1  | 2.29                     | 0.44              |
| 3:L:101:THR:HA   | 3:L:137:ILE:O    | 2.18                     | 0.44              |
| 4:3:193:LEU:O    | 4:3:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:3:253:GLU:CD   | 4:3:253:GLU:H    | 2.25                     | 0.44              |
| 4:3:287:ILE:HB   | 4:5:204:ALA:H    | 1.83                     | 0.44              |
| 4:5:193:LEU:O    | 4:5:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:Y:253:GLU:H    | 4:Y:253:GLU:CD   | 2.25                     | 0.44              |
| 1:A:174:SER:OG   | 1:A:669:PRO:HA   | 2.18                     | 0.44              |
| 1:A:391:GLY:HA3  | 1:A:616:VAL:HG23 | 2.00                     | 0.44              |
| 1:A:641:LYS:C    | 4:8:22:ALA:O     | 2.60                     | 0.44              |
| 1:A:715:VAL:HG12 | 1:A:720:PHE:HB2  | 2.00                     | 0.44              |
| 1:A:787:ILE:HG23 | 1:A:791:GLN:HG3  | 2.00                     | 0.44              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:HE2  | 2.29                     | 0.44              |
| 1:A:839:MLY:CE   | 2:B:159:HIS:HB3  | 2.48                     | 0.44              |
| 2:B:113:LYS:C    | 2:B:147:ASN:HB2  | 2.43                     | 0.44              |
| 2:B:137:TRP:CZ3  | 2:B:145:ALA:N    | 2.81                     | 0.44              |
| 1:D:55:MLY:HH23  | 1:D:60:VAL:HG22  | 1.99                     | 0.44              |
| 1:D:485:GLU:OE2  | 1:D:584:TYR:N    | 2.50                     | 0.44              |
| 1:D:516:GLY:O    | 1:D:518:ASP:N    | 2.51                     | 0.44              |
| 1:D:788:THR:HG22 | 3:F:81:GLN:HE22  | 1.83                     | 0.44              |
| 1:D:793:ARG:HE   | 3:F:147:MET:CG   | 2.30                     | 0.44              |
| 2:E:88:LEU:HB3   | 2:E:91:ALA:HB2   | 1.98                     | 0.44              |
| 1:J:202:SER:C    | 1:J:207:LYS:HE3  | 2.43                     | 0.44              |
| 1:J:206:LYS:CE   | 1:J:217:THR:HG23 | 2.29                     | 0.44              |
| 1:J:576:GLU:CG   | 1:J:577:ALA:N    | 2.43                     | 0.44              |
| 1:J:747:LEU:HD23 | 1:J:747:LEU:C    | 2.43                     | 0.44              |
| 3:L:69:LEU:HB3   | 3:L:70:PRO:HD3   | 1.99                     | 0.44              |
| 4:1:204:ALA:H    | 4:Z:287:ILE:HG22 | 1.75                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:47:MET:HE2   | 4:2:47:MET:HB2   | 1.79                     | 0.44              |
| 4:2:205:GLU:O    | 4:2:208:ILE:HG22 | 2.18                     | 0.44              |
| 4:3:220:ALA:HB3  | 4:3:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:4:149:THR:HA   | 4:4:165:ILE:O    | 2.18                     | 0.44              |
| 4:4:193:LEU:O    | 4:4:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:7:193:LEU:O    | 4:7:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:7:253:GLU:H    | 4:7:253:GLU:CD   | 2.25                     | 0.44              |
| 4:8:220:ALA:HB3  | 4:8:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:X:223:PHE:HB3  | 4:X:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:X:287:ILE:O    | 4:Z:205:GLU:OE2  | 2.36                     | 0.44              |
| 4:Z:223:PHE:HB3  | 4:Z:259:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:HD13 | 2.00                     | 0.43              |
| 1:A:502:GLU:HG2  | 1:A:766:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:541:MET:CE   | 4:8:346:LEU:HD12 | 2.48                     | 0.43              |
| 3:C:50:LEU:O     | 3:C:53:PRO:HG2   | 2.18                     | 0.43              |
| 1:D:48:VAL:HA    | 1:D:104:TYR:OH   | 2.17                     | 0.43              |
| 1:D:173:GLN:HG3  | 1:D:670:HIS:HD2  | 1.82                     | 0.43              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG13 | 1.95                     | 0.43              |
| 1:D:346:ASP:O    | 1:D:350:ALA:N    | 2.46                     | 0.43              |
| 1:D:485:GLU:HA   | 1:D:584:TYR:HE2  | 1.83                     | 0.43              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:N    | 2.33                     | 0.43              |
| 1:D:507:GLY:C    | 1:D:762:HIS:H    | 2.26                     | 0.43              |
| 1:D:530:MET:CB   | 4:9:354:GLN:CB   | 2.95                     | 0.43              |
| 1:D:641:LYS:C    | 4:9:22:ALA:O     | 2.60                     | 0.43              |
| 1:G:123:CYS:CB   | 1:G:158:ILE:HD13 | 2.48                     | 0.43              |
| 1:G:266:GLU:OE1  | 1:G:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:G:439:LEU:N    | 1:G:439:LEU:CD1  | 2.81                     | 0.43              |
| 1:G:787:ILE:HG23 | 1:G:791:GLN:HG3  | 2.00                     | 0.43              |
| 1:J:246:PHE:HB3  | 1:J:270:LEU:HD12 | 2.00                     | 0.43              |
| 1:J:529:PRO:HB3  | 4:W:354:GLN:HA   | 1.99                     | 0.43              |
| 1:J:795:ARG:HH22 | 3:L:43:ASN:HB2   | 1.83                     | 0.43              |
| 1:J:817:GLN:CB   | 2:K:127:ARG:HH11 | 2.22                     | 0.43              |
| 1:J:818:TYR:CB   | 2:K:90:GLY:HA3   | 2.37                     | 0.43              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HD11  | 2.37                     | 0.43              |
| 4:2:253:GLU:CD   | 4:2:253:GLU:H    | 2.25                     | 0.43              |
| 4:2:290:ARG:NH1  | 4:4:202:THR:CG2  | 2.75                     | 0.43              |
| 4:7:287:ILE:CB   | 4:9:204:ALA:H    | 2.13                     | 0.43              |
| 4:8:149:THR:HA   | 4:8:165:ILE:O    | 2.18                     | 0.43              |
| 4:8:253:GLU:CD   | 4:8:253:GLU:H    | 2.25                     | 0.43              |
| 4:V:193:LEU:O    | 4:V:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:X:290:ARG:NH2  | 4:Z:201:VAL:HG21 | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Z:193:LEU:O    | 4:Z:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:201:ALA:O    | 1:A:202:SER:OG   | 2.36                     | 0.43              |
| 1:A:217:THR:HG22 | 1:A:218:LEU:N    | 2.34                     | 0.43              |
| 1:A:348:MLY:HH12 | 1:A:348:MLY:HD2  | 1.82                     | 0.43              |
| 1:A:409:GLY:HA3  | 4:8:332:PRO:C    | 2.43                     | 0.43              |
| 1:A:436:MLY:HE3  | 1:A:626:TYR:HE1  | 1.77                     | 0.43              |
| 1:A:534:SER:CB   | 4:8:351:THR:HA   | 2.48                     | 0.43              |
| 1:A:725:ARG:CZ   | 1:A:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:C    | 2.43                     | 0.43              |
| 2:B:129:THR:HG23 | 2:B:132:GLU:OE1  | 2.18                     | 0.43              |
| 3:C:101:THR:HA   | 3:C:137:ILE:O    | 2.18                     | 0.43              |
| 1:D:40:VAL:HG23  | 1:D:76:GLN:O     | 2.18                     | 0.43              |
| 1:D:768:MLY:O    | 1:D:771:LEU:HD12 | 0.62                     | 0.43              |
| 2:E:112:ILE:O    | 2:E:148:VAL:N    | 2.50                     | 0.43              |
| 3:F:101:THR:HA   | 3:F:137:ILE:O    | 2.18                     | 0.43              |
| 1:G:166:MET:HE1  | 1:G:254:PHE:CB   | 2.46                     | 0.43              |
| 1:G:322:VAL:CG1  | 1:G:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:G:391:GLY:HA3  | 1:G:616:VAL:HG23 | 2.00                     | 0.43              |
| 1:G:409:GLY:HA3  | 4:V:332:PRO:C    | 2.43                     | 0.43              |
| 1:G:639:GLY:H    | 4:V:344:SER:HB3  | 1.83                     | 0.43              |
| 2:H:113:LYS:C    | 2:H:147:ASN:HB2  | 2.43                     | 0.43              |
| 1:J:48:VAL:HA    | 1:J:104:TYR:OH   | 2.18                     | 0.43              |
| 1:J:391:GLY:HA3  | 1:J:616:VAL:HG23 | 2.00                     | 0.43              |
| 1:J:409:GLY:N    | 1:J:636:LYS:CD   | 2.70                     | 0.43              |
| 1:J:541:MET:HB3  | 4:W:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:J:641:LYS:C    | 4:W:22:ALA:O     | 2.60                     | 0.43              |
| 1:J:711:PHE:HB3  | 1:J:766:PHE:HB3  | 1.99                     | 0.43              |
| 1:J:751:GLY:C    | 1:J:753:VAL:HG22 | 2.43                     | 0.43              |
| 4:0:149:THR:HA   | 4:0:165:ILE:O    | 2.19                     | 0.43              |
| 4:1:193:LEU:O    | 4:1:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:3:47:MET:HB2   | 4:3:47:MET:HE2   | 1.79                     | 0.43              |
| 4:4:205:GLU:O    | 4:4:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:4:223:PHE:HB3  | 4:4:259:GLU:OE2  | 2.18                     | 0.43              |
| 4:9:253:GLU:HA   | 4:9:256:ARG:CG   | 2.42                     | 0.43              |
| 4:V:253:GLU:CD   | 4:V:253:GLU:H    | 2.25                     | 0.43              |
| 4:Y:205:GLU:O    | 4:Y:208:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:109:ARG:CD   | 1:A:117:THR:HB   | 2.48                     | 0.43              |
| 1:A:295:MLY:CE   | 1:A:332:MET:CE   | 2.96                     | 0.43              |
| 1:A:496:PHE:HB2  | 1:A:515:PHE:CD2  | 2.53                     | 0.43              |
| 3:C:119:THR:O    | 3:C:123:VAL:HG23 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:122:GLU:HA   | 3:C:125:GLU:OE1  | 2.18                     | 0.43              |
| 1:D:64:THR:CG2   | 1:D:65:GLU:H     | 2.32                     | 0.43              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:HD13 | 2.00                     | 0.43              |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:CD1  | 2.48                     | 0.43              |
| 1:D:322:VAL:CG1  | 1:D:325:ILE:HG13 | 2.48                     | 0.43              |
| 1:D:400:ALA:CB   | 1:D:606:THR:HG22 | 2.48                     | 0.43              |
| 1:D:530:MET:CE   | 4:9:354:GLN:HG3  | 2.35                     | 0.43              |
| 1:D:541:MET:CE   | 4:9:346:LEU:HD12 | 2.47                     | 0.43              |
| 1:D:639:GLY:H    | 4:9:344:SER:HB3  | 1.83                     | 0.43              |
| 1:D:747:LEU:HD23 | 1:D:747:LEU:C    | 2.43                     | 0.43              |
| 1:D:831:TRP:CA   | 2:E:51:PHE:CZ    | 3.01                     | 0.43              |
| 2:E:144:VAL:C    | 2:E:153:ILE:HD11 | 2.42                     | 0.43              |
| 1:G:48:VAL:HA    | 1:G:104:TYR:OH   | 2.18                     | 0.43              |
| 1:G:84:MLY:NZ    | 1:G:719:ASP:O    | 2.17                     | 0.43              |
| 1:G:174:SER:OG   | 1:G:669:PRO:HA   | 2.18                     | 0.43              |
| 1:G:217:THR:HG22 | 1:G:218:LEU:N    | 2.34                     | 0.43              |
| 1:G:568:PRO:CG   | 1:G:578:HIS:H    | 2.29                     | 0.43              |
| 1:G:578:HIS:HB3  | 1:G:592:ILE:CD1  | 2.38                     | 0.43              |
| 1:G:643:GLY:CA   | 4:V:24:ASP:OD1   | 2.62                     | 0.43              |
| 1:G:754:ASP:C    | 1:G:756:THR:H    | 2.27                     | 0.43              |
| 1:G:783:LEU:N    | 1:G:783:LEU:CD1  | 2.78                     | 0.43              |
| 1:J:496:PHE:HB2  | 1:J:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:J:835:PHE:O    | 1:J:839:MLY:N    | 2.49                     | 0.43              |
| 4:2:149:THR:HA   | 4:2:165:ILE:O    | 2.19                     | 0.43              |
| 4:7:149:THR:HA   | 4:7:165:ILE:O    | 2.19                     | 0.43              |
| 4:7:205:GLU:O    | 4:7:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:W:149:THR:HA   | 4:W:165:ILE:O    | 2.19                     | 0.43              |
| 4:X:286:ASP:OD2  | 4:Z:203:THR:HG22 | 2.18                     | 0.43              |
| 4:Z:253:GLU:H    | 4:Z:253:GLU:CD   | 2.25                     | 0.43              |
| 1:A:14:ALA:N     | 1:A:15:PRO:CD    | 2.81                     | 0.43              |
| 1:A:40:VAL:HG23  | 1:A:76:GLN:O     | 2.19                     | 0.43              |
| 1:A:129:TYR:HD1  | 1:A:129:TYR:HA   | 1.65                     | 0.43              |
| 1:A:155:ILE:HG22 | 1:A:156:PHE:N    | 2.33                     | 0.43              |
| 1:A:322:VAL:CG1  | 1:A:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:A:529:PRO:HB3  | 4:8:354:GLN:HA   | 1.99                     | 0.43              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:568:PRO:CG   | 1:A:578:HIS:H    | 2.30                     | 0.43              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:H    | 2.14                     | 0.43              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:OD1  | 2.52                     | 0.43              |
| 1:D:202:SER:C    | 1:D:207:LYS:HE3  | 2.44                     | 0.43              |
| 1:D:223:ILE:C    | 1:D:225:ALA:N    | 2.76                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:226:ASN:HB2  | 1:D:227:PRO:CD   | 2.47                     | 0.43              |
| 1:D:246:PHE:HB3  | 1:D:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:391:GLY:HA3  | 1:D:616:VAL:HG23 | 2.00                     | 0.43              |
| 1:D:508:ILE:HG12 | 1:D:766:PHE:HE1  | 1.35                     | 0.43              |
| 1:D:723:ARG:CG   | 1:D:723:ARG:NH1  | 2.79                     | 0.43              |
| 1:D:751:GLY:C    | 1:D:753:VAL:HG22 | 2.43                     | 0.43              |
| 1:D:754:ASP:C    | 1:D:756:THR:H    | 2.26                     | 0.43              |
| 1:D:818:TYR:CB   | 2:E:89:LYS:HB2   | 2.48                     | 0.43              |
| 1:G:226:ASN:N    | 1:G:227:PRO:HD2  | 2.32                     | 0.43              |
| 1:G:295:MLY:CE   | 1:G:332:MET:CE   | 2.97                     | 0.43              |
| 1:G:689:GLU:HA   | 1:G:692:LEU:HB2  | 1.99                     | 0.43              |
| 1:G:692:LEU:HD23 | 1:G:692:LEU:HA   | 1.84                     | 0.43              |
| 1:G:725:ARG:CZ   | 1:G:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:G:747:LEU:HD23 | 1:G:747:LEU:C    | 2.43                     | 0.43              |
| 1:J:217:THR:HG22 | 1:J:218:LEU:N    | 2.34                     | 0.43              |
| 1:J:322:VAL:CG1  | 1:J:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:J:322:VAL:HA   | 1:J:323:PRO:HD3  | 1.87                     | 0.43              |
| 1:J:400:ALA:CB   | 1:J:606:THR:HG22 | 2.49                     | 0.43              |
| 1:J:754:ASP:HB3  | 1:J:776:GLU:HG3  | 1.71                     | 0.43              |
| 2:K:140:PHE:HA   | 2:K:141:PRO:HD2  | 1.56                     | 0.43              |
| 4:1:223:PHE:HB3  | 4:1:259:GLU:OE2  | 2.18                     | 0.43              |
| 4:2:290:ARG:CZ   | 4:4:202:THR:HG22 | 2.37                     | 0.43              |
| 4:3:223:PHE:HB3  | 4:3:259:GLU:OE2  | 2.18                     | 0.43              |
| 4:V:290:ARG:NH1  | 4:X:202:THR:CG2  | 2.81                     | 0.43              |
| 4:Y:193:LEU:O    | 4:Y:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:86:ASP:OD2   | 1:A:87:MLY:HH22  | 2.19                     | 0.43              |
| 1:A:266:GLU:OE1  | 1:A:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:A:537:GLU:OE1  | 4:8:350:SER:HA   | 2.19                     | 0.43              |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:CD1  | 2.49                     | 0.43              |
| 1:D:144:ARG:HA   | 1:D:144:ARG:HD2  | 1.78                     | 0.43              |
| 1:D:155:ILE:HG22 | 1:D:156:PHE:N    | 2.33                     | 0.43              |
| 1:D:224:SER:O    | 1:D:227:PRO:HD2  | 2.17                     | 0.43              |
| 1:D:493:HIS:O    | 1:D:496:PHE:HB3  | 2.18                     | 0.43              |
| 1:D:813:ILE:HG22 | 2:E:127:ARG:NH1  | 2.07                     | 0.43              |
| 1:G:40:VAL:HG23  | 1:G:76:GLN:O     | 2.19                     | 0.43              |
| 1:G:86:ASP:OD2   | 1:G:87:MLY:HH22  | 2.19                     | 0.43              |
| 1:G:201:ALA:O    | 1:G:202:SER:OG   | 2.36                     | 0.43              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG13 | 1.95                     | 0.43              |
| 1:G:496:PHE:HB2  | 1:G:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:G:516:GLY:O    | 1:G:518:ASP:N    | 2.51                     | 0.43              |
| 1:G:541:MET:CE   | 4:V:346:LEU:HD12 | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:641:LYS:C    | 4:V:22:ALA:O     | 2.60                     | 0.43              |
| 1:G:655:GLU:CD   | 4:V:1:ASP:HB2    | 2.44                     | 0.43              |
| 1:G:711:PHE:HB3  | 1:G:766:PHE:HB3  | 1.99                     | 0.43              |
| 1:J:64:THR:CG2   | 1:J:65:GLU:H     | 2.31                     | 0.43              |
| 1:J:266:GLU:OE1  | 1:J:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:J:537:GLU:OE1  | 4:W:350:SER:HA   | 2.19                     | 0.43              |
| 3:L:119:THR:O    | 3:L:123:VAL:HG23 | 2.18                     | 0.43              |
| 4:0:220:ALA:HB3  | 4:0:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:0:243:PRO:CA   | 4:Y:291:LYS:HD2  | 2.48                     | 0.43              |
| 4:0:253:GLU:CD   | 4:0:253:GLU:H    | 2.25                     | 0.43              |
| 4:1:253:GLU:H    | 4:1:253:GLU:CD   | 2.25                     | 0.43              |
| 4:V:149:THR:HA   | 4:V:165:ILE:O    | 2.19                     | 0.43              |
| 1:A:151:ALA:HB1  | 1:A:152:PRO:HD2  | 2.01                     | 0.43              |
| 1:A:400:ALA:CB   | 1:A:606:THR:HG22 | 2.48                     | 0.43              |
| 1:A:442:VAL:O    | 1:A:445:ILE:HB   | 2.19                     | 0.43              |
| 1:A:533:PHE:HD1  | 1:A:533:PHE:HA   | 1.78                     | 0.43              |
| 1:A:751:GLY:C    | 1:A:753:VAL:HG22 | 2.43                     | 0.43              |
| 1:G:332:MET:H    | 1:G:332:MET:HG2  | 1.52                     | 0.43              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:G:725:ARG:HA   | 1:G:732:ILE:HG22 | 1.99                     | 0.43              |
| 3:I:49:ILE:CA    | 3:I:52:ASN:ND2   | 2.53                     | 0.43              |
| 1:J:14:ALA:N     | 1:J:15:PRO:CD    | 2.81                     | 0.43              |
| 1:J:224:SER:O    | 1:J:227:PRO:HD2  | 2.17                     | 0.43              |
| 1:J:485:GLU:OE2  | 1:J:584:TYR:N    | 2.50                     | 0.43              |
| 1:J:725:ARG:CZ   | 1:J:737:PHE:CE1  | 3.02                     | 0.43              |
| 2:K:144:VAL:C    | 2:K:153:ILE:HD11 | 2.42                     | 0.43              |
| 4:1:47:MET:HB2   | 4:1:47:MET:HE2   | 1.79                     | 0.43              |
| 4:4:220:ALA:HB3  | 4:4:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:5:149:THR:HA   | 4:5:165:ILE:O    | 2.19                     | 0.43              |
| 4:5:220:ALA:HB3  | 4:5:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:V:299:MET:HE2  | 4:V:299:MET:HB2  | 1.82                     | 0.43              |
| 4:W:220:ALA:HB3  | 4:W:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:330:GLU:O    | 1:A:333:ALA:HB3  | 2.17                     | 0.43              |
| 1:A:369:MLY:HH22 | 1:A:369:MLY:HD3  | 1.79                     | 0.43              |
| 1:A:541:MET:HB3  | 4:8:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:725:ARG:HA   | 1:A:732:ILE:HG22 | 1.99                     | 0.43              |
| 1:A:754:ASP:C    | 1:A:756:THR:H    | 2.26                     | 0.43              |
| 3:C:69:LEU:HB3   | 3:C:70:PRO:HD3   | 1.99                     | 0.43              |
| 1:D:14:ALA:N     | 1:D:15:PRO:CD    | 2.81                     | 0.43              |
| 1:D:17:LEU:HA    | 1:D:17:LEU:HD12  | 1.67                     | 0.43              |
| 1:D:174:SER:OG   | 1:D:669:PRO:HA   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:712:PRO:HB2  | 1:D:713:SER:H    | 1.61                     | 0.43              |
| 1:D:723:ARG:HE   | 1:D:779:ARG:HA   | 1.83                     | 0.43              |
| 1:D:725:ARG:CZ   | 1:D:737:PHE:CE1  | 3.02                     | 0.43              |
| 1:G:246:PHE:HB3  | 1:G:270:LEU:HD12 | 2.00                     | 0.43              |
| 1:G:294:ASN:OD1  | 1:G:307:THR:HG21 | 2.19                     | 0.43              |
| 1:G:530:MET:HE3  | 4:V:354:GLN:HG2  | 1.89                     | 0.43              |
| 1:G:725:ARG:CZ   | 1:G:737:PHE:CE1  | 3.02                     | 0.43              |
| 1:G:733:PRO:C    | 1:G:737:PHE:CE1  | 2.96                     | 0.43              |
| 1:G:800:ARG:CD   | 3:I:149:VAL:HG22 | 2.43                     | 0.43              |
| 1:G:834:LEU:HD11 | 2:H:51:PHE:CD1   | 2.52                     | 0.43              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:HD13 | 2.00                     | 0.43              |
| 1:J:503:TYR:CZ   | 1:J:711:PHE:CE2  | 3.06                     | 0.43              |
| 1:J:553:MLY:HE2  | 4:Y:45:VAL:HB    | 2.01                     | 0.43              |
| 1:J:584:TYR:CD1  | 1:J:584:TYR:C    | 2.96                     | 0.43              |
| 1:J:724:TYR:HB3  | 1:J:727:LEU:CD1  | 2.49                     | 0.43              |
| 1:J:725:ARG:CZ   | 1:J:737:PHE:CZ   | 3.01                     | 0.43              |
| 4:2:220:ALA:HB3  | 4:2:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:Y:149:THR:HA   | 4:Y:165:ILE:O    | 2.19                     | 0.43              |
| 4:Y:220:ALA:HB3  | 4:Y:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:449:LEU:HD12 | 1:A:449:LEU:HA   | 1.60                     | 0.43              |
| 1:A:485:GLU:OE1  | 1:A:583:HIS:ND1  | 2.49                     | 0.43              |
| 1:A:500:GLN:HB2  | 1:A:512:PHE:CZ   | 2.54                     | 0.43              |
| 1:A:504:MLY:CB   | 1:A:762:HIS:NE2  | 2.81                     | 0.43              |
| 1:A:551:MLY:C    | 4:V:47:MET:HA    | 2.48                     | 0.43              |
| 1:D:274:ARG:HH22 | 1:D:282:GLU:CD   | 2.27                     | 0.43              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:HG23 | 2.01                     | 0.43              |
| 1:D:715:VAL:HG12 | 1:D:720:PHE:HB2  | 2.00                     | 0.43              |
| 1:D:829:TRP:O    | 1:D:832:MET:N    | 2.50                     | 0.43              |
| 3:F:69:LEU:HB3   | 3:F:70:PRO:HD3   | 1.99                     | 0.43              |
| 1:G:93:MET:CE    | 1:G:764:MLY:HG3  | 2.38                     | 0.43              |
| 1:G:109:ARG:CD   | 1:G:117:THR:HB   | 2.48                     | 0.43              |
| 1:G:206:LYS:CE   | 1:G:217:THR:HG23 | 2.30                     | 0.43              |
| 1:G:500:GLN:HB2  | 1:G:512:PHE:CZ   | 2.54                     | 0.43              |
| 3:I:11:LYS:HE2   | 3:I:11:LYS:HB3   | 1.83                     | 0.43              |
| 1:J:109:ARG:CD   | 1:J:117:THR:HB   | 2.49                     | 0.43              |
| 1:J:201:ALA:O    | 1:J:202:SER:OG   | 2.36                     | 0.43              |
| 1:J:320:ILE:O    | 1:J:320:ILE:HG22 | 2.17                     | 0.43              |
| 1:J:442:VAL:O    | 1:J:445:ILE:HB   | 2.19                     | 0.43              |
| 1:J:783:LEU:HA   | 1:J:786:ILE:HB   | 1.99                     | 0.43              |
| 1:J:787:ILE:HG23 | 1:J:791:GLN:HG3  | 2.00                     | 0.43              |
| 4:1:203:THR:HG21 | 4:Z:288:ASP:CB   | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:287:ILE:HG13 | 4:4:202:THR:HG22 | 1.89                     | 0.43              |
| 4:X:193:LEU:O    | 4:X:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:Z:149:THR:HA   | 4:Z:165:ILE:O    | 2.19                     | 0.43              |
| 1:A:64:THR:CG2   | 1:A:65:GLU:H     | 2.32                     | 0.43              |
| 1:A:294:ASN:OD1  | 1:A:307:THR:HG21 | 2.19                     | 0.43              |
| 1:A:408:VAL:HG22 | 1:A:636:LYS:HG2  | 1.51                     | 0.43              |
| 2:B:140:PHE:CD2  | 2:B:144:VAL:HG11 | 2.54                     | 0.43              |
| 1:D:409:GLY:HA3  | 4:9:332:PRO:C    | 2.43                     | 0.43              |
| 1:D:442:VAL:O    | 1:D:445:ILE:HB   | 2.19                     | 0.43              |
| 1:D:725:ARG:HA   | 1:D:732:ILE:HG22 | 1.99                     | 0.43              |
| 1:D:822:SER:OG   | 2:E:87:LYS:C     | 2.62                     | 0.43              |
| 3:F:119:THR:O    | 3:F:123:VAL:HG23 | 2.18                     | 0.43              |
| 1:G:129:TYR:HD1  | 1:G:129:TYR:HA   | 1.65                     | 0.43              |
| 1:G:151:ALA:HB1  | 1:G:152:PRO:HD2  | 2.01                     | 0.43              |
| 1:G:442:VAL:O    | 1:G:445:ILE:HB   | 2.19                     | 0.43              |
| 1:G:771:LEU:C    | 1:G:773:GLY:N    | 2.75                     | 0.43              |
| 1:J:169:ASP:O    | 1:J:170:ARG:HB2  | 2.19                     | 0.43              |
| 1:J:195:TYR:CD2  | 1:J:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:J:406:VAL:O    | 1:J:412:ALA:HA   | 2.19                     | 0.43              |
| 1:J:409:GLY:HA3  | 4:W:332:PRO:C    | 2.43                     | 0.43              |
| 1:J:754:ASP:C    | 1:J:756:THR:H    | 2.26                     | 0.43              |
| 4:1:149:THR:HA   | 4:1:165:ILE:O    | 2.19                     | 0.43              |
| 4:4:47:MET:HB2   | 4:4:47:MET:HE2   | 1.79                     | 0.43              |
| 4:4:180:LEU:HD11 | 4:4:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:5:205:GLU:O    | 4:5:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:7:180:LEU:HD11 | 4:7:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:8:205:GLU:O    | 4:8:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:W:47:MET:HE2   | 4:W:47:MET:HB2   | 1.79                     | 0.43              |
| 4:W:193:LEU:O    | 4:W:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:195:TYR:CD2  | 1:A:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:A:330:GLU:HG2  | 1:A:330:GLU:H    | 1.55                     | 0.43              |
| 1:A:409:GLY:N    | 1:A:636:LYS:CD   | 2.70                     | 0.43              |
| 1:A:445:ILE:HG22 | 1:A:449:LEU:HD22 | 2.01                     | 0.43              |
| 1:A:493:HIS:O    | 1:A:496:PHE:HB3  | 2.18                     | 0.43              |
| 1:A:578:HIS:HB3  | 1:A:592:ILE:CD1  | 2.38                     | 0.43              |
| 1:A:636:LYS:CB   | 4:8:334:GLU:OE1  | 2.67                     | 0.43              |
| 1:A:733:PRO:C    | 1:A:737:PHE:CE1  | 2.96                     | 0.43              |
| 1:D:195:TYR:CD2  | 1:D:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:D:673:ARG:HD2  | 1:D:673:ARG:HA   | 1.79                     | 0.43              |
| 1:D:787:ILE:HG23 | 1:D:791:GLN:HG3  | 2.00                     | 0.43              |
| 1:D:799:MET:CE   | 3:F:32:ASP:CB    | 2.81                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:141:LEU:HD12 | 1:G:141:LEU:N    | 2.32                     | 0.43              |
| 1:G:195:TYR:CD2  | 1:G:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:OD2  | 2.19                     | 0.43              |
| 1:G:223:ILE:C    | 1:G:225:ALA:N    | 2.76                     | 0.43              |
| 1:G:445:ILE:HG22 | 1:G:449:LEU:HD22 | 2.01                     | 0.43              |
| 3:I:63:ILE:CG2   | 3:I:64:THR:H     | 2.32                     | 0.43              |
| 1:J:223:ILE:C    | 1:J:225:ALA:N    | 2.76                     | 0.43              |
| 1:J:294:ASN:OD1  | 1:J:307:THR:HG21 | 2.19                     | 0.43              |
| 1:J:568:PRO:O    | 1:J:570:PRO:HD3  | 2.19                     | 0.43              |
| 1:J:661:MET:HE3  | 1:J:661:MET:HB3  | 1.74                     | 0.43              |
| 1:J:747:LEU:O    | 1:J:749:GLY:N    | 2.52                     | 0.43              |
| 4:0:180:LEU:HD11 | 4:0:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:2:180:LEU:HD11 | 4:2:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:5:180:LEU:HD11 | 4:5:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:8:180:LEU:HD11 | 4:8:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:9:180:LEU:HD11 | 4:9:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:9:220:ALA:HB3  | 4:9:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:42:HIS:C     | 1:A:42:HIS:ND1   | 2.77                     | 0.42              |
| 1:A:62:VAL:O     | 1:A:69:THR:HA    | 2.19                     | 0.42              |
| 1:A:246:PHE:HB3  | 1:A:270:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:537:GLU:C    | 4:8:350:SER:N    | 2.77                     | 0.42              |
| 1:A:625:THR:H    | 1:A:625:THR:HG22 | 1.48                     | 0.42              |
| 1:A:692:LEU:HA   | 1:A:692:LEU:HD23 | 1.84                     | 0.42              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:CE   | 2.30                     | 0.42              |
| 1:D:169:ASP:O    | 1:D:170:ARG:HB2  | 2.19                     | 0.42              |
| 1:D:217:THR:HG22 | 1:D:218:LEU:N    | 2.34                     | 0.42              |
| 1:D:529:PRO:HB3  | 4:9:354:GLN:HA   | 2.00                     | 0.42              |
| 1:D:655:GLU:CD   | 4:9:1:ASP:HB2    | 2.43                     | 0.42              |
| 1:D:692:LEU:HD23 | 1:D:692:LEU:HA   | 1.84                     | 0.42              |
| 1:D:789:ALA:O    | 3:F:87:PHE:HZ    | 1.98                     | 0.42              |
| 1:G:64:THR:CG2   | 1:G:65:GLU:H     | 2.32                     | 0.42              |
| 1:G:406:VAL:O    | 1:G:412:ALA:HA   | 2.19                     | 0.42              |
| 1:G:443:ILE:HG22 | 1:G:444:ARG:N    | 2.29                     | 0.42              |
| 1:G:568:PRO:O    | 1:G:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:G:715:VAL:HG12 | 1:G:720:PHE:HB2  | 2.00                     | 0.42              |
| 1:G:795:ARG:HH22 | 3:I:43:ASN:CB    | 2.32                     | 0.42              |
| 1:G:829:TRP:O    | 1:G:832:MET:N    | 2.50                     | 0.42              |
| 1:J:87:MLY:HD3   | 1:J:87:MLY:HH12  | 1.61                     | 0.42              |
| 1:J:97:LEU:HA    | 1:J:97:LEU:HD12  | 1.67                     | 0.42              |
| 1:J:530:MET:CB   | 4:W:354:GLN:CB   | 2.95                     | 0.42              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:HG23 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:797:PHE:HB2  | 3:L:149:VAL:HG13 | 1.94                     | 0.42              |
| 2:K:112:ILE:O    | 2:K:148:VAL:N    | 2.50                     | 0.42              |
| 4:3:322:PRO:CA   | 4:5:244:ASP:HB2  | 2.49                     | 0.42              |
| 4:X:222:ASP:OD1  | 4:X:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:Y:180:LEU:HD11 | 4:Y:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:Z:315:LYS:HD2  | 4:Z:315:LYS:HA   | 1.92                     | 0.42              |
| 1:A:136:ASN:C    | 1:A:138:MLY:N    | 2.75                     | 0.42              |
| 1:A:214:MET:CA   | 1:A:340:ILE:HD11 | 2.46                     | 0.42              |
| 1:A:689:GLU:HA   | 1:A:692:LEU:HB2  | 2.00                     | 0.42              |
| 1:A:724:TYR:HB3  | 1:A:727:LEU:CD1  | 2.48                     | 0.42              |
| 1:A:800:ARG:HD3  | 3:C:149:VAL:C    | 2.37                     | 0.42              |
| 1:D:445:ILE:HG22 | 1:D:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:D:449:LEU:N    | 1:D:449:LEU:CD1  | 2.81                     | 0.42              |
| 1:D:496:PHE:HB2  | 1:D:515:PHE:CD2  | 2.54                     | 0.42              |
| 1:D:519:LEU:HD12 | 1:D:519:LEU:H    | 1.83                     | 0.42              |
| 1:D:701:LEU:HD12 | 1:D:701:LEU:HA   | 1.55                     | 0.42              |
| 1:D:725:ARG:CZ   | 1:D:737:PHE:CZ   | 3.01                     | 0.42              |
| 3:F:50:LEU:O     | 3:F:53:PRO:HG2   | 2.18                     | 0.42              |
| 1:G:529:PRO:HB3  | 4:V:354:GLN:HA   | 2.00                     | 0.42              |
| 1:G:798:LEU:HA   | 1:G:798:LEU:HD12 | 1.36                     | 0.42              |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:HD13 | 1.92                     | 0.42              |
| 1:J:40:VAL:HG23  | 1:J:76:GLN:O     | 2.19                     | 0.42              |
| 1:J:445:ILE:HG22 | 1:J:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:J:567:LYS:HZ1  | 4:Y:92:ASN:HA    | 1.81                     | 0.42              |
| 1:J:733:PRO:C    | 1:J:737:PHE:CE1  | 2.96                     | 0.42              |
| 4:1:180:LEU:HD11 | 4:1:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:2:193:LEU:O    | 4:2:198:TYR:HD2  | 2.01                     | 0.42              |
| 4:4:171:LEU:HA   | 4:4:172:PRO:HD2  | 1.84                     | 0.42              |
| 4:8:206:ARG:O    | 4:8:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:X:149:THR:HA   | 4:X:165:ILE:O    | 2.19                     | 0.42              |
| 4:X:180:LEU:HD11 | 4:X:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:Z:180:LEU:HD11 | 4:Z:261:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:530:MET:CE   | 4:8:354:GLN:HG3  | 2.35                     | 0.42              |
| 1:A:819:ASN:CG   | 2:B:91:ALA:C     | 2.72                     | 0.42              |
| 1:A:829:TRP:O    | 1:A:832:MET:N    | 2.50                     | 0.42              |
| 1:D:295:MLY:CE   | 1:D:332:MET:CE   | 2.97                     | 0.42              |
| 2:E:140:PHE:CD2  | 2:E:144:VAL:HG11 | 2.54                     | 0.42              |
| 1:G:62:VAL:O     | 1:G:69:THR:HA    | 2.19                     | 0.42              |
| 1:G:534:SER:CB   | 4:V:351:THR:HA   | 2.49                     | 0.42              |
| 1:G:747:LEU:O    | 1:G:749:GLY:N    | 2.52                     | 0.42              |
| 1:G:791:GLN:HB3  | 3:I:118:MET:CE   | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:84:MLY:HH13  | 1:J:715:VAL:CG1  | 2.07                     | 0.42              |
| 1:J:86:ASP:OD2   | 1:J:87:MLY:HH22  | 2.18                     | 0.42              |
| 1:J:214:MET:C    | 1:J:340:ILE:HD13 | 2.45                     | 0.42              |
| 1:J:278:GLN:HE21 | 1:J:278:GLN:HB3  | 1.42                     | 0.42              |
| 1:J:295:MLY:CE   | 1:J:332:MET:CE   | 2.97                     | 0.42              |
| 1:J:449:LEU:N    | 1:J:449:LEU:CD1  | 2.81                     | 0.42              |
| 1:J:502:GLU:C    | 1:J:504:MLY:N    | 2.77                     | 0.42              |
| 1:J:534:SER:CB   | 4:W:351:THR:HA   | 2.49                     | 0.42              |
| 1:J:757:GLN:OE1  | 1:J:773:GLY:CA   | 2.67                     | 0.42              |
| 3:L:63:ILE:CG2   | 3:L:64:THR:H     | 2.33                     | 0.42              |
| 4:3:149:THR:HA   | 4:3:165:ILE:O    | 2.19                     | 0.42              |
| 4:8:222:ASP:OD1  | 4:8:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:9:193:LEU:O    | 4:9:198:TYR:HD2  | 2.01                     | 0.42              |
| 4:V:180:LEU:HD11 | 4:V:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:V:205:GLU:O    | 4:V:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:Z:205:GLU:O    | 4:Z:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:A:38:VAL:HG13  | 1:A:39:PHE:N     | 2.35                     | 0.42              |
| 1:A:202:SER:C    | 1:A:207:LYS:HE3  | 2.43                     | 0.42              |
| 1:A:584:TYR:CD1  | 1:A:584:TYR:C    | 2.96                     | 0.42              |
| 2:B:113:LYS:O    | 2:B:147:ASN:HB2  | 2.20                     | 0.42              |
| 2:B:114:LYS:CG   | 2:B:146:GLY:HA2  | 2.46                     | 0.42              |
| 1:D:14:ALA:HB3   | 1:D:15:PRO:CD    | 2.45                     | 0.42              |
| 1:D:109:ARG:CD   | 1:D:117:THR:HB   | 2.49                     | 0.42              |
| 1:D:206:LYS:HD2  | 1:D:217:THR:CG2  | 2.17                     | 0.42              |
| 1:D:210:GLN:C    | 1:D:211:SER:HG   | 2.22                     | 0.42              |
| 1:D:354:LEU:HD12 | 1:D:354:LEU:HA   | 1.56                     | 0.42              |
| 1:D:406:VAL:O    | 1:D:412:ALA:HA   | 2.19                     | 0.42              |
| 2:E:140:PHE:HA   | 2:E:141:PRO:HD2  | 1.57                     | 0.42              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:HD13 | 2.00                     | 0.42              |
| 1:G:556:ASP:HB2  | 4:X:47:MET:HE2   | 1.05                     | 0.42              |
| 1:J:62:VAL:O     | 1:J:69:THR:HA    | 2.19                     | 0.42              |
| 1:J:173:GLN:HG3  | 1:J:670:HIS:CD2  | 2.54                     | 0.42              |
| 1:J:174:SER:HA   | 1:J:460:GLY:O    | 2.20                     | 0.42              |
| 1:J:226:ASN:HB2  | 1:J:227:PRO:CD   | 2.47                     | 0.42              |
| 1:J:271:GLU:OE1  | 1:J:274:ARG:NH1  | 2.53                     | 0.42              |
| 1:J:354:LEU:HD12 | 1:J:354:LEU:HA   | 1.56                     | 0.42              |
| 1:J:462:LEU:HD11 | 1:J:464:ILE:CD1  | 2.50                     | 0.42              |
| 1:J:537:GLU:C    | 4:W:350:SER:N    | 2.77                     | 0.42              |
| 1:J:556:ASP:HB3  | 4:Y:47:MET:HB2   | 1.00                     | 0.42              |
| 1:J:665:ARG:C    | 1:J:667:THR:N    | 2.74                     | 0.42              |
| 4:2:206:ARG:O    | 4:2:209:VAL:HG12 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:180:LEU:HD11 | 4:3:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:4:315:LYS:HD2  | 4:4:315:LYS:HA   | 1.92                     | 0.42              |
| 4:8:196:ARG:HH21 | 4:8:249:THR:HG23 | 1.85                     | 0.42              |
| 4:9:149:THR:HA   | 4:9:165:ILE:O    | 2.18                     | 0.42              |
| 4:9:205:GLU:O    | 4:9:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:9:324:THR:N    | 4:W:245:GLY:CA   | 2.69                     | 0.42              |
| 4:W:180:LEU:HD11 | 4:W:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:W:222:ASP:OD1  | 4:W:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:60:VAL:O     | 1:A:72:VAL:N     | 2.51                     | 0.42              |
| 1:A:712:PRO:HB2  | 1:A:713:SER:H    | 1.61                     | 0.42              |
| 1:A:747:LEU:O    | 1:A:749:GLY:N    | 2.52                     | 0.42              |
| 3:C:96:LYS:H     | 3:C:96:LYS:HG3   | 1.67                     | 0.42              |
| 1:D:214:MET:C    | 1:D:340:ILE:HD13 | 2.45                     | 0.42              |
| 1:D:320:ILE:O    | 1:D:320:ILE:HG22 | 2.17                     | 0.42              |
| 1:D:502:GLU:C    | 1:D:504:MLY:N    | 2.77                     | 0.42              |
| 1:D:733:PRO:CB   | 1:D:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:D:829:TRP:CD1  | 2:E:67:MET:HE2   | 2.54                     | 0.42              |
| 1:D:842:LEU:N    | 1:D:842:LEU:CD1  | 2.82                     | 0.42              |
| 1:G:173:GLN:HG3  | 1:G:670:HIS:CD2  | 2.55                     | 0.42              |
| 1:G:346:ASP:O    | 1:G:350:ALA:N    | 2.46                     | 0.42              |
| 1:G:578:HIS:CD2  | 1:G:592:ILE:H    | 2.38                     | 0.42              |
| 2:H:140:PHE:CD2  | 2:H:144:VAL:HG11 | 2.54                     | 0.42              |
| 1:J:132:LEU:C    | 1:J:134:VAL:H    | 2.28                     | 0.42              |
| 1:J:485:GLU:HA   | 1:J:584:TYR:HE2  | 1.83                     | 0.42              |
| 1:J:533:PHE:HD1  | 1:J:533:PHE:HA   | 1.79                     | 0.42              |
| 1:J:578:HIS:CD2  | 1:J:592:ILE:H    | 2.38                     | 0.42              |
| 1:J:715:VAL:HG12 | 1:J:720:PHE:HB2  | 2.00                     | 0.42              |
| 4:1:205:GLU:O    | 4:1:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:8:322:PRO:CB   | 4:V:244:ASP:CG   | 2.71                     | 0.42              |
| 4:X:206:ARG:O    | 4:X:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:X:325:MET:HE1  | 4:Z:244:ASP:OD2  | 2.18                     | 0.42              |
| 4:Y:222:ASP:OD1  | 4:Y:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:141:LEU:HD12 | 1:A:141:LEU:N    | 2.32                     | 0.42              |
| 1:A:166:MET:HE1  | 1:A:254:PHE:CB   | 2.46                     | 0.42              |
| 1:A:169:ASP:O    | 1:A:170:ARG:HB2  | 2.19                     | 0.42              |
| 1:A:568:PRO:O    | 1:A:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:A:744:SER:O    | 1:A:748:LEU:HD12 | 2.20                     | 0.42              |
| 1:A:791:GLN:OE1  | 3:C:116:GLU:HB2  | 2.20                     | 0.42              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:CG   | 2.32                     | 0.42              |
| 1:D:204:GLU:N    | 1:D:207:LYS:HE3  | 2.22                     | 0.42              |
| 1:D:584:TYR:CD1  | 1:D:584:TYR:C    | 2.96                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:636:LYS:CB   | 4:9:334:GLU:OE1  | 2.68                     | 0.42              |
| 1:D:659:MLY:HH22 | 1:D:659:MLY:HD2  | 1.42                     | 0.42              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:HB3   | 2.54                     | 0.42              |
| 1:G:42:HIS:C     | 1:G:42:HIS:ND1   | 2.77                     | 0.42              |
| 1:G:132:LEU:C    | 1:G:134:VAL:H    | 2.28                     | 0.42              |
| 1:G:530:MET:CE   | 4:V:354:GLN:HG3  | 2.34                     | 0.42              |
| 1:G:537:GLU:C    | 4:V:350:SER:N    | 2.77                     | 0.42              |
| 1:G:842:LEU:N    | 1:G:842:LEU:CD1  | 2.82                     | 0.42              |
| 1:J:214:MET:CA   | 1:J:340:ILE:HD11 | 2.45                     | 0.42              |
| 1:J:418:THR:CG2  | 1:J:419:VAL:N    | 2.79                     | 0.42              |
| 1:J:636:LYS:C    | 1:J:637:LYS:HG3  | 2.44                     | 0.42              |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CZ   | 2.54                     | 0.42              |
| 1:J:826:VAL:O    | 1:J:828:HIS:N    | 2.53                     | 0.42              |
| 4:0:193:LEU:O    | 4:0:198:TYR:HD2  | 2.01                     | 0.42              |
| 4:1:196:ARG:HH21 | 4:1:249:THR:HG23 | 1.85                     | 0.42              |
| 4:2:222:ASP:OD1  | 4:2:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:7:220:ALA:HB3  | 4:7:223:PHE:CD1  | 2.53                     | 0.42              |
| 4:W:221:LEU:HA   | 4:W:312:ARG:HG2  | 2.02                     | 0.42              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:406:VAL:O    | 1:A:412:ALA:HA   | 2.19                     | 0.42              |
| 1:A:771:LEU:C    | 1:A:773:GLY:N    | 2.75                     | 0.42              |
| 1:D:86:ASP:OD2   | 1:D:87:MLY:HH22  | 2.19                     | 0.42              |
| 1:D:279:LEU:CB   | 1:D:280:PRO:HD2  | 2.49                     | 0.42              |
| 1:D:294:ASN:OD1  | 1:D:307:THR:HG21 | 2.19                     | 0.42              |
| 1:D:409:GLY:N    | 1:D:636:LYS:CD   | 2.71                     | 0.42              |
| 1:D:534:SER:CB   | 4:9:351:THR:HA   | 2.49                     | 0.42              |
| 1:D:537:GLU:C    | 4:9:350:SER:N    | 2.77                     | 0.42              |
| 1:D:537:GLU:OE1  | 4:9:350:SER:HA   | 2.19                     | 0.42              |
| 1:D:636:LYS:C    | 1:D:637:LYS:HG3  | 2.44                     | 0.42              |
| 1:D:725:ARG:HA   | 1:D:732:ILE:CG2  | 2.50                     | 0.42              |
| 1:D:759:ALA:O    | 1:D:766:PHE:N    | 2.32                     | 0.42              |
| 1:D:799:MET:SD   | 3:F:32:ASP:HA    | 2.49                     | 0.42              |
| 1:G:400:ALA:CB   | 1:G:606:THR:HG22 | 2.49                     | 0.42              |
| 1:G:584:TYR:CD1  | 1:G:584:TYR:C    | 2.96                     | 0.42              |
| 1:J:42:HIS:C     | 1:J:42:HIS:ND1   | 2.78                     | 0.42              |
| 1:J:831:TRP:CH2  | 2:K:34:ILE:CG2   | 2.95                     | 0.42              |
| 2:K:140:PHE:CD2  | 2:K:144:VAL:HG11 | 2.54                     | 0.42              |
| 4:2:193:LEU:HD11 | 4:2:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:7:221:LEU:HA   | 4:7:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:7:369:ILE:HG23 | 4:7:370:VAL:N    | 2.35                     | 0.42              |
| 4:9:222:ASP:OD1  | 4:9:224:GLU:HB3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Z:47:MET:HB2   | 4:Z:47:MET:HE2   | 1.79                     | 0.42              |
| 4:Z:206:ARG:O    | 4:Z:209:VAL:HG12 | 2.20                     | 0.42              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:HD13 | 2.55                     | 0.42              |
| 1:A:214:MET:C    | 1:A:340:ILE:HD13 | 2.45                     | 0.42              |
| 1:A:553:MLY:HE2  | 4:V:45:VAL:CA    | 2.38                     | 0.42              |
| 1:A:725:ARG:CZ   | 1:A:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:A:797:PHE:CD2  | 1:A:798:LEU:HD12 | 2.55                     | 0.42              |
| 1:D:462:LEU:HD11 | 1:D:464:ILE:CD1  | 2.50                     | 0.42              |
| 1:D:744:SER:O    | 1:D:748:LEU:HD12 | 2.20                     | 0.42              |
| 1:G:81:ASN:CG    | 1:G:96:HIS:HB2   | 2.45                     | 0.42              |
| 1:G:97:LEU:HD12  | 1:G:97:LEU:HA    | 1.67                     | 0.42              |
| 1:G:274:ARG:HH22 | 1:G:282:GLU:CD   | 2.27                     | 0.42              |
| 1:G:633:GLY:HA2  | 4:V:25:ASP:HA    | 1.26                     | 0.42              |
| 1:G:725:ARG:HA   | 1:G:732:ILE:CG2  | 2.50                     | 0.42              |
| 1:J:11:GLY:O     | 1:J:14:ALA:HB3   | 2.20                     | 0.42              |
| 1:J:151:ALA:HB1  | 1:J:152:PRO:HD2  | 2.01                     | 0.42              |
| 1:J:500:GLN:HB2  | 1:J:512:PHE:CZ   | 2.54                     | 0.42              |
| 1:J:771:LEU:C    | 1:J:773:GLY:N    | 2.75                     | 0.42              |
| 4:1:222:ASP:OD1  | 4:1:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:3:206:ARG:O    | 4:3:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:3:222:ASP:OD1  | 4:3:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:4:193:LEU:HD11 | 4:4:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:5:196:ARG:HH21 | 4:5:249:THR:HG23 | 1.85                     | 0.42              |
| 4:5:206:ARG:O    | 4:5:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:9:221:LEU:HA   | 4:9:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:V:222:ASP:OD1  | 4:V:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:X:205:GLU:O    | 4:X:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:HB3  | 2.09                     | 0.42              |
| 4:Y:221:LEU:HA   | 4:Y:312:ARG:HG2  | 2.02                     | 0.42              |
| 1:A:173:GLN:HG3  | 1:A:670:HIS:CD2  | 2.54                     | 0.42              |
| 1:A:642:LYS:HB3  | 4:8:24:ASP:HB2   | 1.37                     | 0.42              |
| 1:A:842:LEU:N    | 1:A:842:LEU:CD1  | 2.82                     | 0.42              |
| 1:D:174:SER:HA   | 1:D:460:GLY:O    | 2.20                     | 0.42              |
| 1:D:471:ASP:CB   | 1:D:573:GLY:O    | 2.68                     | 0.42              |
| 1:D:578:HIS:CD2  | 1:D:592:ILE:H    | 2.38                     | 0.42              |
| 1:D:747:LEU:O    | 1:D:749:GLY:N    | 2.52                     | 0.42              |
| 1:D:839:MLY:N    | 1:D:840:PRO:HD2  | 2.35                     | 0.42              |
| 1:G:38:VAL:HG13  | 1:G:39:PHE:N     | 2.35                     | 0.42              |
| 1:G:62:VAL:HG12  | 1:G:63:MLY:N     | 2.34                     | 0.42              |
| 1:G:539:GLU:OE2  | 1:G:553:MLY:HD3  | 2.20                     | 0.42              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HD12 | 0.95                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:733:PRO:CB   | 1:G:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:CB   | 2.50                     | 0.42              |
| 1:G:798:LEU:HD22 | 3:I:126:LEU:CD1  | 2.43                     | 0.42              |
| 1:J:332:MET:H    | 1:J:332:MET:HG2  | 1.52                     | 0.42              |
| 1:J:821:ARG:HH12 | 2:K:127:ARG:CZ   | 2.33                     | 0.42              |
| 4:0:193:LEU:HD11 | 4:0:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:0:222:ASP:OD1  | 4:0:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:1:206:ARG:O    | 4:1:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:3:205:GLU:O    | 4:3:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:3:221:LEU:HA   | 4:3:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:5:193:LEU:HD11 | 4:5:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:7:287:ILE:HA   | 4:9:202:THR:HG21 | 1.59                     | 0.42              |
| 4:9:369:ILE:HG23 | 4:9:370:VAL:N    | 2.35                     | 0.42              |
| 4:V:196:ARG:HH21 | 4:V:249:THR:HG23 | 1.85                     | 0.42              |
| 4:W:206:ARG:O    | 4:W:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:W:369:ILE:HG23 | 4:W:370:VAL:N    | 2.35                     | 0.42              |
| 4:X:369:ILE:HG23 | 4:X:370:VAL:N    | 2.35                     | 0.42              |
| 4:Y:369:ILE:HG23 | 4:Y:370:VAL:N    | 2.35                     | 0.42              |
| 4:Z:222:ASP:OD1  | 4:Z:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:81:ASN:CG    | 1:A:96:HIS:HB2   | 2.45                     | 0.42              |
| 1:A:110:TYR:O    | 1:A:113:TRP:N    | 2.42                     | 0.42              |
| 1:A:501:GLU:HA   | 1:A:762:HIS:CE1  | 2.55                     | 0.42              |
| 1:A:578:HIS:CD2  | 1:A:592:ILE:H    | 2.38                     | 0.42              |
| 1:A:725:ARG:HA   | 1:A:732:ILE:CG2  | 2.50                     | 0.42              |
| 1:A:826:VAL:O    | 1:A:828:HIS:N    | 2.53                     | 0.42              |
| 1:D:215:GLN:H    | 1:D:340:ILE:CD1  | 2.21                     | 0.42              |
| 1:D:271:GLU:OE1  | 1:D:274:ARG:NH1  | 2.53                     | 0.42              |
| 1:D:506:GLU:O    | 1:D:762:HIS:HB2  | 2.20                     | 0.42              |
| 1:D:690:LEU:O    | 1:D:694:GLN:HG3  | 2.20                     | 0.42              |
| 1:D:741:LYS:HG2  | 1:D:742:LYS:N    | 2.35                     | 0.42              |
| 3:F:63:ILE:CG2   | 3:F:64:THR:H     | 2.32                     | 0.42              |
| 1:G:11:GLY:O     | 1:G:14:ALA:HB3   | 2.20                     | 0.42              |
| 1:G:369:MLY:HH22 | 1:G:369:MLY:HD3  | 1.79                     | 0.42              |
| 1:G:568:PRO:CG   | 1:G:578:HIS:N    | 2.83                     | 0.42              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:CD1  | 0.65                     | 0.42              |
| 1:G:826:VAL:O    | 1:G:828:HIS:N    | 2.53                     | 0.42              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:HD13 | 2.55                     | 0.42              |
| 1:J:739:ASP:OD1  | 1:J:739:ASP:C    | 2.58                     | 0.42              |
| 1:J:797:PHE:CD2  | 1:J:798:LEU:HD12 | 2.55                     | 0.42              |
| 4:0:206:ARG:O    | 4:0:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:7:193:LEU:HD11 | 4:7:250:ILE:HG13 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:315:LYS:HD2  | 4:8:315:LYS:HA   | 1.92                     | 0.42              |
| 4:8:369:ILE:HG23 | 4:8:370:VAL:N    | 2.35                     | 0.42              |
| 4:V:193:LEU:HD11 | 4:V:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:V:206:ARG:O    | 4:V:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:V:369:ILE:HG23 | 4:V:370:VAL:N    | 2.35                     | 0.42              |
| 4:X:315:LYS:HD2  | 4:X:315:LYS:HA   | 1.92                     | 0.42              |
| 1:A:11:GLY:O     | 1:A:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:A:25:ILE:HG23  | 1:A:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:A:322:VAL:HA   | 1:A:323:PRO:HD3  | 1.87                     | 0.41              |
| 1:A:330:GLU:OE1  | 1:A:330:GLU:HA   | 2.20                     | 0.41              |
| 1:A:462:LEU:HD11 | 1:A:464:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:501:GLU:CB   | 1:A:762:HIS:ND1  | 2.82                     | 0.41              |
| 1:A:659:MLY:HD2  | 1:A:659:MLY:HH22 | 1.42                     | 0.41              |
| 2:B:140:PHE:HA   | 2:B:141:PRO:HD2  | 1.56                     | 0.41              |
| 3:C:95:ASP:OD1   | 3:C:139:TYR:HE1  | 2.03                     | 0.41              |
| 1:D:129:TYR:HD1  | 1:D:129:TYR:HA   | 1.65                     | 0.41              |
| 1:D:151:ALA:HB1  | 1:D:152:PRO:HD2  | 2.01                     | 0.41              |
| 1:D:508:ILE:CG2  | 1:D:766:PHE:CD1  | 3.03                     | 0.41              |
| 1:D:568:PRO:CG   | 1:D:578:HIS:N    | 2.83                     | 0.41              |
| 1:G:169:ASP:O    | 1:G:170:ARG:HB2  | 2.19                     | 0.41              |
| 1:G:538:GLU:OE1  | 4:V:355:MET:HE1  | 2.18                     | 0.41              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:CB   | 2.74                     | 0.41              |
| 1:G:797:PHE:CD2  | 1:G:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:G:818:TYR:C    | 2:H:90:GLY:HA3   | 2.45                     | 0.41              |
| 3:I:95:ASP:OD1   | 3:I:139:TYR:HE1  | 2.03                     | 0.41              |
| 1:J:93:MET:CA    | 1:J:714:ARG:HG3  | 2.45                     | 0.41              |
| 1:J:530:MET:CE   | 4:W:354:GLN:CB   | 2.95                     | 0.41              |
| 1:J:655:GLU:CD   | 4:W:1:ASP:HB2    | 2.43                     | 0.41              |
| 1:J:690:LEU:O    | 1:J:694:GLN:HG3  | 2.20                     | 0.41              |
| 1:J:725:ARG:HA   | 1:J:732:ILE:CG2  | 2.50                     | 0.41              |
| 4:3:193:LEU:HD11 | 4:3:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:4:196:ARG:HH21 | 4:4:249:THR:HG23 | 1.85                     | 0.41              |
| 4:4:222:ASP:OD1  | 4:4:224:GLU:HB3  | 2.19                     | 0.41              |
| 4:7:222:ASP:OD1  | 4:7:224:GLU:HB3  | 2.19                     | 0.41              |
| 4:8:193:LEU:HD11 | 4:8:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:9:287:ILE:CB   | 4:W:204:ALA:H    | 2.13                     | 0.41              |
| 4:Y:193:LEU:HD11 | 4:Y:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:Y:206:ARG:O    | 4:Y:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:Z:193:LEU:HD11 | 4:Z:250:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:221:GLN:HG2  | 1:A:221:GLN:H    | 1.47                     | 0.41              |
| 1:A:223:ILE:C    | 1:A:225:ALA:N    | 2.76                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:274:ARG:HH22 | 1:A:282:GLU:CD   | 2.27                     | 0.41              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:HG23 | 2.01                     | 0.41              |
| 1:A:568:PRO:CG   | 1:A:578:HIS:N    | 2.84                     | 0.41              |
| 1:A:741:LYS:HG2  | 1:A:742:LYS:N    | 2.34                     | 0.41              |
| 1:A:839:MLY:N    | 1:A:840:PRO:HD2  | 2.34                     | 0.41              |
| 1:D:25:ILE:HG23  | 1:D:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:D:87:MLY:HH12  | 1:D:87:MLY:HD3   | 1.61                     | 0.41              |
| 1:D:132:LEU:C    | 1:D:134:VAL:H    | 2.28                     | 0.41              |
| 1:D:356:GLY:HA2  | 1:D:359:MET:HG3  | 2.02                     | 0.41              |
| 1:D:466:GLY:CA   | 1:D:484:ASN:HD21 | 2.32                     | 0.41              |
| 1:D:500:GLN:HB2  | 1:D:512:PHE:CZ   | 2.54                     | 0.41              |
| 1:D:530:MET:CA   | 4:9:354:GLN:CD   | 2.86                     | 0.41              |
| 1:D:568:PRO:O    | 1:D:570:PRO:HD3  | 2.19                     | 0.41              |
| 1:D:718:ALA:C    | 1:D:720:PHE:N    | 2.79                     | 0.41              |
| 1:D:787:ILE:HD13 | 1:D:787:ILE:HG21 | 1.67                     | 0.41              |
| 1:D:812:SER:O    | 1:D:816:ILE:HG13 | 2.20                     | 0.41              |
| 1:G:60:VAL:O     | 1:G:72:VAL:N     | 2.51                     | 0.41              |
| 1:G:110:TYR:C    | 1:G:112:ALA:N    | 2.78                     | 0.41              |
| 1:G:136:ASN:O    | 1:G:138:MLY:N    | 2.54                     | 0.41              |
| 1:G:202:SER:C    | 1:G:207:LYS:HE3  | 2.44                     | 0.41              |
| 1:G:462:LEU:HD11 | 1:G:464:ILE:CD1  | 2.50                     | 0.41              |
| 1:G:762:HIS:CD2  | 1:G:762:HIS:N    | 2.78                     | 0.41              |
| 3:I:25:ILE:O     | 3:I:63:ILE:CB    | 2.66                     | 0.41              |
| 1:J:136:ASN:O    | 1:J:138:MLY:N    | 2.54                     | 0.41              |
| 1:J:229:LEU:HD12 | 1:J:229:LEU:HA   | 1.75                     | 0.41              |
| 1:J:568:PRO:CG   | 1:J:578:HIS:N    | 2.84                     | 0.41              |
| 1:J:636:LYS:CB   | 4:W:334:GLU:OE1  | 2.68                     | 0.41              |
| 1:J:793:ARG:HD2  | 3:L:146:ILE:O    | 2.20                     | 0.41              |
| 4:1:193:LEU:HD11 | 4:1:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:2:196:ARG:HH21 | 4:2:249:THR:HG23 | 1.85                     | 0.41              |
| 4:2:369:ILE:HG23 | 4:2:370:VAL:N    | 2.35                     | 0.41              |
| 4:3:369:ILE:HG23 | 4:3:370:VAL:N    | 2.35                     | 0.41              |
| 4:4:226:GLU:HG3  | 4:4:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:5:221:LEU:HA   | 4:5:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:7:287:ILE:N    | 4:9:202:THR:CG2  | 2.77                     | 0.41              |
| 4:8:227:MET:O    | 4:8:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:8:324:THR:HG23 | 4:V:245:GLY:HA2  | 1.09                     | 0.41              |
| 4:W:193:LEU:HD11 | 4:W:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:Z:369:ILE:HG23 | 4:Z:370:VAL:N    | 2.35                     | 0.41              |
| 1:A:132:LEU:C    | 1:A:134:VAL:H    | 2.28                     | 0.41              |
| 1:A:502:GLU:HG2  | 1:A:766:PHE:HE1  | 1.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:690:LEU:O    | 1:A:694:GLN:HG3  | 2.20                     | 0.41              |
| 1:D:81:ASN:CG    | 1:D:96:HIS:HB2   | 2.45                     | 0.41              |
| 1:D:554:LEU:HA   | 1:D:554:LEU:HD12 | 1.77                     | 0.41              |
| 1:D:625:THR:H    | 1:D:625:THR:HG22 | 1.48                     | 0.41              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:CB   | 2.74                     | 0.41              |
| 1:D:793:ARG:HG2  | 3:F:147:MET:HG2  | 2.01                     | 0.41              |
| 1:D:795:ARG:NE   | 3:F:43:ASN:OD1   | 2.53                     | 0.41              |
| 1:G:217:THR:CA   | 1:G:221:GLN:HE21 | 2.33                     | 0.41              |
| 1:G:330:GLU:OE1  | 1:G:330:GLU:HA   | 2.20                     | 0.41              |
| 1:G:541:MET:HB3  | 4:V:345:ILE:HG22 | 2.01                     | 0.41              |
| 1:G:553:MLY:CB   | 4:X:46:GLY:HA3   | 2.49                     | 0.41              |
| 1:G:775:LEU:HD12 | 1:G:775:LEU:HA   | 1.71                     | 0.41              |
| 1:J:84:MLY:CG    | 1:J:719:ASP:OD2  | 2.68                     | 0.41              |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:CH2  | 2.48                     | 0.41              |
| 4:0:196:ARG:HH21 | 4:0:249:THR:HG23 | 1.85                     | 0.41              |
| 4:3:148:THR:HG21 | 4:5:45:VAL:CG2   | 2.50                     | 0.41              |
| 4:3:288:ASP:CA   | 4:5:203:THR:CG2  | 2.99                     | 0.41              |
| 4:3:324:THR:CG2  | 4:5:244:ASP:O    | 2.68                     | 0.41              |
| 4:5:222:ASP:OD1  | 4:5:224:GLU:HB3  | 2.19                     | 0.41              |
| 4:5:369:ILE:HG23 | 4:5:370:VAL:N    | 2.35                     | 0.41              |
| 4:7:206:ARG:O    | 4:7:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:9:193:LEU:HD11 | 4:9:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:9:196:ARG:HH21 | 4:9:249:THR:HG23 | 1.85                     | 0.41              |
| 4:9:226:GLU:HG3  | 4:9:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:V:315:LYS:HD2  | 4:V:315:LYS:HA   | 1.92                     | 0.41              |
| 1:A:62:VAL:HG12  | 1:A:63:MLY:N     | 2.35                     | 0.41              |
| 1:A:110:TYR:C    | 1:A:112:ALA:N    | 2.78                     | 0.41              |
| 1:A:636:LYS:C    | 1:A:637:LYS:HG3  | 2.44                     | 0.41              |
| 1:D:11:GLY:O     | 1:D:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:D:135:TYR:CD2  | 1:D:191:ARG:HD3  | 2.55                     | 0.41              |
| 1:D:173:GLN:HG3  | 1:D:670:HIS:CD2  | 2.54                     | 0.41              |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:CH2  | 2.48                     | 0.41              |
| 1:D:771:LEU:C    | 1:D:773:GLY:N    | 2.75                     | 0.41              |
| 1:D:797:PHE:CD2  | 1:D:798:LEU:HD12 | 2.55                     | 0.41              |
| 2:E:113:LYS:O    | 2:E:147:ASN:HB2  | 2.20                     | 0.41              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:CG   | 2.33                     | 0.41              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:G:471:ASP:CB   | 1:G:573:GLY:O    | 2.68                     | 0.41              |
| 1:G:553:MLY:C    | 4:X:46:GLY:HA3   | 2.50                     | 0.41              |
| 1:G:636:LYS:C    | 1:G:637:LYS:HG3  | 2.44                     | 0.41              |
| 1:G:642:LYS:HE2  | 4:V:344:SER:HA   | 1.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:744:SER:O    | 1:G:748:LEU:HD12 | 2.20                     | 0.41              |
| 1:G:768:MLY:CD   | 1:G:772:LEU:HB2  | 2.50                     | 0.41              |
| 1:J:14:ALA:HB3   | 1:J:15:PRO:CD    | 2.46                     | 0.41              |
| 1:J:471:ASP:CB   | 1:J:573:GLY:O    | 2.68                     | 0.41              |
| 1:J:718:ALA:C    | 1:J:720:PHE:N    | 2.79                     | 0.41              |
| 1:J:829:TRP:O    | 1:J:832:MET:N    | 2.50                     | 0.41              |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD13 | 1.92                     | 0.41              |
| 4:2:221:LEU:HA   | 4:2:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:4:206:ARG:O    | 4:4:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:7:226:GLU:HG3  | 4:7:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:W:226:GLU:HG3  | 4:W:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:X:193:LEU:HD11 | 4:X:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:X:227:MET:O    | 4:X:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:Y:226:GLU:HG3  | 4:Y:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:Z:226:GLU:HG3  | 4:Z:255:PHE:CE2  | 2.56                     | 0.41              |
| 1:A:174:SER:HA   | 1:A:460:GLY:O    | 2.20                     | 0.41              |
| 1:A:797:PHE:HE2  | 3:C:126:LEU:CD2  | 1.92                     | 0.41              |
| 1:A:817:GLN:CB   | 2:B:127:ARG:CZ   | 2.69                     | 0.41              |
| 1:D:166:MET:HE1  | 1:D:254:PHE:CB   | 2.46                     | 0.41              |
| 1:D:408:VAL:HG22 | 1:D:636:LYS:HG2  | 1.51                     | 0.41              |
| 1:D:826:VAL:O    | 1:D:828:HIS:N    | 2.53                     | 0.41              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:HD3  | 2.48                     | 0.41              |
| 1:G:56:GLU:HB2   | 1:G:59:MLY:CB    | 2.30                     | 0.41              |
| 1:G:185:LYS:H    | 1:G:185:LYS:HG3  | 1.63                     | 0.41              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:HG23 | 2.02                     | 0.41              |
| 1:G:690:LEU:O    | 1:G:694:GLN:HG3  | 2.20                     | 0.41              |
| 1:G:840:PRO:C    | 1:G:842:LEU:N    | 2.79                     | 0.41              |
| 1:J:25:ILE:HG23  | 1:J:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:J:335:ASP:O    | 1:J:338:ILE:HB   | 2.20                     | 0.41              |
| 1:J:346:ASP:O    | 1:J:350:ALA:N    | 2.46                     | 0.41              |
| 1:J:826:VAL:CG2  | 2:K:88:LEU:CD2   | 2.86                     | 0.41              |
| 4:0:227:MET:O    | 4:0:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:1:144:ALA:HB2  | 4:1:342:GLY:CA   | 2.51                     | 0.41              |
| 4:2:144:ALA:HB2  | 4:2:342:GLY:CA   | 2.51                     | 0.41              |
| 4:5:32:PRO:HB2   | 4:5:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:7:32:PRO:HB2   | 4:7:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:8:226:GLU:HG3  | 4:8:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:Z:144:ALA:HB2  | 4:Z:342:GLY:CA   | 2.51                     | 0.41              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:CG   | 2.33                     | 0.41              |
| 1:A:136:ASN:O    | 1:A:138:MLY:N    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:149:GLN:HG2  | 1:A:719:ASP:CG   | 2.38                     | 0.41              |
| 1:A:812:SER:O    | 1:A:816:ILE:HG13 | 2.21                     | 0.41              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:HG11 | 2.03                     | 0.41              |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:HD11 | 1.75                     | 0.41              |
| 2:B:150:TYR:HB3  | 2:B:151:LYS:HG3  | 2.03                     | 0.41              |
| 3:C:63:ILE:CG2   | 3:C:64:THR:H     | 2.33                     | 0.41              |
| 1:D:62:VAL:O     | 1:D:69:THR:HA    | 2.19                     | 0.41              |
| 1:D:733:PRO:C    | 1:D:737:PHE:CE1  | 2.97                     | 0.41              |
| 3:F:48:LYS:HA    | 3:F:48:LYS:HD3   | 1.17                     | 0.41              |
| 1:G:174:SER:HA   | 1:G:460:GLY:O    | 2.20                     | 0.41              |
| 1:G:636:LYS:CB   | 4:V:334:GLU:OE1  | 2.68                     | 0.41              |
| 1:G:717:TYR:OH   | 1:G:760:PHE:HB3  | 2.21                     | 0.41              |
| 1:J:610:LEU:N    | 1:J:610:LEU:CD1  | 2.84                     | 0.41              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:H    | 2.14                     | 0.41              |
| 4:1:148:THR:OG1  | 4:3:45:VAL:HG23  | 2.21                     | 0.41              |
| 4:2:32:PRO:HB2   | 4:2:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:2:227:MET:O    | 4:2:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:3:196:ARG:HH21 | 4:3:249:THR:HG23 | 1.85                     | 0.41              |
| 4:3:287:ILE:CG2  | 4:5:204:ALA:N    | 2.68                     | 0.41              |
| 4:7:196:ARG:HH21 | 4:7:249:THR:HG23 | 1.85                     | 0.41              |
| 4:7:290:ARG:HH22 | 4:9:202:THR:CG2  | 2.17                     | 0.41              |
| 4:9:32:PRO:HB2   | 4:9:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:9:287:ILE:N    | 4:W:202:THR:CG2  | 2.77                     | 0.41              |
| 4:V:144:ALA:HB2  | 4:V:342:GLY:CA   | 2.51                     | 0.41              |
| 4:W:144:ALA:HB2  | 4:W:342:GLY:CA   | 2.51                     | 0.41              |
| 4:X:32:PRO:HB2   | 4:X:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:Y:196:ARG:HH21 | 4:Y:249:THR:HG23 | 1.85                     | 0.41              |
| 1:A:194:GLN:HE21 | 1:A:194:GLN:HB3  | 1.43                     | 0.41              |
| 1:A:530:MET:HE3  | 4:8:354:GLN:HG2  | 1.90                     | 0.41              |
| 1:D:136:ASN:O    | 1:D:138:MLY:N    | 2.54                     | 0.41              |
| 1:D:322:VAL:HG12 | 1:D:325:ILE:HG13 | 2.03                     | 0.41              |
| 1:D:330:GLU:HA   | 1:D:330:GLU:OE1  | 2.21                     | 0.41              |
| 1:D:831:TRP:CE2  | 2:E:51:PHE:CZ    | 3.09                     | 0.41              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HG2   | 1.98                     | 0.41              |
| 2:E:150:TYR:HB3  | 2:E:151:LYS:HG3  | 2.03                     | 0.41              |
| 1:G:14:ALA:HB3   | 1:G:15:PRO:CD    | 2.45                     | 0.41              |
| 1:G:193:ILE:CD1  | 1:G:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:G:449:LEU:N    | 1:G:449:LEU:CD1  | 2.82                     | 0.41              |
| 1:G:795:ARG:NH2  | 3:I:43:ASN:OD1   | 1.61                     | 0.41              |
| 1:G:810:ARG:HG2  | 1:G:810:ARG:NH1  | 2.28                     | 0.41              |
| 1:J:204:GLU:N    | 1:J:207:LYS:HE3  | 2.23                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:464:ILE:HD13 | 1:J:464:ILE:HG21 | 1.69                     | 0.41              |
| 1:J:635:GLY:C    | 4:W:341:ILE:HG21 | 2.45                     | 0.41              |
| 1:J:741:LYS:HG2  | 1:J:742:LYS:N    | 2.35                     | 0.41              |
| 1:J:744:SER:O    | 1:J:748:LEU:HD12 | 2.20                     | 0.41              |
| 1:J:821:ARG:CZ   | 2:K:127:ARG:HD3  | 2.51                     | 0.41              |
| 4:O:32:PRO:HB2   | 4:O:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:1:324:THR:H    | 4:3:244:ASP:HA   | 1.86                     | 0.41              |
| 4:3:226:GLU:HG3  | 4:3:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:4:32:PRO:HB2   | 4:4:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:4:369:ILE:HG23 | 4:4:370:VAL:N    | 2.35                     | 0.41              |
| 4:5:226:GLU:HG3  | 4:5:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:7:299:MET:HE2  | 4:7:299:MET:HB2  | 1.81                     | 0.41              |
| 4:8:144:ALA:HB2  | 4:8:342:GLY:CA   | 2.51                     | 0.41              |
| 4:8:288:ASP:OD1  | 4:V:204:ALA:HA   | 2.21                     | 0.41              |
| 4:9:206:ARG:O    | 4:9:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:V:226:GLU:HG3  | 4:V:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:W:227:MET:O    | 4:W:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:Y:144:ALA:HB2  | 4:Y:342:GLY:CA   | 2.51                     | 0.41              |
| 4:Z:196:ARG:HH21 | 4:Z:249:THR:HG23 | 1.85                     | 0.41              |
| 1:A:711:PHE:O    | 1:A:714:ARG:NH2  | 2.54                     | 0.41              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD13 | 1.37                     | 0.41              |
| 1:A:739:ASP:OD1  | 1:A:739:ASP:C    | 2.58                     | 0.41              |
| 3:C:56:GLU:OE1   | 3:C:59:ASN:ND2   | 2.54                     | 0.41              |
| 1:D:38:VAL:HG13  | 1:D:39:PHE:N     | 2.34                     | 0.41              |
| 1:D:42:HIS:ND1   | 1:D:42:HIS:C     | 2.77                     | 0.41              |
| 1:D:62:VAL:HG12  | 1:D:63:MLY:N     | 2.35                     | 0.41              |
| 1:D:110:TYR:C    | 1:D:112:ALA:N    | 2.79                     | 0.41              |
| 1:D:308:ASN:HA   | 1:D:309:PRO:HD2  | 1.88                     | 0.41              |
| 1:D:335:ASP:O    | 1:D:338:ILE:HB   | 2.20                     | 0.41              |
| 1:D:407:GLY:HA2  | 1:D:411:GLU:O    | 2.21                     | 0.41              |
| 1:D:534:SER:HB2  | 4:9:354:GLN:HE22 | 1.56                     | 0.41              |
| 1:G:335:ASP:O    | 1:G:338:ILE:HB   | 2.20                     | 0.41              |
| 1:G:384:ASP:HA   | 1:G:394:SER:OG   | 2.21                     | 0.41              |
| 1:G:485:GLU:OE2  | 1:G:584:TYR:N    | 2.50                     | 0.41              |
| 1:G:555:TYR:C    | 1:G:557:GLU:N    | 2.77                     | 0.41              |
| 1:G:741:LYS:HG2  | 1:G:742:LYS:N    | 2.35                     | 0.41              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:CB    | 3.02                     | 0.41              |
| 1:J:62:VAL:HG12  | 1:J:63:MLY:N     | 2.34                     | 0.41              |
| 1:J:90:ASP:CB    | 1:J:764:MLY:HH11 | 2.42                     | 0.41              |
| 1:J:322:VAL:HG12 | 1:J:325:ILE:HG13 | 2.03                     | 0.41              |
| 1:J:812:SER:O    | 1:J:816:ILE:HG13 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:839:MLY:N    | 1:J:840:PRO:HD2  | 2.34                     | 0.41              |
| 4:0:171:LEU:HA   | 4:0:172:PRO:HD2  | 1.84                     | 0.41              |
| 4:0:201:VAL:CG2  | 4:Y:287:ILE:HG13 | 2.49                     | 0.41              |
| 4:4:144:ALA:HB2  | 4:4:342:GLY:CA   | 2.51                     | 0.41              |
| 1:A:72:VAL:O     | 1:A:73:LYS:O     | 2.39                     | 0.41              |
| 1:A:172:ASN:OD1  | 1:A:457:TYR:HA   | 2.21                     | 0.41              |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:193:ILE:CD1  | 1:A:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:A:226:ASN:HB2  | 1:A:227:PRO:CD   | 2.47                     | 0.41              |
| 1:A:303:LEU:O    | 1:A:304:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:356:GLY:HA2  | 1:A:359:MET:HG3  | 2.02                     | 0.41              |
| 1:A:471:ASP:CB   | 1:A:573:GLY:O    | 2.68                     | 0.41              |
| 1:A:840:PRO:C    | 1:A:842:LEU:N    | 2.78                     | 0.41              |
| 2:B:139:ALA:O    | 2:B:141:PRO:CD   | 2.51                     | 0.41              |
| 1:D:47:PHE:HE1   | 1:D:78:PHE:CE1   | 2.39                     | 0.41              |
| 1:D:48:VAL:CG2   | 1:D:49:MLY:N     | 2.84                     | 0.41              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:D:242:ASN:OD1  | 1:D:286:HIS:NE2  | 2.49                     | 0.41              |
| 1:D:309:PRO:C    | 1:D:311:ASP:N    | 2.79                     | 0.41              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:HD12 | 2.03                     | 0.41              |
| 1:D:398:LEU:HA   | 1:D:398:LEU:HD12 | 1.83                     | 0.41              |
| 1:D:493:HIS:O    | 1:D:496:PHE:N    | 2.54                     | 0.41              |
| 1:D:528:MLY:HB2  | 1:D:529:PRO:HD2  | 2.02                     | 0.41              |
| 1:D:736:GLN:C    | 1:D:743:ALA:HB2  | 2.46                     | 0.41              |
| 1:D:822:SER:OG   | 2:E:88:LEU:CG    | 2.64                     | 0.41              |
| 1:D:829:TRP:HE1  | 2:E:67:MET:CB    | 2.27                     | 0.41              |
| 1:D:830:PRO:C    | 2:E:51:PHE:CZ    | 2.98                     | 0.41              |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:G:322:VAL:HA   | 1:G:323:PRO:HD3  | 1.87                     | 0.41              |
| 1:G:356:GLY:HA2  | 1:G:359:MET:HG3  | 2.02                     | 0.41              |
| 1:G:829:TRP:HH2  | 2:H:83:MET:HE3   | 1.85                     | 0.41              |
| 2:H:113:LYS:O    | 2:H:147:ASN:HB2  | 2.20                     | 0.41              |
| 2:H:140:PHE:HA   | 2:H:141:PRO:HD2  | 1.57                     | 0.41              |
| 1:J:81:ASN:CG    | 1:J:96:HIS:HB2   | 2.45                     | 0.41              |
| 1:J:135:TYR:CD2  | 1:J:191:ARG:HD3  | 2.55                     | 0.41              |
| 1:J:193:ILE:CD1  | 1:J:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:J:309:PRO:C    | 1:J:311:ASP:N    | 2.79                     | 0.41              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:HD12 | 2.02                     | 0.41              |
| 1:J:330:GLU:OE1  | 1:J:330:GLU:HA   | 2.20                     | 0.41              |
| 1:J:356:GLY:HA2  | 1:J:359:MET:HG3  | 2.02                     | 0.41              |
| 1:J:384:ASP:HA   | 1:J:394:SER:OG   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:508:ILE:HD13 | 1:J:759:ALA:HB2  | 1.79                     | 0.41              |
| 1:J:539:GLU:OE2  | 1:J:553:MLY:HD3  | 2.20                     | 0.41              |
| 1:J:657:LEU:HD12 | 1:J:657:LEU:O    | 2.21                     | 0.41              |
| 1:J:776:GLU:O    | 1:J:780:ASP:N    | 2.45                     | 0.41              |
| 1:J:789:ALA:C    | 3:L:87:PHE:CZ    | 2.99                     | 0.41              |
| 4:0:167:GLU:OE1  | 4:2:43:VAL:N     | 2.54                     | 0.41              |
| 4:0:221:LEU:HA   | 4:0:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:1:227:MET:O    | 4:1:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:1:369:ILE:HG23 | 4:1:370:VAL:N    | 2.35                     | 0.41              |
| 4:2:226:GLU:HG3  | 4:2:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:2:237:GLU:HA   | 4:2:251:GLY:CA   | 2.43                     | 0.41              |
| 4:3:32:PRO:HB2   | 4:3:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:3:219:VAL:HG22 | 4:3:258:PRO:CB   | 2.51                     | 0.41              |
| 4:3:287:ILE:CB   | 4:5:203:THR:HG22 | 2.44                     | 0.41              |
| 4:4:227:MET:O    | 4:4:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:7:227:MET:O    | 4:7:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:9:144:ALA:HB2  | 4:9:342:GLY:CA   | 2.51                     | 0.41              |
| 4:9:227:MET:O    | 4:9:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:9:288:ASP:OD1  | 4:W:204:ALA:HA   | 2.20                     | 0.41              |
| 4:V:32:PRO:HB2   | 4:V:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:V:227:MET:O    | 4:V:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:W:32:PRO:HB2   | 4:W:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:X:144:ALA:HB2  | 4:X:342:GLY:CA   | 2.51                     | 0.41              |
| 4:X:219:VAL:HG22 | 4:X:258:PRO:CB   | 2.51                     | 0.41              |
| 4:X:221:LEU:HA   | 4:X:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:X:226:GLU:HG3  | 4:X:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:Y:32:PRO:HB2   | 4:Y:34:ILE:CD1   | 2.51                     | 0.41              |
| 1:A:384:ASP:HA   | 1:A:394:SER:OG   | 2.21                     | 0.41              |
| 1:A:410:ASN:HA   | 4:8:334:GLU:HB3  | 1.29                     | 0.41              |
| 1:A:502:GLU:C    | 1:A:504:MLY:N    | 2.77                     | 0.41              |
| 2:B:63:GLU:O     | 2:B:67:MET:HG3   | 2.21                     | 0.41              |
| 2:B:111:SER:OG   | 2:B:148:VAL:CA   | 2.69                     | 0.41              |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:OD2  | 2.19                     | 0.41              |
| 1:D:348:MLY:HH12 | 1:D:348:MLY:HD2  | 1.81                     | 0.41              |
| 1:D:361:TYR:C    | 1:D:363:ASN:N    | 2.79                     | 0.41              |
| 1:G:25:ILE:HG23  | 1:G:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:G:172:ASN:OD1  | 1:G:457:TYR:HA   | 2.21                     | 0.41              |
| 1:G:214:MET:C    | 1:G:340:ILE:HD13 | 2.45                     | 0.41              |
| 1:G:534:SER:HB2  | 4:V:354:GLN:HE22 | 1.57                     | 0.41              |
| 1:G:537:GLU:OE1  | 4:V:350:SER:HA   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:553:MLY:HA   | 4:X:45:VAL:O     | 2.21                     | 0.41              |
| 1:G:657:LEU:HD12 | 1:G:657:LEU:O    | 2.21                     | 0.41              |
| 1:G:712:PRO:HB2  | 1:G:713:SER:H    | 1.61                     | 0.41              |
| 1:G:812:SER:O    | 1:G:816:ILE:HG13 | 2.21                     | 0.41              |
| 3:I:56:GLU:OE1   | 3:I:59:ASN:ND2   | 2.54                     | 0.41              |
| 1:J:144:ARG:HH11 | 1:J:160:ASP:CG   | 2.28                     | 0.41              |
| 1:J:330:GLU:HG2  | 1:J:330:GLU:H    | 1.54                     | 0.41              |
| 1:J:493:HIS:O    | 1:J:496:PHE:N    | 2.54                     | 0.41              |
| 1:J:642:LYS:HE2  | 4:W:344:SER:HA   | 1.56                     | 0.41              |
| 1:J:668:HIS:CD2  | 1:J:668:HIS:C    | 2.99                     | 0.41              |
| 1:J:701:LEU:HD12 | 1:J:701:LEU:HA   | 1.55                     | 0.41              |
| 1:J:733:PRO:CB   | 1:J:737:PHE:CE1  | 3.03                     | 0.41              |
| 1:J:842:LEU:N    | 1:J:842:LEU:CD1  | 2.83                     | 0.41              |
| 3:L:95:ASP:OD1   | 3:L:139:TYR:HE1  | 2.03                     | 0.41              |
| 4:3:144:ALA:HB2  | 4:3:342:GLY:CA   | 2.51                     | 0.41              |
| 4:4:219:VAL:HG22 | 4:4:258:PRO:CB   | 2.51                     | 0.41              |
| 4:5:227:MET:O    | 4:5:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:8:219:VAL:HG22 | 4:8:258:PRO:CB   | 2.51                     | 0.41              |
| 4:8:221:LEU:HA   | 4:8:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:9:287:ILE:HA   | 4:W:202:THR:HG21 | 1.59                     | 0.41              |
| 4:V:219:VAL:HG22 | 4:V:258:PRO:CB   | 2.51                     | 0.41              |
| 4:X:196:ARG:HH21 | 4:X:249:THR:HG23 | 1.85                     | 0.41              |
| 4:X:291:LYS:HG3  | 4:Z:244:ASP:HA   | 1.20                     | 0.41              |
| 1:A:335:ASP:O    | 1:A:338:ILE:HB   | 2.20                     | 0.40              |
| 1:D:94:MET:HE1   | 1:D:101:ALA:CB   | 2.50                     | 0.40              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:CG   | 2.32                     | 0.40              |
| 1:D:556:ASP:OD1  | 4:W:50:LYS:CG    | 2.69                     | 0.40              |
| 1:G:110:TYR:O    | 1:G:113:TRP:N    | 2.42                     | 0.40              |
| 1:G:528:MLY:HB2  | 1:G:529:PRO:HD2  | 2.03                     | 0.40              |
| 1:G:668:HIS:CD2  | 1:G:668:HIS:C    | 2.99                     | 0.40              |
| 1:G:835:PHE:CZ   | 2:H:27:PHE:CE1   | 3.09                     | 0.40              |
| 1:J:172:ASN:OD1  | 1:J:457:TYR:HA   | 2.21                     | 0.40              |
| 1:J:519:LEU:HD12 | 1:J:519:LEU:H    | 1.83                     | 0.40              |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:HB3  | 1.86                     | 0.40              |
| 2:K:113:LYS:O    | 2:K:147:ASN:HB2  | 2.20                     | 0.40              |
| 3:L:56:GLU:OE1   | 3:L:59:ASN:ND2   | 2.54                     | 0.40              |
| 4:0:369:ILE:HG23 | 4:0:370:VAL:N    | 2.35                     | 0.40              |
| 4:1:219:VAL:HG22 | 4:1:258:PRO:CB   | 2.52                     | 0.40              |
| 4:1:226:GLU:HG3  | 4:1:255:PHE:CE2  | 2.55                     | 0.40              |
| 4:V:221:LEU:HA   | 4:V:312:ARG:HG2  | 2.02                     | 0.40              |
| 4:Y:227:MET:O    | 4:Y:230:ALA:HB3  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Z:227:MET:O    | 4:Z:230:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:443:ILE:HG22 | 1:A:444:ARG:N    | 2.29                     | 0.40              |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:H    | 1.87                     | 0.40              |
| 1:A:555:TYR:C    | 1:A:557:GLU:N    | 2.77                     | 0.40              |
| 1:A:798:LEU:HD12 | 1:A:798:LEU:HA   | 1.37                     | 0.40              |
| 1:D:193:ILE:CD1  | 1:D:250:ILE:HD13 | 2.51                     | 0.40              |
| 1:D:237:THR:CG2  | 1:D:238:VAL:N    | 2.85                     | 0.40              |
| 1:D:635:GLY:C    | 4:9:341:ILE:HG21 | 2.45                     | 0.40              |
| 1:D:657:LEU:O    | 1:D:657:LEU:HD12 | 2.21                     | 0.40              |
| 1:D:717:TYR:OH   | 1:D:760:PHE:HB3  | 2.21                     | 0.40              |
| 3:F:56:GLU:OE1   | 3:F:59:ASN:ND2   | 2.54                     | 0.40              |
| 1:G:224:SER:C    | 1:G:227:PRO:HD2  | 2.47                     | 0.40              |
| 1:G:303:LEU:O    | 1:G:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:G:407:GLY:HA2  | 1:G:411:GLU:O    | 2.21                     | 0.40              |
| 1:G:493:HIS:O    | 1:G:496:PHE:N    | 2.54                     | 0.40              |
| 1:G:839:MLY:N    | 1:G:840:PRO:HD2  | 2.35                     | 0.40              |
| 1:J:303:LEU:O    | 1:J:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:J:553:MLY:HH12 | 4:Y:45:VAL:HG11  | 2.00                     | 0.40              |
| 1:J:659:MLY:HD2  | 1:J:659:MLY:HH22 | 1.42                     | 0.40              |
| 1:J:717:TYR:OH   | 1:J:760:PHE:HB3  | 2.20                     | 0.40              |
| 1:J:840:PRO:C    | 1:J:842:LEU:H    | 2.30                     | 0.40              |
| 4:0:120:THR:HG21 | 4:0:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:3:227:MET:O    | 4:3:230:ALA:HB3  | 2.21                     | 0.40              |
| 4:7:144:ALA:HB2  | 4:7:342:GLY:CA   | 2.51                     | 0.40              |
| 4:9:120:THR:HG21 | 4:9:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:9:299:MET:HE2  | 4:9:299:MET:HB2  | 1.82                     | 0.40              |
| 4:V:286:ASP:HA   | 4:X:202:THR:HG22 | 1.63                     | 0.40              |
| 4:X:120:THR:HG21 | 4:X:370:VAL:CG1  | 2.52                     | 0.40              |
| 1:A:322:VAL:HB   | 1:A:325:ILE:CG1  | 2.51                     | 0.40              |
| 1:A:398:LEU:HA   | 1:A:398:LEU:HD12 | 1.84                     | 0.40              |
| 1:A:817:GLN:HG3  | 2:B:127:ARG:HD3  | 1.01                     | 0.40              |
| 1:D:60:VAL:O     | 1:D:72:VAL:N     | 2.51                     | 0.40              |
| 1:D:176:LEU:N    | 1:D:176:LEU:CD1  | 2.75                     | 0.40              |
| 1:D:201:ALA:O    | 1:D:202:SER:OG   | 2.36                     | 0.40              |
| 1:D:668:HIS:CD2  | 1:D:668:HIS:C    | 2.99                     | 0.40              |
| 1:D:840:PRO:C    | 1:D:842:LEU:H    | 2.29                     | 0.40              |
| 2:E:163:ALA:O    | 2:K:20:ASP:OD2   | 2.38                     | 0.40              |
| 1:G:144:ARG:HH11 | 1:G:160:ASP:CG   | 2.28                     | 0.40              |
| 1:G:166:MET:CE   | 1:G:254:PHE:HB2  | 2.46                     | 0.40              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:OH   | 2.21                     | 0.40              |
| 1:G:673:ARG:HD2  | 1:G:673:ARG:HA   | 1.79                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:795:ARG:HE   | 3:I:118:MET:CE   | 2.32                     | 0.40              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:CG   | 2.93                     | 0.40              |
| 1:J:38:VAL:HG13  | 1:J:39:PHE:N     | 2.35                     | 0.40              |
| 1:J:361:TYR:C    | 1:J:363:ASN:N    | 2.78                     | 0.40              |
| 1:J:544:LYS:N    | 4:W:146:GLY:O    | 2.54                     | 0.40              |
| 3:L:62:ALA:O     | 3:L:63:ILE:CB    | 2.63                     | 0.40              |
| 4:0:112:PRO:HG3  | 4:1:195:GLU:HA   | 2.03                     | 0.40              |
| 4:0:226:GLU:HG3  | 4:0:255:PHE:CE2  | 2.55                     | 0.40              |
| 4:0:244:ASP:HA   | 4:Y:291:LYS:HG3  | 1.53                     | 0.40              |
| 4:8:32:PRO:HB2   | 4:8:34:ILE:CD1   | 2.51                     | 0.40              |
| 4:V:120:THR:HG21 | 4:V:370:VAL:CG1  | 2.51                     | 0.40              |
| 1:A:757:GLN:OE1  | 1:A:771:LEU:CD1  | 2.69                     | 0.40              |
| 2:B:112:ILE:O    | 2:B:148:VAL:N    | 2.50                     | 0.40              |
| 1:D:64:THR:OG1   | 1:D:68:GLU:HB3   | 2.22                     | 0.40              |
| 1:D:172:ASN:OD1  | 1:D:457:TYR:HA   | 2.21                     | 0.40              |
| 1:D:303:LEU:O    | 1:D:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:D:610:LEU:N    | 1:D:610:LEU:CD1  | 2.84                     | 0.40              |
| 1:D:795:ARG:O    | 3:F:35:ARG:HD3   | 2.20                     | 0.40              |
| 1:G:193:ILE:HD13 | 1:G:252:ILE:HD11 | 2.03                     | 0.40              |
| 1:G:194:GLN:HE21 | 1:G:194:GLN:HB3  | 1.43                     | 0.40              |
| 1:G:308:ASN:HA   | 1:G:309:PRO:HD2  | 1.88                     | 0.40              |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:H    | 1.87                     | 0.40              |
| 1:G:831:TRP:HZ2  | 2:H:67:MET:SD    | 2.32                     | 0.40              |
| 1:J:47:PHE:HE1   | 1:J:78:PHE:CE1   | 2.40                     | 0.40              |
| 1:J:63:MLY:HD3   | 1:J:63:MLY:HH23  | 1.76                     | 0.40              |
| 1:J:110:TYR:C    | 1:J:112:ALA:N    | 2.79                     | 0.40              |
| 1:J:311:ASP:C    | 1:J:312:TYR:CD1  | 3.00                     | 0.40              |
| 1:J:400:ALA:CB   | 1:J:606:THR:CG2  | 3.00                     | 0.40              |
| 1:J:528:MLY:HB2  | 1:J:529:PRO:HD2  | 2.03                     | 0.40              |
| 1:J:648:THR:CG2  | 1:J:651:ALA:CB   | 2.92                     | 0.40              |
| 1:J:712:PRO:HB2  | 1:J:713:SER:H    | 1.61                     | 0.40              |
| 1:J:756:THR:HB   | 1:J:757:GLN:H    | 1.63                     | 0.40              |
| 3:L:48:LYS:HD3   | 3:L:48:LYS:HA    | 1.17                     | 0.40              |
| 4:0:144:ALA:HB2  | 4:0:342:GLY:CA   | 2.51                     | 0.40              |
| 4:1:221:LEU:HA   | 4:1:312:ARG:HG2  | 2.02                     | 0.40              |
| 4:3:120:THR:HG21 | 4:3:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:7:219:VAL:HG22 | 4:7:258:PRO:CB   | 2.51                     | 0.40              |
| 4:W:196:ARG:HH21 | 4:W:249:THR:HG23 | 1.85                     | 0.40              |
| 4:X:291:LYS:HE2  | 4:Z:243:PRO:CA   | 2.41                     | 0.40              |
| 4:Z:171:LEU:HA   | 4:Z:172:PRO:HD2  | 1.84                     | 0.40              |
| 1:A:237:THR:CG2  | 1:A:238:VAL:N    | 2.84                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:400:ALA:CB   | 1:A:606:THR:CG2  | 3.00                     | 0.40              |
| 1:A:538:GLU:OE1  | 4:8:355:MET:HE1  | 2.17                     | 0.40              |
| 1:A:556:ASP:OD1  | 4:V:50:LYS:CG    | 2.69                     | 0.40              |
| 1:A:800:ARG:CZ   | 3:C:149:VAL:O    | 2.64                     | 0.40              |
| 1:D:89:GLU:HB3   | 1:D:153:PRO:HG3  | 2.03                     | 0.40              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:CD2  | 2.87                     | 0.40              |
| 1:D:724:TYR:HB3  | 1:D:727:LEU:CD1  | 2.48                     | 0.40              |
| 1:D:793:ARG:CA   | 3:F:40:ASN:ND2   | 2.78                     | 0.40              |
| 1:D:840:PRO:C    | 1:D:842:LEU:N    | 2.78                     | 0.40              |
| 2:E:149:ASP:O    | 2:E:150:TYR:CD1  | 2.75                     | 0.40              |
| 3:F:95:ASP:OD1   | 3:F:139:TYR:HE1  | 2.04                     | 0.40              |
| 1:G:221:GLN:HG2  | 1:G:221:GLN:H    | 1.47                     | 0.40              |
| 1:G:435:GLU:O    | 1:G:438:PHE:N    | 2.55                     | 0.40              |
| 1:G:502:GLU:C    | 1:G:504:MLY:N    | 2.77                     | 0.40              |
| 1:G:554:LEU:HD12 | 1:G:554:LEU:HA   | 1.76                     | 0.40              |
| 1:G:580:SER:O    | 1:G:581:LEU:HD12 | 2.22                     | 0.40              |
| 1:G:797:PHE:CD1  | 3:I:149:VAL:CB   | 2.85                     | 0.40              |
| 1:G:797:PHE:HD2  | 3:I:126:LEU:HD21 | 1.87                     | 0.40              |
| 2:H:63:GLU:O     | 2:H:67:MET:HG3   | 2.22                     | 0.40              |
| 1:J:60:VAL:O     | 1:J:72:VAL:N     | 2.51                     | 0.40              |
| 1:J:64:THR:HG22  | 1:J:65:GLU:H     | 1.87                     | 0.40              |
| 1:J:224:SER:C    | 1:J:227:PRO:HD2  | 2.47                     | 0.40              |
| 1:J:725:ARG:CZ   | 1:J:733:PRO:CB   | 2.83                     | 0.40              |
| 2:K:149:ASP:O    | 2:K:150:TYR:CD1  | 2.75                     | 0.40              |
| 4:1:32:PRO:HB2   | 4:1:34:ILE:CD1   | 2.51                     | 0.40              |
| 4:1:299:MET:HE2  | 4:1:299:MET:HB2  | 1.81                     | 0.40              |
| 4:1:315:LYS:HD2  | 4:1:315:LYS:HA   | 1.92                     | 0.40              |
| 4:3:250:ILE:HG22 | 4:3:254:ARG:HB2  | 2.04                     | 0.40              |
| 4:7:120:THR:HG21 | 4:7:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:8:287:ILE:N    | 4:V:202:THR:CG2  | 2.77                     | 0.40              |
| 4:Y:219:VAL:HG22 | 4:Y:258:PRO:CB   | 2.51                     | 0.40              |
| 4:Z:88:HIS:HA    | 4:Z:92:ASN:OD1   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 789/840 (94%)   | 650 (82%)  | 113 (14%) | 26 (3%)  | 3           | 21  |
| 1   | D     | 789/840 (94%)   | 650 (82%)  | 113 (14%) | 26 (3%)  | 3           | 21  |
| 1   | G     | 789/840 (94%)   | 650 (82%)  | 112 (14%) | 27 (3%)  | 3           | 21  |
| 1   | J     | 791/840 (94%)   | 652 (82%)  | 112 (14%) | 27 (3%)  | 3           | 21  |
| 2   | B     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 1           | 14  |
| 2   | E     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 1           | 14  |
| 2   | H     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 1           | 14  |
| 2   | K     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 1           | 14  |
| 3   | C     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 3   | F     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 3   | I     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 3   | L     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 4   | 0     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 1     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 2     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 3     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 4     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 5     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 7     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 8     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | 9     | 370/375 (99%)   | 333 (90%)  | 31 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | V     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | W     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | X     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | Y     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 7           | 38  |
| 4   | Z     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 7           | 38  |
| All | All   | 9482/9778 (97%) | 8316 (88%) | 944 (10%) | 222 (2%) | 7           | 28  |

All (222) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 73  | LYS  |
| 1   | A     | 202 | SER  |
| 1   | A     | 572 | LYS  |
| 1   | A     | 712 | PRO  |
| 1   | A     | 729 | ALA  |
| 1   | A     | 757 | GLN  |
| 1   | A     | 762 | HIS  |
| 2   | B     | 131 | GLU  |
| 2   | B     | 141 | PRO  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 202 | SER  |
| 1   | D     | 572 | LYS  |
| 1   | D     | 712 | PRO  |
| 1   | D     | 729 | ALA  |
| 1   | D     | 757 | GLN  |
| 1   | D     | 762 | HIS  |
| 2   | E     | 131 | GLU  |
| 2   | E     | 141 | PRO  |
| 1   | G     | 73  | LYS  |
| 1   | G     | 202 | SER  |
| 1   | G     | 572 | LYS  |
| 1   | G     | 712 | PRO  |
| 1   | G     | 729 | ALA  |
| 1   | G     | 757 | GLN  |
| 1   | G     | 762 | HIS  |
| 2   | H     | 131 | GLU  |
| 2   | H     | 141 | PRO  |
| 1   | J     | 73  | LYS  |
| 1   | J     | 202 | SER  |
| 1   | J     | 572 | LYS  |
| 1   | J     | 712 | PRO  |
| 1   | J     | 729 | ALA  |
| 1   | J     | 757 | GLN  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 785 | GLU  |
| 2   | K     | 131 | GLU  |
| 2   | K     | 141 | PRO  |
| 4   | 0     | 246 | GLN  |
| 4   | 1     | 246 | GLN  |
| 4   | 2     | 246 | GLN  |
| 4   | 3     | 246 | GLN  |
| 4   | 4     | 246 | GLN  |
| 4   | 5     | 246 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 7     | 246 | GLN  |
| 4   | 8     | 246 | GLN  |
| 4   | 9     | 246 | GLN  |
| 4   | V     | 246 | GLN  |
| 4   | W     | 246 | GLN  |
| 4   | X     | 246 | GLN  |
| 4   | Y     | 246 | GLN  |
| 4   | Z     | 246 | GLN  |
| 1   | A     | 11  | GLY  |
| 1   | A     | 21  | GLU  |
| 1   | A     | 219 | GLU  |
| 1   | A     | 517 | MET  |
| 1   | A     | 637 | LYS  |
| 2   | B     | 130 | PRO  |
| 2   | B     | 147 | ASN  |
| 2   | B     | 151 | LYS  |
| 2   | B     | 161 | GLU  |
| 1   | D     | 11  | GLY  |
| 1   | D     | 21  | GLU  |
| 1   | D     | 219 | GLU  |
| 1   | D     | 517 | MET  |
| 1   | D     | 637 | LYS  |
| 2   | E     | 130 | PRO  |
| 2   | E     | 147 | ASN  |
| 2   | E     | 151 | LYS  |
| 2   | E     | 161 | GLU  |
| 1   | G     | 11  | GLY  |
| 1   | G     | 21  | GLU  |
| 1   | G     | 219 | GLU  |
| 1   | G     | 517 | MET  |
| 1   | G     | 532 | ILE  |
| 1   | G     | 637 | LYS  |
| 1   | G     | 785 | GLU  |
| 2   | H     | 130 | PRO  |
| 2   | H     | 147 | ASN  |
| 2   | H     | 151 | LYS  |
| 1   | J     | 11  | GLY  |
| 1   | J     | 21  | GLU  |
| 1   | J     | 219 | GLU  |
| 1   | J     | 517 | MET  |
| 1   | J     | 637 | LYS  |
| 2   | K     | 130 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 147 | ASN  |
| 2   | K     | 151 | LYS  |
| 2   | K     | 161 | GLU  |
| 4   | 0     | 274 | ILE  |
| 4   | 1     | 274 | ILE  |
| 4   | 2     | 274 | ILE  |
| 4   | 3     | 274 | ILE  |
| 4   | 4     | 274 | ILE  |
| 4   | 5     | 274 | ILE  |
| 4   | 7     | 274 | ILE  |
| 4   | 8     | 274 | ILE  |
| 4   | 9     | 274 | ILE  |
| 4   | V     | 274 | ILE  |
| 4   | W     | 274 | ILE  |
| 4   | X     | 274 | ILE  |
| 4   | Y     | 274 | ILE  |
| 4   | Z     | 274 | ILE  |
| 1   | A     | 58  | GLY  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 532 | ILE  |
| 1   | A     | 644 | SER  |
| 1   | D     | 58  | GLY  |
| 1   | D     | 294 | ASN  |
| 1   | D     | 532 | ILE  |
| 1   | D     | 644 | SER  |
| 1   | G     | 58  | GLY  |
| 1   | G     | 294 | ASN  |
| 1   | G     | 644 | SER  |
| 2   | H     | 161 | GLU  |
| 1   | J     | 58  | GLY  |
| 1   | J     | 294 | ASN  |
| 1   | J     | 532 | ILE  |
| 1   | J     | 644 | SER  |
| 4   | 0     | 233 | SER  |
| 4   | 1     | 233 | SER  |
| 4   | 2     | 233 | SER  |
| 4   | 3     | 233 | SER  |
| 4   | 4     | 233 | SER  |
| 4   | 5     | 233 | SER  |
| 4   | 7     | 233 | SER  |
| 4   | 8     | 233 | SER  |
| 4   | 9     | 233 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | V     | 233 | SER  |
| 4   | W     | 233 | SER  |
| 4   | X     | 233 | SER  |
| 4   | Y     | 233 | SER  |
| 4   | Z     | 233 | SER  |
| 1   | A     | 435 | GLU  |
| 1   | A     | 817 | GLN  |
| 1   | D     | 435 | GLU  |
| 1   | D     | 817 | GLN  |
| 1   | G     | 269 | LEU  |
| 1   | G     | 435 | GLU  |
| 1   | G     | 817 | GLN  |
| 1   | J     | 435 | GLU  |
| 1   | J     | 817 | GLN  |
| 4   | 0     | 2   | GLU  |
| 4   | 1     | 2   | GLU  |
| 4   | 2     | 2   | GLU  |
| 4   | 3     | 2   | GLU  |
| 4   | 4     | 2   | GLU  |
| 4   | 5     | 2   | GLU  |
| 4   | 5     | 253 | GLU  |
| 4   | 7     | 2   | GLU  |
| 4   | 8     | 2   | GLU  |
| 4   | 9     | 2   | GLU  |
| 4   | 9     | 253 | GLU  |
| 4   | V     | 2   | GLU  |
| 4   | W     | 2   | GLU  |
| 4   | X     | 2   | GLU  |
| 4   | Y     | 2   | GLU  |
| 4   | Z     | 2   | GLU  |
| 1   | A     | 8   | ALA  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 578 | HIS  |
| 2   | B     | 140 | PHE  |
| 1   | D     | 8   | ALA  |
| 1   | D     | 269 | LEU  |
| 1   | D     | 578 | HIS  |
| 2   | E     | 140 | PHE  |
| 1   | G     | 8   | ALA  |
| 1   | G     | 79  | SER  |
| 1   | G     | 578 | HIS  |
| 2   | H     | 140 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 8   | ALA  |
| 1   | J     | 269 | LEU  |
| 1   | J     | 578 | HIS  |
| 2   | K     | 140 | PHE  |
| 4   | 0     | 253 | GLU  |
| 4   | 1     | 253 | GLU  |
| 4   | 2     | 253 | GLU  |
| 4   | 3     | 253 | GLU  |
| 4   | 4     | 253 | GLU  |
| 4   | 7     | 253 | GLU  |
| 4   | 8     | 253 | GLU  |
| 4   | V     | 253 | GLU  |
| 4   | W     | 253 | GLU  |
| 4   | X     | 253 | GLU  |
| 4   | Y     | 253 | GLU  |
| 4   | Z     | 253 | GLU  |
| 1   | A     | 79  | SER  |
| 1   | A     | 199 | ILE  |
| 1   | A     | 556 | ASP  |
| 2   | B     | 142 | PRO  |
| 1   | D     | 79  | SER  |
| 1   | D     | 199 | ILE  |
| 1   | D     | 556 | ASP  |
| 2   | E     | 142 | PRO  |
| 1   | G     | 199 | ILE  |
| 1   | G     | 556 | ASP  |
| 2   | H     | 142 | PRO  |
| 1   | J     | 79  | SER  |
| 1   | J     | 199 | ILE  |
| 1   | J     | 556 | ASP  |
| 2   | K     | 142 | PRO  |
| 1   | A     | 840 | PRO  |
| 1   | D     | 287 | ILE  |
| 1   | D     | 840 | PRO  |
| 1   | G     | 287 | ILE  |
| 1   | G     | 840 | PRO  |
| 1   | J     | 287 | ILE  |
| 1   | J     | 840 | PRO  |
| 4   | 0     | 242 | LEU  |
| 4   | 1     | 242 | LEU  |
| 4   | 2     | 242 | LEU  |
| 4   | 3     | 242 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 242 | LEU  |
| 4   | 5     | 242 | LEU  |
| 4   | 7     | 242 | LEU  |
| 4   | 8     | 242 | LEU  |
| 4   | 9     | 242 | LEU  |
| 4   | V     | 242 | LEU  |
| 4   | W     | 242 | LEU  |
| 4   | X     | 242 | LEU  |
| 4   | Y     | 242 | LEU  |
| 4   | Z     | 242 | LEU  |
| 1   | A     | 287 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 672/672 (100%) | 490 (73%)  | 182 (27%) | 0           | 3   |
| 1   | D     | 672/672 (100%) | 490 (73%)  | 182 (27%) | 0           | 3   |
| 1   | G     | 672/672 (100%) | 492 (73%)  | 180 (27%) | 0           | 3   |
| 1   | J     | 672/672 (100%) | 491 (73%)  | 181 (27%) | 0           | 3   |
| 2   | B     | 120/120 (100%) | 120 (100%) | 0         | 100         | 100 |
| 2   | E     | 120/120 (100%) | 119 (99%)  | 1 (1%)    | 73          | 80  |
| 2   | H     | 120/120 (100%) | 120 (100%) | 0         | 100         | 100 |
| 2   | K     | 120/120 (100%) | 120 (100%) | 0         | 100         | 100 |
| 3   | C     | 117/117 (100%) | 113 (97%)  | 4 (3%)    | 32          | 54  |
| 3   | F     | 117/117 (100%) | 113 (97%)  | 4 (3%)    | 32          | 54  |
| 3   | I     | 117/117 (100%) | 113 (97%)  | 4 (3%)    | 32          | 54  |
| 3   | L     | 117/117 (100%) | 113 (97%)  | 4 (3%)    | 32          | 54  |
| 4   | 0     | 315/318 (99%)  | 264 (84%)  | 51 (16%)  | 2           | 11  |
| 4   | 1     | 315/318 (99%)  | 265 (84%)  | 50 (16%)  | 2           | 11  |
| 4   | 2     | 315/318 (99%)  | 264 (84%)  | 51 (16%)  | 2           | 11  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 4   | 3     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | 4     | 315/318 (99%)    | 265 (84%)  | 50 (16%)   | 2           | 11 |
| 4   | 5     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | 7     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | 8     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | 9     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | V     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | W     | 315/318 (99%)    | 265 (84%)  | 50 (16%)   | 2           | 11 |
| 4   | X     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | Y     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| 4   | Z     | 315/318 (99%)    | 264 (84%)  | 51 (16%)   | 2           | 11 |
| All | All   | 8046/8088 (100%) | 6593 (82%) | 1453 (18%) | 3           | 9  |

All (1453) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | MET  |
| 1   | A     | 12  | GLU  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 20  | SER  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 23  | GLU  |
| 1   | A     | 25  | ILE  |
| 1   | A     | 36  | SER  |
| 1   | A     | 37  | SER  |
| 1   | A     | 38  | VAL  |
| 1   | A     | 40  | VAL  |
| 1   | A     | 41  | VAL  |
| 1   | A     | 46  | SER  |
| 1   | A     | 52  | ILE  |
| 1   | A     | 61  | THR  |
| 1   | A     | 65  | GLU  |
| 1   | A     | 69  | THR  |
| 1   | A     | 70  | LEU  |
| 1   | A     | 72  | VAL  |
| 1   | A     | 73  | LYS  |
| 1   | A     | 75  | ASP  |
| 1   | A     | 76  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 88  | ILE  |
| 1   | A     | 97  | LEU  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 109 | ARG  |
| 1   | A     | 114 | MET  |
| 1   | A     | 117 | THR  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 125 | THR  |
| 1   | A     | 126 | VAL  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 136 | ASN  |
| 1   | A     | 146 | LYS  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 155 | ILE  |
| 1   | A     | 157 | SER  |
| 1   | A     | 158 | ILE  |
| 1   | A     | 159 | SER  |
| 1   | A     | 166 | MET  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 169 | ASP  |
| 1   | A     | 170 | ARG  |
| 1   | A     | 173 | GLN  |
| 1   | A     | 175 | ILE  |
| 1   | A     | 178 | THR  |
| 1   | A     | 180 | GLU  |
| 1   | A     | 185 | LYS  |
| 1   | A     | 186 | THR  |
| 1   | A     | 187 | VAL  |
| 1   | A     | 189 | THR  |
| 1   | A     | 191 | ARG  |
| 1   | A     | 193 | ILE  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 198 | THR  |
| 1   | A     | 199 | ILE  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 219 | GLU  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 223 | ILE  |
| 1   | A     | 229 | LEU  |
| 1   | A     | 244 | SER  |
| 1   | A     | 245 | ARG  |
| 1   | A     | 251 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 273 | SER  |
| 1   | A     | 274 | ARG  |
| 1   | A     | 278 | GLN  |
| 1   | A     | 282 | GLU  |
| 1   | A     | 287 | ILE  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 291 | ILE  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 298 | GLU  |
| 1   | A     | 300 | ILE  |
| 1   | A     | 302 | MET  |
| 1   | A     | 303 | LEU  |
| 1   | A     | 305 | ILE  |
| 1   | A     | 315 | VAL  |
| 1   | A     | 325 | ILE  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 332 | MET  |
| 1   | A     | 336 | SER  |
| 1   | A     | 351 | ILE  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 359 | MET  |
| 1   | A     | 364 | LEU  |
| 1   | A     | 365 | LYS  |
| 1   | A     | 372 | GLU  |
| 1   | A     | 376 | GLU  |
| 1   | A     | 381 | GLU  |
| 1   | A     | 389 | LEU  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 394 | SER  |
| 1   | A     | 399 | LYS  |
| 1   | A     | 401 | LEU  |
| 1   | A     | 405 | ARG  |
| 1   | A     | 410 | ASN  |
| 1   | A     | 411 | GLU  |
| 1   | A     | 439 | LEU  |
| 1   | A     | 448 | GLN  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 452 | LYS  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 455 | ARG  |
| 1   | A     | 456 | GLN  |
| 1   | A     | 457 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 462 | LEU  |
| 1   | A     | 471 | ASP  |
| 1   | A     | 480 | ILE  |
| 1   | A     | 487 | LEU  |
| 1   | A     | 495 | MET  |
| 1   | A     | 498 | LEU  |
| 1   | A     | 499 | GLU  |
| 1   | A     | 506 | GLU  |
| 1   | A     | 513 | ILE  |
| 1   | A     | 524 | GLU  |
| 1   | A     | 530 | MET  |
| 1   | A     | 532 | ILE  |
| 1   | A     | 534 | SER  |
| 1   | A     | 537 | GLU  |
| 1   | A     | 549 | SER  |
| 1   | A     | 561 | LYS  |
| 1   | A     | 562 | SER  |
| 1   | A     | 569 | LYS  |
| 1   | A     | 580 | SER  |
| 1   | A     | 593 | SER  |
| 1   | A     | 596 | LEU  |
| 1   | A     | 597 | GLU  |
| 1   | A     | 604 | ASN  |
| 1   | A     | 608 | ILE  |
| 1   | A     | 610 | LEU  |
| 1   | A     | 615 | SER  |
| 1   | A     | 621 | LEU  |
| 1   | A     | 625 | THR  |
| 1   | A     | 664 | LEU  |
| 1   | A     | 666 | SER  |
| 1   | A     | 673 | ARG  |
| 1   | A     | 675 | ILE  |
| 1   | A     | 676 | ILE  |
| 1   | A     | 686 | MET  |
| 1   | A     | 689 | GLU  |
| 1   | A     | 690 | LEU  |
| 1   | A     | 693 | HIS  |
| 1   | A     | 698 | ASN  |
| 1   | A     | 700 | VAL  |
| 1   | A     | 701 | LEU  |
| 1   | A     | 702 | GLU  |
| 1   | A     | 704 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 705 | ARG  |
| 1   | A     | 707 | CYS  |
| 1   | A     | 708 | ARG  |
| 1   | A     | 713 | SER  |
| 1   | A     | 714 | ARG  |
| 1   | A     | 716 | LEU  |
| 1   | A     | 722 | GLN  |
| 1   | A     | 723 | ARG  |
| 1   | A     | 727 | LEU  |
| 1   | A     | 728 | ASN  |
| 1   | A     | 744 | SER  |
| 1   | A     | 745 | GLU  |
| 1   | A     | 748 | LEU  |
| 1   | A     | 752 | ASP  |
| 1   | A     | 753 | VAL  |
| 1   | A     | 754 | ASP  |
| 1   | A     | 762 | HIS  |
| 1   | A     | 772 | LEU  |
| 1   | A     | 774 | LEU  |
| 1   | A     | 785 | GLU  |
| 1   | A     | 787 | ILE  |
| 1   | A     | 793 | ARG  |
| 1   | A     | 798 | LEU  |
| 1   | A     | 799 | MET  |
| 1   | A     | 802 | GLU  |
| 1   | A     | 810 | ARG  |
| 1   | A     | 816 | ILE  |
| 1   | A     | 819 | ASN  |
| 1   | A     | 822 | SER  |
| 1   | A     | 832 | MET  |
| 1   | A     | 834 | LEU  |
| 1   | A     | 838 | ILE  |
| 1   | A     | 842 | LEU  |
| 1   | A     | 843 | LYS  |
| 3   | C     | 48  | LYS  |
| 3   | C     | 83  | THR  |
| 3   | C     | 85  | GLU  |
| 3   | C     | 96  | LYS  |
| 1   | D     | 7   | MET  |
| 1   | D     | 12  | GLU  |
| 1   | D     | 17  | LEU  |
| 1   | D     | 20  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 22  | LYS  |
| 1   | D     | 23  | GLU  |
| 1   | D     | 25  | ILE  |
| 1   | D     | 36  | SER  |
| 1   | D     | 37  | SER  |
| 1   | D     | 38  | VAL  |
| 1   | D     | 40  | VAL  |
| 1   | D     | 41  | VAL  |
| 1   | D     | 46  | SER  |
| 1   | D     | 52  | ILE  |
| 1   | D     | 61  | THR  |
| 1   | D     | 65  | GLU  |
| 1   | D     | 69  | THR  |
| 1   | D     | 70  | LEU  |
| 1   | D     | 72  | VAL  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 75  | ASP  |
| 1   | D     | 76  | GLN  |
| 1   | D     | 88  | ILE  |
| 1   | D     | 97  | LEU  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 109 | ARG  |
| 1   | D     | 114 | MET  |
| 1   | D     | 117 | THR  |
| 1   | D     | 121 | LEU  |
| 1   | D     | 125 | THR  |
| 1   | D     | 126 | VAL  |
| 1   | D     | 127 | ASN  |
| 1   | D     | 136 | ASN  |
| 1   | D     | 146 | LYS  |
| 1   | D     | 149 | GLN  |
| 1   | D     | 155 | ILE  |
| 1   | D     | 157 | SER  |
| 1   | D     | 158 | ILE  |
| 1   | D     | 159 | SER  |
| 1   | D     | 166 | MET  |
| 1   | D     | 167 | LEU  |
| 1   | D     | 169 | ASP  |
| 1   | D     | 170 | ARG  |
| 1   | D     | 173 | GLN  |
| 1   | D     | 175 | ILE  |
| 1   | D     | 178 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 180 | GLU  |
| 1   | D     | 185 | LYS  |
| 1   | D     | 186 | THR  |
| 1   | D     | 187 | VAL  |
| 1   | D     | 189 | THR  |
| 1   | D     | 191 | ARG  |
| 1   | D     | 193 | ILE  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 198 | THR  |
| 1   | D     | 199 | ILE  |
| 1   | D     | 218 | LEU  |
| 1   | D     | 219 | GLU  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 223 | ILE  |
| 1   | D     | 229 | LEU  |
| 1   | D     | 244 | SER  |
| 1   | D     | 245 | ARG  |
| 1   | D     | 251 | ARG  |
| 1   | D     | 273 | SER  |
| 1   | D     | 274 | ARG  |
| 1   | D     | 278 | GLN  |
| 1   | D     | 282 | GLU  |
| 1   | D     | 287 | ILE  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 291 | ILE  |
| 1   | D     | 294 | ASN  |
| 1   | D     | 298 | GLU  |
| 1   | D     | 300 | ILE  |
| 1   | D     | 302 | MET  |
| 1   | D     | 303 | LEU  |
| 1   | D     | 305 | ILE  |
| 1   | D     | 315 | VAL  |
| 1   | D     | 325 | ILE  |
| 1   | D     | 331 | LEU  |
| 1   | D     | 332 | MET  |
| 1   | D     | 336 | SER  |
| 1   | D     | 351 | ILE  |
| 1   | D     | 354 | LEU  |
| 1   | D     | 359 | MET  |
| 1   | D     | 364 | LEU  |
| 1   | D     | 365 | LYS  |
| 1   | D     | 372 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 376 | GLU  |
| 1   | D     | 381 | GLU  |
| 1   | D     | 389 | LEU  |
| 1   | D     | 392 | LEU  |
| 1   | D     | 394 | SER  |
| 1   | D     | 399 | LYS  |
| 1   | D     | 401 | LEU  |
| 1   | D     | 405 | ARG  |
| 1   | D     | 410 | ASN  |
| 1   | D     | 411 | GLU  |
| 1   | D     | 439 | LEU  |
| 1   | D     | 448 | GLN  |
| 1   | D     | 449 | LEU  |
| 1   | D     | 452 | LYS  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 455 | ARG  |
| 1   | D     | 456 | GLN  |
| 1   | D     | 457 | TYR  |
| 1   | D     | 462 | LEU  |
| 1   | D     | 471 | ASP  |
| 1   | D     | 480 | ILE  |
| 1   | D     | 487 | LEU  |
| 1   | D     | 495 | MET  |
| 1   | D     | 498 | LEU  |
| 1   | D     | 499 | GLU  |
| 1   | D     | 506 | GLU  |
| 1   | D     | 513 | ILE  |
| 1   | D     | 524 | GLU  |
| 1   | D     | 530 | MET  |
| 1   | D     | 532 | ILE  |
| 1   | D     | 534 | SER  |
| 1   | D     | 537 | GLU  |
| 1   | D     | 549 | SER  |
| 1   | D     | 561 | LYS  |
| 1   | D     | 562 | SER  |
| 1   | D     | 569 | LYS  |
| 1   | D     | 580 | SER  |
| 1   | D     | 593 | SER  |
| 1   | D     | 596 | LEU  |
| 1   | D     | 597 | GLU  |
| 1   | D     | 604 | ASN  |
| 1   | D     | 608 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 610 | LEU  |
| 1   | D     | 615 | SER  |
| 1   | D     | 621 | LEU  |
| 1   | D     | 625 | THR  |
| 1   | D     | 664 | LEU  |
| 1   | D     | 666 | SER  |
| 1   | D     | 673 | ARG  |
| 1   | D     | 675 | ILE  |
| 1   | D     | 676 | ILE  |
| 1   | D     | 686 | MET  |
| 1   | D     | 689 | GLU  |
| 1   | D     | 690 | LEU  |
| 1   | D     | 693 | HIS  |
| 1   | D     | 698 | ASN  |
| 1   | D     | 700 | VAL  |
| 1   | D     | 701 | LEU  |
| 1   | D     | 702 | GLU  |
| 1   | D     | 704 | ILE  |
| 1   | D     | 705 | ARG  |
| 1   | D     | 707 | CYS  |
| 1   | D     | 708 | ARG  |
| 1   | D     | 713 | SER  |
| 1   | D     | 714 | ARG  |
| 1   | D     | 716 | LEU  |
| 1   | D     | 722 | GLN  |
| 1   | D     | 723 | ARG  |
| 1   | D     | 727 | LEU  |
| 1   | D     | 728 | ASN  |
| 1   | D     | 744 | SER  |
| 1   | D     | 745 | GLU  |
| 1   | D     | 748 | LEU  |
| 1   | D     | 752 | ASP  |
| 1   | D     | 753 | VAL  |
| 1   | D     | 754 | ASP  |
| 1   | D     | 762 | HIS  |
| 1   | D     | 772 | LEU  |
| 1   | D     | 774 | LEU  |
| 1   | D     | 785 | GLU  |
| 1   | D     | 787 | ILE  |
| 1   | D     | 793 | ARG  |
| 1   | D     | 798 | LEU  |
| 1   | D     | 799 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 802 | GLU  |
| 1   | D     | 810 | ARG  |
| 1   | D     | 816 | ILE  |
| 1   | D     | 819 | ASN  |
| 1   | D     | 822 | SER  |
| 1   | D     | 832 | MET  |
| 1   | D     | 834 | LEU  |
| 1   | D     | 838 | ILE  |
| 1   | D     | 842 | LEU  |
| 1   | D     | 843 | LYS  |
| 2   | E     | 129 | THR  |
| 3   | F     | 48  | LYS  |
| 3   | F     | 83  | THR  |
| 3   | F     | 85  | GLU  |
| 3   | F     | 96  | LYS  |
| 1   | G     | 7   | MET  |
| 1   | G     | 12  | GLU  |
| 1   | G     | 17  | LEU  |
| 1   | G     | 20  | SER  |
| 1   | G     | 22  | LYS  |
| 1   | G     | 23  | GLU  |
| 1   | G     | 25  | ILE  |
| 1   | G     | 36  | SER  |
| 1   | G     | 37  | SER  |
| 1   | G     | 38  | VAL  |
| 1   | G     | 40  | VAL  |
| 1   | G     | 41  | VAL  |
| 1   | G     | 46  | SER  |
| 1   | G     | 52  | ILE  |
| 1   | G     | 61  | THR  |
| 1   | G     | 65  | GLU  |
| 1   | G     | 69  | THR  |
| 1   | G     | 70  | LEU  |
| 1   | G     | 72  | VAL  |
| 1   | G     | 73  | LYS  |
| 1   | G     | 75  | ASP  |
| 1   | G     | 76  | GLN  |
| 1   | G     | 88  | ILE  |
| 1   | G     | 97  | LEU  |
| 1   | G     | 106 | LEU  |
| 1   | G     | 109 | ARG  |
| 1   | G     | 114 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 117 | THR  |
| 1   | G     | 121 | LEU  |
| 1   | G     | 125 | THR  |
| 1   | G     | 126 | VAL  |
| 1   | G     | 127 | ASN  |
| 1   | G     | 136 | ASN  |
| 1   | G     | 146 | LYS  |
| 1   | G     | 149 | GLN  |
| 1   | G     | 155 | ILE  |
| 1   | G     | 157 | SER  |
| 1   | G     | 158 | ILE  |
| 1   | G     | 159 | SER  |
| 1   | G     | 166 | MET  |
| 1   | G     | 167 | LEU  |
| 1   | G     | 169 | ASP  |
| 1   | G     | 170 | ARG  |
| 1   | G     | 173 | GLN  |
| 1   | G     | 175 | ILE  |
| 1   | G     | 178 | THR  |
| 1   | G     | 180 | GLU  |
| 1   | G     | 185 | LYS  |
| 1   | G     | 186 | THR  |
| 1   | G     | 187 | VAL  |
| 1   | G     | 189 | THR  |
| 1   | G     | 191 | ARG  |
| 1   | G     | 193 | ILE  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 198 | THR  |
| 1   | G     | 199 | ILE  |
| 1   | G     | 218 | LEU  |
| 1   | G     | 219 | GLU  |
| 1   | G     | 221 | GLN  |
| 1   | G     | 223 | ILE  |
| 1   | G     | 229 | LEU  |
| 1   | G     | 244 | SER  |
| 1   | G     | 245 | ARG  |
| 1   | G     | 251 | ARG  |
| 1   | G     | 273 | SER  |
| 1   | G     | 274 | ARG  |
| 1   | G     | 278 | GLN  |
| 1   | G     | 282 | GLU  |
| 1   | G     | 287 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 290 | GLN  |
| 1   | G     | 291 | ILE  |
| 1   | G     | 294 | ASN  |
| 1   | G     | 298 | GLU  |
| 1   | G     | 300 | ILE  |
| 1   | G     | 302 | MET  |
| 1   | G     | 303 | LEU  |
| 1   | G     | 305 | ILE  |
| 1   | G     | 315 | VAL  |
| 1   | G     | 325 | ILE  |
| 1   | G     | 331 | LEU  |
| 1   | G     | 332 | MET  |
| 1   | G     | 336 | SER  |
| 1   | G     | 351 | ILE  |
| 1   | G     | 354 | LEU  |
| 1   | G     | 359 | MET  |
| 1   | G     | 364 | LEU  |
| 1   | G     | 365 | LYS  |
| 1   | G     | 372 | GLU  |
| 1   | G     | 376 | GLU  |
| 1   | G     | 381 | GLU  |
| 1   | G     | 389 | LEU  |
| 1   | G     | 392 | LEU  |
| 1   | G     | 394 | SER  |
| 1   | G     | 399 | LYS  |
| 1   | G     | 401 | LEU  |
| 1   | G     | 405 | ARG  |
| 1   | G     | 410 | ASN  |
| 1   | G     | 411 | GLU  |
| 1   | G     | 439 | LEU  |
| 1   | G     | 448 | GLN  |
| 1   | G     | 449 | LEU  |
| 1   | G     | 452 | LYS  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 455 | ARG  |
| 1   | G     | 456 | GLN  |
| 1   | G     | 457 | TYR  |
| 1   | G     | 462 | LEU  |
| 1   | G     | 471 | ASP  |
| 1   | G     | 480 | ILE  |
| 1   | G     | 487 | LEU  |
| 1   | G     | 495 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 498 | LEU  |
| 1   | G     | 506 | GLU  |
| 1   | G     | 513 | ILE  |
| 1   | G     | 524 | GLU  |
| 1   | G     | 530 | MET  |
| 1   | G     | 532 | ILE  |
| 1   | G     | 534 | SER  |
| 1   | G     | 537 | GLU  |
| 1   | G     | 549 | SER  |
| 1   | G     | 561 | LYS  |
| 1   | G     | 562 | SER  |
| 1   | G     | 569 | LYS  |
| 1   | G     | 580 | SER  |
| 1   | G     | 596 | LEU  |
| 1   | G     | 597 | GLU  |
| 1   | G     | 604 | ASN  |
| 1   | G     | 608 | ILE  |
| 1   | G     | 610 | LEU  |
| 1   | G     | 615 | SER  |
| 1   | G     | 621 | LEU  |
| 1   | G     | 625 | THR  |
| 1   | G     | 664 | LEU  |
| 1   | G     | 666 | SER  |
| 1   | G     | 673 | ARG  |
| 1   | G     | 675 | ILE  |
| 1   | G     | 676 | ILE  |
| 1   | G     | 686 | MET  |
| 1   | G     | 689 | GLU  |
| 1   | G     | 690 | LEU  |
| 1   | G     | 693 | HIS  |
| 1   | G     | 698 | ASN  |
| 1   | G     | 700 | VAL  |
| 1   | G     | 701 | LEU  |
| 1   | G     | 702 | GLU  |
| 1   | G     | 704 | ILE  |
| 1   | G     | 705 | ARG  |
| 1   | G     | 707 | CYS  |
| 1   | G     | 708 | ARG  |
| 1   | G     | 713 | SER  |
| 1   | G     | 714 | ARG  |
| 1   | G     | 716 | LEU  |
| 1   | G     | 722 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 723 | ARG  |
| 1   | G     | 727 | LEU  |
| 1   | G     | 728 | ASN  |
| 1   | G     | 744 | SER  |
| 1   | G     | 745 | GLU  |
| 1   | G     | 748 | LEU  |
| 1   | G     | 752 | ASP  |
| 1   | G     | 753 | VAL  |
| 1   | G     | 754 | ASP  |
| 1   | G     | 762 | HIS  |
| 1   | G     | 772 | LEU  |
| 1   | G     | 774 | LEU  |
| 1   | G     | 785 | GLU  |
| 1   | G     | 787 | ILE  |
| 1   | G     | 793 | ARG  |
| 1   | G     | 798 | LEU  |
| 1   | G     | 799 | MET  |
| 1   | G     | 802 | GLU  |
| 1   | G     | 810 | ARG  |
| 1   | G     | 816 | ILE  |
| 1   | G     | 819 | ASN  |
| 1   | G     | 822 | SER  |
| 1   | G     | 832 | MET  |
| 1   | G     | 834 | LEU  |
| 1   | G     | 838 | ILE  |
| 1   | G     | 842 | LEU  |
| 1   | G     | 843 | LYS  |
| 3   | I     | 48  | LYS  |
| 3   | I     | 83  | THR  |
| 3   | I     | 85  | GLU  |
| 3   | I     | 96  | LYS  |
| 1   | J     | 7   | MET  |
| 1   | J     | 12  | GLU  |
| 1   | J     | 17  | LEU  |
| 1   | J     | 20  | SER  |
| 1   | J     | 22  | LYS  |
| 1   | J     | 23  | GLU  |
| 1   | J     | 25  | ILE  |
| 1   | J     | 36  | SER  |
| 1   | J     | 37  | SER  |
| 1   | J     | 38  | VAL  |
| 1   | J     | 40  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 41  | VAL  |
| 1   | J     | 46  | SER  |
| 1   | J     | 52  | ILE  |
| 1   | J     | 61  | THR  |
| 1   | J     | 65  | GLU  |
| 1   | J     | 69  | THR  |
| 1   | J     | 70  | LEU  |
| 1   | J     | 72  | VAL  |
| 1   | J     | 73  | LYS  |
| 1   | J     | 75  | ASP  |
| 1   | J     | 76  | GLN  |
| 1   | J     | 88  | ILE  |
| 1   | J     | 97  | LEU  |
| 1   | J     | 106 | LEU  |
| 1   | J     | 109 | ARG  |
| 1   | J     | 114 | MET  |
| 1   | J     | 117 | THR  |
| 1   | J     | 121 | LEU  |
| 1   | J     | 125 | THR  |
| 1   | J     | 126 | VAL  |
| 1   | J     | 127 | ASN  |
| 1   | J     | 136 | ASN  |
| 1   | J     | 146 | LYS  |
| 1   | J     | 149 | GLN  |
| 1   | J     | 155 | ILE  |
| 1   | J     | 157 | SER  |
| 1   | J     | 158 | ILE  |
| 1   | J     | 159 | SER  |
| 1   | J     | 166 | MET  |
| 1   | J     | 167 | LEU  |
| 1   | J     | 169 | ASP  |
| 1   | J     | 170 | ARG  |
| 1   | J     | 173 | GLN  |
| 1   | J     | 175 | ILE  |
| 1   | J     | 178 | THR  |
| 1   | J     | 180 | GLU  |
| 1   | J     | 185 | LYS  |
| 1   | J     | 186 | THR  |
| 1   | J     | 187 | VAL  |
| 1   | J     | 189 | THR  |
| 1   | J     | 191 | ARG  |
| 1   | J     | 193 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 194 | GLN  |
| 1   | J     | 198 | THR  |
| 1   | J     | 199 | ILE  |
| 1   | J     | 218 | LEU  |
| 1   | J     | 219 | GLU  |
| 1   | J     | 221 | GLN  |
| 1   | J     | 223 | ILE  |
| 1   | J     | 229 | LEU  |
| 1   | J     | 244 | SER  |
| 1   | J     | 245 | ARG  |
| 1   | J     | 251 | ARG  |
| 1   | J     | 273 | SER  |
| 1   | J     | 274 | ARG  |
| 1   | J     | 278 | GLN  |
| 1   | J     | 282 | GLU  |
| 1   | J     | 287 | ILE  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 291 | ILE  |
| 1   | J     | 294 | ASN  |
| 1   | J     | 298 | GLU  |
| 1   | J     | 300 | ILE  |
| 1   | J     | 302 | MET  |
| 1   | J     | 303 | LEU  |
| 1   | J     | 305 | ILE  |
| 1   | J     | 315 | VAL  |
| 1   | J     | 325 | ILE  |
| 1   | J     | 331 | LEU  |
| 1   | J     | 332 | MET  |
| 1   | J     | 336 | SER  |
| 1   | J     | 351 | ILE  |
| 1   | J     | 354 | LEU  |
| 1   | J     | 359 | MET  |
| 1   | J     | 364 | LEU  |
| 1   | J     | 365 | LYS  |
| 1   | J     | 372 | GLU  |
| 1   | J     | 376 | GLU  |
| 1   | J     | 381 | GLU  |
| 1   | J     | 389 | LEU  |
| 1   | J     | 392 | LEU  |
| 1   | J     | 394 | SER  |
| 1   | J     | 399 | LYS  |
| 1   | J     | 401 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 405 | ARG  |
| 1   | J     | 410 | ASN  |
| 1   | J     | 411 | GLU  |
| 1   | J     | 439 | LEU  |
| 1   | J     | 448 | GLN  |
| 1   | J     | 449 | LEU  |
| 1   | J     | 452 | LYS  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 455 | ARG  |
| 1   | J     | 456 | GLN  |
| 1   | J     | 457 | TYR  |
| 1   | J     | 462 | LEU  |
| 1   | J     | 471 | ASP  |
| 1   | J     | 480 | ILE  |
| 1   | J     | 487 | LEU  |
| 1   | J     | 495 | MET  |
| 1   | J     | 498 | LEU  |
| 1   | J     | 506 | GLU  |
| 1   | J     | 513 | ILE  |
| 1   | J     | 524 | GLU  |
| 1   | J     | 530 | MET  |
| 1   | J     | 532 | ILE  |
| 1   | J     | 534 | SER  |
| 1   | J     | 537 | GLU  |
| 1   | J     | 549 | SER  |
| 1   | J     | 561 | LYS  |
| 1   | J     | 562 | SER  |
| 1   | J     | 569 | LYS  |
| 1   | J     | 580 | SER  |
| 1   | J     | 593 | SER  |
| 1   | J     | 596 | LEU  |
| 1   | J     | 597 | GLU  |
| 1   | J     | 604 | ASN  |
| 1   | J     | 608 | ILE  |
| 1   | J     | 610 | LEU  |
| 1   | J     | 615 | SER  |
| 1   | J     | 621 | LEU  |
| 1   | J     | 625 | THR  |
| 1   | J     | 664 | LEU  |
| 1   | J     | 666 | SER  |
| 1   | J     | 673 | ARG  |
| 1   | J     | 675 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 676 | ILE  |
| 1   | J     | 686 | MET  |
| 1   | J     | 689 | GLU  |
| 1   | J     | 690 | LEU  |
| 1   | J     | 693 | HIS  |
| 1   | J     | 698 | ASN  |
| 1   | J     | 700 | VAL  |
| 1   | J     | 701 | LEU  |
| 1   | J     | 702 | GLU  |
| 1   | J     | 704 | ILE  |
| 1   | J     | 705 | ARG  |
| 1   | J     | 707 | CYS  |
| 1   | J     | 708 | ARG  |
| 1   | J     | 713 | SER  |
| 1   | J     | 714 | ARG  |
| 1   | J     | 716 | LEU  |
| 1   | J     | 722 | GLN  |
| 1   | J     | 723 | ARG  |
| 1   | J     | 727 | LEU  |
| 1   | J     | 728 | ASN  |
| 1   | J     | 744 | SER  |
| 1   | J     | 745 | GLU  |
| 1   | J     | 748 | LEU  |
| 1   | J     | 752 | ASP  |
| 1   | J     | 753 | VAL  |
| 1   | J     | 754 | ASP  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 772 | LEU  |
| 1   | J     | 774 | LEU  |
| 1   | J     | 785 | GLU  |
| 1   | J     | 787 | ILE  |
| 1   | J     | 793 | ARG  |
| 1   | J     | 798 | LEU  |
| 1   | J     | 799 | MET  |
| 1   | J     | 802 | GLU  |
| 1   | J     | 810 | ARG  |
| 1   | J     | 816 | ILE  |
| 1   | J     | 819 | ASN  |
| 1   | J     | 822 | SER  |
| 1   | J     | 832 | MET  |
| 1   | J     | 834 | LEU  |
| 1   | J     | 838 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 842 | LEU  |
| 1   | J     | 843 | LYS  |
| 3   | L     | 48  | LYS  |
| 3   | L     | 83  | THR  |
| 3   | L     | 85  | GLU  |
| 3   | L     | 96  | LYS  |
| 4   | 0     | 16  | LEU  |
| 4   | 0     | 33  | SER  |
| 4   | 0     | 34  | ILE  |
| 4   | 0     | 37  | ARG  |
| 4   | 0     | 65  | LEU  |
| 4   | 0     | 66  | THR  |
| 4   | 0     | 67  | LEU  |
| 4   | 0     | 72  | GLU  |
| 4   | 0     | 80  | ASP  |
| 4   | 0     | 99  | GLU  |
| 4   | 0     | 100 | GLU  |
| 4   | 0     | 109 | PRO  |
| 4   | 0     | 145 | SER  |
| 4   | 0     | 153 | LEU  |
| 4   | 0     | 159 | VAL  |
| 4   | 0     | 180 | LEU  |
| 4   | 0     | 196 | ARG  |
| 4   | 0     | 199 | SER  |
| 4   | 0     | 201 | VAL  |
| 4   | 0     | 206 | ARG  |
| 4   | 0     | 221 | LEU  |
| 4   | 0     | 223 | PHE  |
| 4   | 0     | 229 | THR  |
| 4   | 0     | 238 | LYS  |
| 4   | 0     | 239 | SER  |
| 4   | 0     | 242 | LEU  |
| 4   | 0     | 246 | GLN  |
| 4   | 0     | 253 | GLU  |
| 4   | 0     | 263 | GLN  |
| 4   | 0     | 274 | ILE  |
| 4   | 0     | 281 | SER  |
| 4   | 0     | 283 | MET  |
| 4   | 0     | 287 | ILE  |
| 4   | 0     | 291 | LYS  |
| 4   | 0     | 293 | LEU  |
| 4   | 0     | 297 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 0     | 299 | MET  |
| 4   | 0     | 305 | MET  |
| 4   | 0     | 312 | ARG  |
| 4   | 0     | 315 | LYS  |
| 4   | 0     | 318 | THR  |
| 4   | 0     | 320 | LEU  |
| 4   | 0     | 327 | ILE  |
| 4   | 0     | 334 | GLU  |
| 4   | 0     | 349 | LEU  |
| 4   | 0     | 350 | SER  |
| 4   | 0     | 351 | THR  |
| 4   | 0     | 353 | GLN  |
| 4   | 0     | 354 | GLN  |
| 4   | 0     | 361 | GLU  |
| 4   | 0     | 368 | SER  |
| 4   | 1     | 16  | LEU  |
| 4   | 1     | 33  | SER  |
| 4   | 1     | 34  | ILE  |
| 4   | 1     | 37  | ARG  |
| 4   | 1     | 66  | THR  |
| 4   | 1     | 67  | LEU  |
| 4   | 1     | 72  | GLU  |
| 4   | 1     | 80  | ASP  |
| 4   | 1     | 99  | GLU  |
| 4   | 1     | 100 | GLU  |
| 4   | 1     | 109 | PRO  |
| 4   | 1     | 145 | SER  |
| 4   | 1     | 153 | LEU  |
| 4   | 1     | 159 | VAL  |
| 4   | 1     | 180 | LEU  |
| 4   | 1     | 196 | ARG  |
| 4   | 1     | 199 | SER  |
| 4   | 1     | 201 | VAL  |
| 4   | 1     | 206 | ARG  |
| 4   | 1     | 221 | LEU  |
| 4   | 1     | 223 | PHE  |
| 4   | 1     | 229 | THR  |
| 4   | 1     | 238 | LYS  |
| 4   | 1     | 239 | SER  |
| 4   | 1     | 242 | LEU  |
| 4   | 1     | 246 | GLN  |
| 4   | 1     | 253 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1     | 263 | GLN  |
| 4   | 1     | 274 | ILE  |
| 4   | 1     | 281 | SER  |
| 4   | 1     | 283 | MET  |
| 4   | 1     | 287 | ILE  |
| 4   | 1     | 291 | LYS  |
| 4   | 1     | 293 | LEU  |
| 4   | 1     | 297 | ASN  |
| 4   | 1     | 299 | MET  |
| 4   | 1     | 305 | MET  |
| 4   | 1     | 312 | ARG  |
| 4   | 1     | 315 | LYS  |
| 4   | 1     | 318 | THR  |
| 4   | 1     | 320 | LEU  |
| 4   | 1     | 327 | ILE  |
| 4   | 1     | 334 | GLU  |
| 4   | 1     | 349 | LEU  |
| 4   | 1     | 350 | SER  |
| 4   | 1     | 351 | THR  |
| 4   | 1     | 353 | GLN  |
| 4   | 1     | 354 | GLN  |
| 4   | 1     | 361 | GLU  |
| 4   | 1     | 368 | SER  |
| 4   | 2     | 16  | LEU  |
| 4   | 2     | 33  | SER  |
| 4   | 2     | 34  | ILE  |
| 4   | 2     | 37  | ARG  |
| 4   | 2     | 65  | LEU  |
| 4   | 2     | 66  | THR  |
| 4   | 2     | 67  | LEU  |
| 4   | 2     | 72  | GLU  |
| 4   | 2     | 80  | ASP  |
| 4   | 2     | 99  | GLU  |
| 4   | 2     | 100 | GLU  |
| 4   | 2     | 109 | PRO  |
| 4   | 2     | 145 | SER  |
| 4   | 2     | 153 | LEU  |
| 4   | 2     | 159 | VAL  |
| 4   | 2     | 180 | LEU  |
| 4   | 2     | 196 | ARG  |
| 4   | 2     | 199 | SER  |
| 4   | 2     | 201 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 2     | 206 | ARG  |
| 4   | 2     | 221 | LEU  |
| 4   | 2     | 223 | PHE  |
| 4   | 2     | 229 | THR  |
| 4   | 2     | 238 | LYS  |
| 4   | 2     | 239 | SER  |
| 4   | 2     | 242 | LEU  |
| 4   | 2     | 246 | GLN  |
| 4   | 2     | 253 | GLU  |
| 4   | 2     | 263 | GLN  |
| 4   | 2     | 274 | ILE  |
| 4   | 2     | 281 | SER  |
| 4   | 2     | 283 | MET  |
| 4   | 2     | 287 | ILE  |
| 4   | 2     | 291 | LYS  |
| 4   | 2     | 293 | LEU  |
| 4   | 2     | 297 | ASN  |
| 4   | 2     | 299 | MET  |
| 4   | 2     | 305 | MET  |
| 4   | 2     | 312 | ARG  |
| 4   | 2     | 315 | LYS  |
| 4   | 2     | 318 | THR  |
| 4   | 2     | 320 | LEU  |
| 4   | 2     | 327 | ILE  |
| 4   | 2     | 334 | GLU  |
| 4   | 2     | 349 | LEU  |
| 4   | 2     | 350 | SER  |
| 4   | 2     | 351 | THR  |
| 4   | 2     | 353 | GLN  |
| 4   | 2     | 354 | GLN  |
| 4   | 2     | 361 | GLU  |
| 4   | 2     | 368 | SER  |
| 4   | 3     | 16  | LEU  |
| 4   | 3     | 33  | SER  |
| 4   | 3     | 34  | ILE  |
| 4   | 3     | 37  | ARG  |
| 4   | 3     | 65  | LEU  |
| 4   | 3     | 66  | THR  |
| 4   | 3     | 67  | LEU  |
| 4   | 3     | 72  | GLU  |
| 4   | 3     | 80  | ASP  |
| 4   | 3     | 99  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 100 | GLU  |
| 4   | 3     | 109 | PRO  |
| 4   | 3     | 145 | SER  |
| 4   | 3     | 153 | LEU  |
| 4   | 3     | 159 | VAL  |
| 4   | 3     | 180 | LEU  |
| 4   | 3     | 196 | ARG  |
| 4   | 3     | 199 | SER  |
| 4   | 3     | 201 | VAL  |
| 4   | 3     | 206 | ARG  |
| 4   | 3     | 221 | LEU  |
| 4   | 3     | 223 | PHE  |
| 4   | 3     | 229 | THR  |
| 4   | 3     | 238 | LYS  |
| 4   | 3     | 239 | SER  |
| 4   | 3     | 242 | LEU  |
| 4   | 3     | 246 | GLN  |
| 4   | 3     | 253 | GLU  |
| 4   | 3     | 263 | GLN  |
| 4   | 3     | 274 | ILE  |
| 4   | 3     | 281 | SER  |
| 4   | 3     | 283 | MET  |
| 4   | 3     | 287 | ILE  |
| 4   | 3     | 291 | LYS  |
| 4   | 3     | 293 | LEU  |
| 4   | 3     | 297 | ASN  |
| 4   | 3     | 299 | MET  |
| 4   | 3     | 305 | MET  |
| 4   | 3     | 312 | ARG  |
| 4   | 3     | 315 | LYS  |
| 4   | 3     | 318 | THR  |
| 4   | 3     | 320 | LEU  |
| 4   | 3     | 327 | ILE  |
| 4   | 3     | 334 | GLU  |
| 4   | 3     | 349 | LEU  |
| 4   | 3     | 350 | SER  |
| 4   | 3     | 351 | THR  |
| 4   | 3     | 353 | GLN  |
| 4   | 3     | 354 | GLN  |
| 4   | 3     | 361 | GLU  |
| 4   | 3     | 368 | SER  |
| 4   | 4     | 16  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 33  | SER  |
| 4   | 4     | 34  | ILE  |
| 4   | 4     | 37  | ARG  |
| 4   | 4     | 66  | THR  |
| 4   | 4     | 67  | LEU  |
| 4   | 4     | 72  | GLU  |
| 4   | 4     | 80  | ASP  |
| 4   | 4     | 99  | GLU  |
| 4   | 4     | 100 | GLU  |
| 4   | 4     | 109 | PRO  |
| 4   | 4     | 145 | SER  |
| 4   | 4     | 153 | LEU  |
| 4   | 4     | 159 | VAL  |
| 4   | 4     | 180 | LEU  |
| 4   | 4     | 196 | ARG  |
| 4   | 4     | 199 | SER  |
| 4   | 4     | 201 | VAL  |
| 4   | 4     | 206 | ARG  |
| 4   | 4     | 221 | LEU  |
| 4   | 4     | 223 | PHE  |
| 4   | 4     | 229 | THR  |
| 4   | 4     | 238 | LYS  |
| 4   | 4     | 239 | SER  |
| 4   | 4     | 242 | LEU  |
| 4   | 4     | 246 | GLN  |
| 4   | 4     | 253 | GLU  |
| 4   | 4     | 263 | GLN  |
| 4   | 4     | 274 | ILE  |
| 4   | 4     | 281 | SER  |
| 4   | 4     | 283 | MET  |
| 4   | 4     | 287 | ILE  |
| 4   | 4     | 291 | LYS  |
| 4   | 4     | 293 | LEU  |
| 4   | 4     | 297 | ASN  |
| 4   | 4     | 299 | MET  |
| 4   | 4     | 305 | MET  |
| 4   | 4     | 312 | ARG  |
| 4   | 4     | 315 | LYS  |
| 4   | 4     | 318 | THR  |
| 4   | 4     | 320 | LEU  |
| 4   | 4     | 327 | ILE  |
| 4   | 4     | 334 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 349 | LEU  |
| 4   | 4     | 350 | SER  |
| 4   | 4     | 351 | THR  |
| 4   | 4     | 353 | GLN  |
| 4   | 4     | 354 | GLN  |
| 4   | 4     | 361 | GLU  |
| 4   | 4     | 368 | SER  |
| 4   | 5     | 16  | LEU  |
| 4   | 5     | 33  | SER  |
| 4   | 5     | 34  | ILE  |
| 4   | 5     | 37  | ARG  |
| 4   | 5     | 65  | LEU  |
| 4   | 5     | 66  | THR  |
| 4   | 5     | 67  | LEU  |
| 4   | 5     | 72  | GLU  |
| 4   | 5     | 80  | ASP  |
| 4   | 5     | 99  | GLU  |
| 4   | 5     | 100 | GLU  |
| 4   | 5     | 109 | PRO  |
| 4   | 5     | 145 | SER  |
| 4   | 5     | 153 | LEU  |
| 4   | 5     | 159 | VAL  |
| 4   | 5     | 180 | LEU  |
| 4   | 5     | 196 | ARG  |
| 4   | 5     | 199 | SER  |
| 4   | 5     | 201 | VAL  |
| 4   | 5     | 206 | ARG  |
| 4   | 5     | 221 | LEU  |
| 4   | 5     | 223 | PHE  |
| 4   | 5     | 229 | THR  |
| 4   | 5     | 238 | LYS  |
| 4   | 5     | 239 | SER  |
| 4   | 5     | 242 | LEU  |
| 4   | 5     | 246 | GLN  |
| 4   | 5     | 253 | GLU  |
| 4   | 5     | 263 | GLN  |
| 4   | 5     | 274 | ILE  |
| 4   | 5     | 281 | SER  |
| 4   | 5     | 283 | MET  |
| 4   | 5     | 287 | ILE  |
| 4   | 5     | 291 | LYS  |
| 4   | 5     | 293 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 5     | 297 | ASN  |
| 4   | 5     | 299 | MET  |
| 4   | 5     | 305 | MET  |
| 4   | 5     | 312 | ARG  |
| 4   | 5     | 315 | LYS  |
| 4   | 5     | 318 | THR  |
| 4   | 5     | 320 | LEU  |
| 4   | 5     | 327 | ILE  |
| 4   | 5     | 334 | GLU  |
| 4   | 5     | 349 | LEU  |
| 4   | 5     | 350 | SER  |
| 4   | 5     | 351 | THR  |
| 4   | 5     | 353 | GLN  |
| 4   | 5     | 354 | GLN  |
| 4   | 5     | 361 | GLU  |
| 4   | 5     | 368 | SER  |
| 4   | 7     | 16  | LEU  |
| 4   | 7     | 33  | SER  |
| 4   | 7     | 34  | ILE  |
| 4   | 7     | 37  | ARG  |
| 4   | 7     | 65  | LEU  |
| 4   | 7     | 66  | THR  |
| 4   | 7     | 67  | LEU  |
| 4   | 7     | 72  | GLU  |
| 4   | 7     | 80  | ASP  |
| 4   | 7     | 99  | GLU  |
| 4   | 7     | 100 | GLU  |
| 4   | 7     | 109 | PRO  |
| 4   | 7     | 145 | SER  |
| 4   | 7     | 153 | LEU  |
| 4   | 7     | 159 | VAL  |
| 4   | 7     | 180 | LEU  |
| 4   | 7     | 196 | ARG  |
| 4   | 7     | 199 | SER  |
| 4   | 7     | 201 | VAL  |
| 4   | 7     | 206 | ARG  |
| 4   | 7     | 221 | LEU  |
| 4   | 7     | 223 | PHE  |
| 4   | 7     | 229 | THR  |
| 4   | 7     | 238 | LYS  |
| 4   | 7     | 239 | SER  |
| 4   | 7     | 242 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 7     | 246 | GLN  |
| 4   | 7     | 253 | GLU  |
| 4   | 7     | 263 | GLN  |
| 4   | 7     | 274 | ILE  |
| 4   | 7     | 281 | SER  |
| 4   | 7     | 283 | MET  |
| 4   | 7     | 287 | ILE  |
| 4   | 7     | 291 | LYS  |
| 4   | 7     | 293 | LEU  |
| 4   | 7     | 297 | ASN  |
| 4   | 7     | 299 | MET  |
| 4   | 7     | 305 | MET  |
| 4   | 7     | 312 | ARG  |
| 4   | 7     | 315 | LYS  |
| 4   | 7     | 318 | THR  |
| 4   | 7     | 320 | LEU  |
| 4   | 7     | 327 | ILE  |
| 4   | 7     | 334 | GLU  |
| 4   | 7     | 349 | LEU  |
| 4   | 7     | 350 | SER  |
| 4   | 7     | 351 | THR  |
| 4   | 7     | 353 | GLN  |
| 4   | 7     | 354 | GLN  |
| 4   | 7     | 361 | GLU  |
| 4   | 7     | 368 | SER  |
| 4   | 8     | 16  | LEU  |
| 4   | 8     | 33  | SER  |
| 4   | 8     | 34  | ILE  |
| 4   | 8     | 37  | ARG  |
| 4   | 8     | 65  | LEU  |
| 4   | 8     | 66  | THR  |
| 4   | 8     | 67  | LEU  |
| 4   | 8     | 72  | GLU  |
| 4   | 8     | 80  | ASP  |
| 4   | 8     | 99  | GLU  |
| 4   | 8     | 100 | GLU  |
| 4   | 8     | 109 | PRO  |
| 4   | 8     | 145 | SER  |
| 4   | 8     | 153 | LEU  |
| 4   | 8     | 159 | VAL  |
| 4   | 8     | 180 | LEU  |
| 4   | 8     | 196 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 8     | 199 | SER  |
| 4   | 8     | 201 | VAL  |
| 4   | 8     | 206 | ARG  |
| 4   | 8     | 221 | LEU  |
| 4   | 8     | 223 | PHE  |
| 4   | 8     | 229 | THR  |
| 4   | 8     | 238 | LYS  |
| 4   | 8     | 239 | SER  |
| 4   | 8     | 242 | LEU  |
| 4   | 8     | 246 | GLN  |
| 4   | 8     | 253 | GLU  |
| 4   | 8     | 263 | GLN  |
| 4   | 8     | 274 | ILE  |
| 4   | 8     | 281 | SER  |
| 4   | 8     | 283 | MET  |
| 4   | 8     | 287 | ILE  |
| 4   | 8     | 291 | LYS  |
| 4   | 8     | 293 | LEU  |
| 4   | 8     | 297 | ASN  |
| 4   | 8     | 299 | MET  |
| 4   | 8     | 305 | MET  |
| 4   | 8     | 312 | ARG  |
| 4   | 8     | 315 | LYS  |
| 4   | 8     | 318 | THR  |
| 4   | 8     | 320 | LEU  |
| 4   | 8     | 327 | ILE  |
| 4   | 8     | 334 | GLU  |
| 4   | 8     | 349 | LEU  |
| 4   | 8     | 350 | SER  |
| 4   | 8     | 351 | THR  |
| 4   | 8     | 353 | GLN  |
| 4   | 8     | 354 | GLN  |
| 4   | 8     | 361 | GLU  |
| 4   | 8     | 368 | SER  |
| 4   | 9     | 16  | LEU  |
| 4   | 9     | 33  | SER  |
| 4   | 9     | 34  | ILE  |
| 4   | 9     | 37  | ARG  |
| 4   | 9     | 65  | LEU  |
| 4   | 9     | 66  | THR  |
| 4   | 9     | 67  | LEU  |
| 4   | 9     | 72  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 9     | 80  | ASP  |
| 4   | 9     | 99  | GLU  |
| 4   | 9     | 100 | GLU  |
| 4   | 9     | 109 | PRO  |
| 4   | 9     | 145 | SER  |
| 4   | 9     | 153 | LEU  |
| 4   | 9     | 159 | VAL  |
| 4   | 9     | 180 | LEU  |
| 4   | 9     | 196 | ARG  |
| 4   | 9     | 199 | SER  |
| 4   | 9     | 201 | VAL  |
| 4   | 9     | 206 | ARG  |
| 4   | 9     | 221 | LEU  |
| 4   | 9     | 223 | PHE  |
| 4   | 9     | 229 | THR  |
| 4   | 9     | 238 | LYS  |
| 4   | 9     | 239 | SER  |
| 4   | 9     | 242 | LEU  |
| 4   | 9     | 246 | GLN  |
| 4   | 9     | 253 | GLU  |
| 4   | 9     | 263 | GLN  |
| 4   | 9     | 274 | ILE  |
| 4   | 9     | 281 | SER  |
| 4   | 9     | 283 | MET  |
| 4   | 9     | 287 | ILE  |
| 4   | 9     | 291 | LYS  |
| 4   | 9     | 293 | LEU  |
| 4   | 9     | 297 | ASN  |
| 4   | 9     | 299 | MET  |
| 4   | 9     | 305 | MET  |
| 4   | 9     | 312 | ARG  |
| 4   | 9     | 315 | LYS  |
| 4   | 9     | 318 | THR  |
| 4   | 9     | 320 | LEU  |
| 4   | 9     | 327 | ILE  |
| 4   | 9     | 334 | GLU  |
| 4   | 9     | 349 | LEU  |
| 4   | 9     | 350 | SER  |
| 4   | 9     | 351 | THR  |
| 4   | 9     | 353 | GLN  |
| 4   | 9     | 354 | GLN  |
| 4   | 9     | 361 | GLU  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 9     | 368 | SER  |
| 4   | V     | 16  | LEU  |
| 4   | V     | 33  | SER  |
| 4   | V     | 34  | ILE  |
| 4   | V     | 37  | ARG  |
| 4   | V     | 65  | LEU  |
| 4   | V     | 66  | THR  |
| 4   | V     | 67  | LEU  |
| 4   | V     | 72  | GLU  |
| 4   | V     | 80  | ASP  |
| 4   | V     | 99  | GLU  |
| 4   | V     | 100 | GLU  |
| 4   | V     | 109 | PRO  |
| 4   | V     | 145 | SER  |
| 4   | V     | 153 | LEU  |
| 4   | V     | 159 | VAL  |
| 4   | V     | 180 | LEU  |
| 4   | V     | 196 | ARG  |
| 4   | V     | 199 | SER  |
| 4   | V     | 201 | VAL  |
| 4   | V     | 206 | ARG  |
| 4   | V     | 221 | LEU  |
| 4   | V     | 223 | PHE  |
| 4   | V     | 229 | THR  |
| 4   | V     | 238 | LYS  |
| 4   | V     | 239 | SER  |
| 4   | V     | 242 | LEU  |
| 4   | V     | 246 | GLN  |
| 4   | V     | 253 | GLU  |
| 4   | V     | 263 | GLN  |
| 4   | V     | 274 | ILE  |
| 4   | V     | 281 | SER  |
| 4   | V     | 283 | MET  |
| 4   | V     | 287 | ILE  |
| 4   | V     | 291 | LYS  |
| 4   | V     | 293 | LEU  |
| 4   | V     | 297 | ASN  |
| 4   | V     | 299 | MET  |
| 4   | V     | 305 | MET  |
| 4   | V     | 312 | ARG  |
| 4   | V     | 315 | LYS  |
| 4   | V     | 318 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | V     | 320 | LEU  |
| 4   | V     | 327 | ILE  |
| 4   | V     | 334 | GLU  |
| 4   | V     | 349 | LEU  |
| 4   | V     | 350 | SER  |
| 4   | V     | 351 | THR  |
| 4   | V     | 353 | GLN  |
| 4   | V     | 354 | GLN  |
| 4   | V     | 361 | GLU  |
| 4   | V     | 368 | SER  |
| 4   | W     | 16  | LEU  |
| 4   | W     | 33  | SER  |
| 4   | W     | 34  | ILE  |
| 4   | W     | 37  | ARG  |
| 4   | W     | 66  | THR  |
| 4   | W     | 67  | LEU  |
| 4   | W     | 72  | GLU  |
| 4   | W     | 80  | ASP  |
| 4   | W     | 99  | GLU  |
| 4   | W     | 100 | GLU  |
| 4   | W     | 109 | PRO  |
| 4   | W     | 145 | SER  |
| 4   | W     | 153 | LEU  |
| 4   | W     | 159 | VAL  |
| 4   | W     | 180 | LEU  |
| 4   | W     | 196 | ARG  |
| 4   | W     | 199 | SER  |
| 4   | W     | 201 | VAL  |
| 4   | W     | 206 | ARG  |
| 4   | W     | 221 | LEU  |
| 4   | W     | 223 | PHE  |
| 4   | W     | 229 | THR  |
| 4   | W     | 238 | LYS  |
| 4   | W     | 239 | SER  |
| 4   | W     | 242 | LEU  |
| 4   | W     | 246 | GLN  |
| 4   | W     | 253 | GLU  |
| 4   | W     | 263 | GLN  |
| 4   | W     | 274 | ILE  |
| 4   | W     | 281 | SER  |
| 4   | W     | 283 | MET  |
| 4   | W     | 287 | ILE  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | W     | 291 | LYS  |
| 4   | W     | 293 | LEU  |
| 4   | W     | 297 | ASN  |
| 4   | W     | 299 | MET  |
| 4   | W     | 305 | MET  |
| 4   | W     | 312 | ARG  |
| 4   | W     | 315 | LYS  |
| 4   | W     | 318 | THR  |
| 4   | W     | 320 | LEU  |
| 4   | W     | 327 | ILE  |
| 4   | W     | 334 | GLU  |
| 4   | W     | 349 | LEU  |
| 4   | W     | 350 | SER  |
| 4   | W     | 351 | THR  |
| 4   | W     | 353 | GLN  |
| 4   | W     | 354 | GLN  |
| 4   | W     | 361 | GLU  |
| 4   | W     | 368 | SER  |
| 4   | X     | 16  | LEU  |
| 4   | X     | 33  | SER  |
| 4   | X     | 34  | ILE  |
| 4   | X     | 37  | ARG  |
| 4   | X     | 65  | LEU  |
| 4   | X     | 66  | THR  |
| 4   | X     | 67  | LEU  |
| 4   | X     | 72  | GLU  |
| 4   | X     | 80  | ASP  |
| 4   | X     | 99  | GLU  |
| 4   | X     | 100 | GLU  |
| 4   | X     | 109 | PRO  |
| 4   | X     | 145 | SER  |
| 4   | X     | 153 | LEU  |
| 4   | X     | 159 | VAL  |
| 4   | X     | 180 | LEU  |
| 4   | X     | 196 | ARG  |
| 4   | X     | 199 | SER  |
| 4   | X     | 201 | VAL  |
| 4   | X     | 206 | ARG  |
| 4   | X     | 221 | LEU  |
| 4   | X     | 223 | PHE  |
| 4   | X     | 229 | THR  |
| 4   | X     | 238 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | X     | 239 | SER  |
| 4   | X     | 242 | LEU  |
| 4   | X     | 246 | GLN  |
| 4   | X     | 253 | GLU  |
| 4   | X     | 263 | GLN  |
| 4   | X     | 274 | ILE  |
| 4   | X     | 281 | SER  |
| 4   | X     | 283 | MET  |
| 4   | X     | 287 | ILE  |
| 4   | X     | 291 | LYS  |
| 4   | X     | 293 | LEU  |
| 4   | X     | 297 | ASN  |
| 4   | X     | 299 | MET  |
| 4   | X     | 305 | MET  |
| 4   | X     | 312 | ARG  |
| 4   | X     | 315 | LYS  |
| 4   | X     | 318 | THR  |
| 4   | X     | 320 | LEU  |
| 4   | X     | 327 | ILE  |
| 4   | X     | 334 | GLU  |
| 4   | X     | 349 | LEU  |
| 4   | X     | 350 | SER  |
| 4   | X     | 351 | THR  |
| 4   | X     | 353 | GLN  |
| 4   | X     | 354 | GLN  |
| 4   | X     | 361 | GLU  |
| 4   | X     | 368 | SER  |
| 4   | Y     | 16  | LEU  |
| 4   | Y     | 33  | SER  |
| 4   | Y     | 34  | ILE  |
| 4   | Y     | 37  | ARG  |
| 4   | Y     | 65  | LEU  |
| 4   | Y     | 66  | THR  |
| 4   | Y     | 67  | LEU  |
| 4   | Y     | 72  | GLU  |
| 4   | Y     | 80  | ASP  |
| 4   | Y     | 99  | GLU  |
| 4   | Y     | 100 | GLU  |
| 4   | Y     | 109 | PRO  |
| 4   | Y     | 145 | SER  |
| 4   | Y     | 153 | LEU  |
| 4   | Y     | 159 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Y     | 180 | LEU  |
| 4   | Y     | 196 | ARG  |
| 4   | Y     | 199 | SER  |
| 4   | Y     | 201 | VAL  |
| 4   | Y     | 206 | ARG  |
| 4   | Y     | 221 | LEU  |
| 4   | Y     | 223 | PHE  |
| 4   | Y     | 229 | THR  |
| 4   | Y     | 238 | LYS  |
| 4   | Y     | 239 | SER  |
| 4   | Y     | 242 | LEU  |
| 4   | Y     | 246 | GLN  |
| 4   | Y     | 253 | GLU  |
| 4   | Y     | 263 | GLN  |
| 4   | Y     | 274 | ILE  |
| 4   | Y     | 281 | SER  |
| 4   | Y     | 283 | MET  |
| 4   | Y     | 287 | ILE  |
| 4   | Y     | 291 | LYS  |
| 4   | Y     | 293 | LEU  |
| 4   | Y     | 297 | ASN  |
| 4   | Y     | 299 | MET  |
| 4   | Y     | 305 | MET  |
| 4   | Y     | 312 | ARG  |
| 4   | Y     | 315 | LYS  |
| 4   | Y     | 318 | THR  |
| 4   | Y     | 320 | LEU  |
| 4   | Y     | 327 | ILE  |
| 4   | Y     | 334 | GLU  |
| 4   | Y     | 349 | LEU  |
| 4   | Y     | 350 | SER  |
| 4   | Y     | 351 | THR  |
| 4   | Y     | 353 | GLN  |
| 4   | Y     | 354 | GLN  |
| 4   | Y     | 361 | GLU  |
| 4   | Y     | 368 | SER  |
| 4   | Z     | 16  | LEU  |
| 4   | Z     | 33  | SER  |
| 4   | Z     | 34  | ILE  |
| 4   | Z     | 37  | ARG  |
| 4   | Z     | 65  | LEU  |
| 4   | Z     | 66  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Z     | 67  | LEU  |
| 4   | Z     | 72  | GLU  |
| 4   | Z     | 80  | ASP  |
| 4   | Z     | 99  | GLU  |
| 4   | Z     | 100 | GLU  |
| 4   | Z     | 109 | PRO  |
| 4   | Z     | 145 | SER  |
| 4   | Z     | 153 | LEU  |
| 4   | Z     | 159 | VAL  |
| 4   | Z     | 180 | LEU  |
| 4   | Z     | 196 | ARG  |
| 4   | Z     | 199 | SER  |
| 4   | Z     | 201 | VAL  |
| 4   | Z     | 206 | ARG  |
| 4   | Z     | 221 | LEU  |
| 4   | Z     | 223 | PHE  |
| 4   | Z     | 229 | THR  |
| 4   | Z     | 238 | LYS  |
| 4   | Z     | 239 | SER  |
| 4   | Z     | 242 | LEU  |
| 4   | Z     | 246 | GLN  |
| 4   | Z     | 253 | GLU  |
| 4   | Z     | 263 | GLN  |
| 4   | Z     | 274 | ILE  |
| 4   | Z     | 281 | SER  |
| 4   | Z     | 283 | MET  |
| 4   | Z     | 287 | ILE  |
| 4   | Z     | 291 | LYS  |
| 4   | Z     | 293 | LEU  |
| 4   | Z     | 297 | ASN  |
| 4   | Z     | 299 | MET  |
| 4   | Z     | 305 | MET  |
| 4   | Z     | 312 | ARG  |
| 4   | Z     | 315 | LYS  |
| 4   | Z     | 318 | THR  |
| 4   | Z     | 320 | LEU  |
| 4   | Z     | 327 | ILE  |
| 4   | Z     | 334 | GLU  |
| 4   | Z     | 349 | LEU  |
| 4   | Z     | 350 | SER  |
| 4   | Z     | 351 | THR  |
| 4   | Z     | 353 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Z     | 354 | GLN  |
| 4   | Z     | 361 | GLU  |
| 4   | Z     | 368 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (233) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | ASN  |
| 1   | A     | 76  | GLN  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 154 | HIS  |
| 1   | A     | 164 | GLN  |
| 1   | A     | 188 | ASN  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 234 | ASN  |
| 1   | A     | 253 | HIS  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 360 | HIS  |
| 1   | A     | 368 | GLN  |
| 1   | A     | 424 | ASN  |
| 1   | A     | 447 | GLN  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 481 | ASN  |
| 1   | A     | 484 | ASN  |
| 1   | A     | 488 | GLN  |
| 1   | A     | 563 | ASN  |
| 1   | A     | 564 | ASN  |
| 1   | A     | 578 | HIS  |
| 1   | A     | 591 | ASN  |
| 1   | A     | 612 | GLN  |
| 1   | A     | 656 | ASN  |
| 1   | A     | 670 | HIS  |
| 1   | A     | 698 | ASN  |
| 1   | A     | 762 | HIS  |
| 1   | A     | 825 | ASN  |
| 2   | B     | 159 | HIS  |
| 3   | C     | 40  | ASN  |
| 3   | C     | 52  | ASN  |
| 3   | C     | 59  | ASN  |
| 1   | D     | 29  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 76  | GLN  |
| 1   | D     | 127 | ASN  |
| 1   | D     | 149 | GLN  |
| 1   | D     | 164 | GLN  |
| 1   | D     | 188 | ASN  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 234 | ASN  |
| 1   | D     | 253 | HIS  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 360 | HIS  |
| 1   | D     | 368 | GLN  |
| 1   | D     | 424 | ASN  |
| 1   | D     | 447 | GLN  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 481 | ASN  |
| 1   | D     | 484 | ASN  |
| 1   | D     | 488 | GLN  |
| 1   | D     | 563 | ASN  |
| 1   | D     | 564 | ASN  |
| 1   | D     | 578 | HIS  |
| 1   | D     | 591 | ASN  |
| 1   | D     | 612 | GLN  |
| 1   | D     | 656 | ASN  |
| 1   | D     | 670 | HIS  |
| 1   | D     | 698 | ASN  |
| 1   | D     | 762 | HIS  |
| 1   | D     | 791 | GLN  |
| 1   | D     | 817 | GLN  |
| 1   | D     | 825 | ASN  |
| 2   | E     | 159 | HIS  |
| 3   | F     | 52  | ASN  |
| 3   | F     | 59  | ASN  |
| 3   | F     | 81  | GLN  |
| 1   | G     | 29  | ASN  |
| 1   | G     | 76  | GLN  |
| 1   | G     | 127 | ASN  |
| 1   | G     | 154 | HIS  |
| 1   | G     | 164 | GLN  |
| 1   | G     | 188 | ASN  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 221 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 253 | HIS  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 360 | HIS  |
| 1   | G     | 368 | GLN  |
| 1   | G     | 424 | ASN  |
| 1   | G     | 447 | GLN  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 481 | ASN  |
| 1   | G     | 484 | ASN  |
| 1   | G     | 563 | ASN  |
| 1   | G     | 564 | ASN  |
| 1   | G     | 578 | HIS  |
| 1   | G     | 591 | ASN  |
| 1   | G     | 612 | GLN  |
| 1   | G     | 656 | ASN  |
| 1   | G     | 670 | HIS  |
| 1   | G     | 698 | ASN  |
| 1   | G     | 728 | ASN  |
| 1   | G     | 762 | HIS  |
| 1   | G     | 825 | ASN  |
| 3   | I     | 40  | ASN  |
| 3   | I     | 52  | ASN  |
| 3   | I     | 59  | ASN  |
| 3   | I     | 81  | GLN  |
| 3   | I     | 109 | HIS  |
| 1   | J     | 29  | ASN  |
| 1   | J     | 76  | GLN  |
| 1   | J     | 127 | ASN  |
| 1   | J     | 154 | HIS  |
| 1   | J     | 164 | GLN  |
| 1   | J     | 188 | ASN  |
| 1   | J     | 194 | GLN  |
| 1   | J     | 221 | GLN  |
| 1   | J     | 234 | ASN  |
| 1   | J     | 253 | HIS  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 360 | HIS  |
| 1   | J     | 368 | GLN  |
| 1   | J     | 424 | ASN  |
| 1   | J     | 447 | GLN  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 481 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 484 | ASN  |
| 1   | J     | 488 | GLN  |
| 1   | J     | 552 | ASN  |
| 1   | J     | 563 | ASN  |
| 1   | J     | 564 | ASN  |
| 1   | J     | 578 | HIS  |
| 1   | J     | 591 | ASN  |
| 1   | J     | 612 | GLN  |
| 1   | J     | 656 | ASN  |
| 1   | J     | 670 | HIS  |
| 1   | J     | 698 | ASN  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 791 | GLN  |
| 1   | J     | 825 | ASN  |
| 2   | K     | 159 | HIS  |
| 3   | L     | 52  | ASN  |
| 3   | L     | 59  | ASN  |
| 4   | 0     | 40  | HIS  |
| 4   | 0     | 41  | GLN  |
| 4   | 0     | 78  | ASN  |
| 4   | 0     | 137 | GLN  |
| 4   | 0     | 252 | ASN  |
| 4   | 0     | 263 | GLN  |
| 4   | 0     | 354 | GLN  |
| 4   | 1     | 40  | HIS  |
| 4   | 1     | 41  | GLN  |
| 4   | 1     | 78  | ASN  |
| 4   | 1     | 137 | GLN  |
| 4   | 1     | 263 | GLN  |
| 4   | 1     | 354 | GLN  |
| 4   | 2     | 40  | HIS  |
| 4   | 2     | 41  | GLN  |
| 4   | 2     | 78  | ASN  |
| 4   | 2     | 137 | GLN  |
| 4   | 2     | 252 | ASN  |
| 4   | 2     | 263 | GLN  |
| 4   | 2     | 354 | GLN  |
| 4   | 2     | 360 | GLN  |
| 4   | 3     | 40  | HIS  |
| 4   | 3     | 41  | GLN  |
| 4   | 3     | 78  | ASN  |
| 4   | 3     | 137 | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 263 | GLN  |
| 4   | 3     | 354 | GLN  |
| 4   | 4     | 40  | HIS  |
| 4   | 4     | 41  | GLN  |
| 4   | 4     | 78  | ASN  |
| 4   | 4     | 111 | ASN  |
| 4   | 4     | 137 | GLN  |
| 4   | 4     | 252 | ASN  |
| 4   | 4     | 263 | GLN  |
| 4   | 4     | 354 | GLN  |
| 4   | 5     | 40  | HIS  |
| 4   | 5     | 41  | GLN  |
| 4   | 5     | 78  | ASN  |
| 4   | 5     | 111 | ASN  |
| 4   | 5     | 263 | GLN  |
| 4   | 5     | 354 | GLN  |
| 4   | 7     | 40  | HIS  |
| 4   | 7     | 41  | GLN  |
| 4   | 7     | 78  | ASN  |
| 4   | 7     | 137 | GLN  |
| 4   | 7     | 252 | ASN  |
| 4   | 7     | 263 | GLN  |
| 4   | 7     | 354 | GLN  |
| 4   | 8     | 40  | HIS  |
| 4   | 8     | 41  | GLN  |
| 4   | 8     | 78  | ASN  |
| 4   | 8     | 137 | GLN  |
| 4   | 8     | 252 | ASN  |
| 4   | 8     | 263 | GLN  |
| 4   | 8     | 360 | GLN  |
| 4   | 9     | 40  | HIS  |
| 4   | 9     | 41  | GLN  |
| 4   | 9     | 78  | ASN  |
| 4   | 9     | 252 | ASN  |
| 4   | 9     | 263 | GLN  |
| 4   | 9     | 360 | GLN  |
| 4   | V     | 40  | HIS  |
| 4   | V     | 41  | GLN  |
| 4   | V     | 78  | ASN  |
| 4   | V     | 137 | GLN  |
| 4   | V     | 252 | ASN  |
| 4   | V     | 263 | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | W     | 40  | HIS  |
| 4   | W     | 41  | GLN  |
| 4   | W     | 78  | ASN  |
| 4   | W     | 137 | GLN  |
| 4   | W     | 252 | ASN  |
| 4   | W     | 263 | GLN  |
| 4   | X     | 40  | HIS  |
| 4   | X     | 41  | GLN  |
| 4   | X     | 78  | ASN  |
| 4   | X     | 92  | ASN  |
| 4   | X     | 137 | GLN  |
| 4   | X     | 252 | ASN  |
| 4   | X     | 263 | GLN  |
| 4   | X     | 354 | GLN  |
| 4   | Y     | 40  | HIS  |
| 4   | Y     | 41  | GLN  |
| 4   | Y     | 78  | ASN  |
| 4   | Y     | 92  | ASN  |
| 4   | Y     | 137 | GLN  |
| 4   | Y     | 252 | ASN  |
| 4   | Y     | 263 | GLN  |
| 4   | Y     | 354 | GLN  |
| 4   | Y     | 360 | GLN  |
| 4   | Z     | 40  | HIS  |
| 4   | Z     | 41  | GLN  |
| 4   | Z     | 78  | ASN  |
| 4   | Z     | 137 | GLN  |
| 4   | Z     | 252 | ASN  |
| 4   | Z     | 263 | GLN  |
| 4   | Z     | 354 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

180 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | D     | 19  | 1    | 9,10,11      | 1.09 | 1 (11%)  | 6,11,13     | 0.58 | 0        |
| 1   | MLY  | D     | 59  | 1    | 9,10,11      | 0.85 | 0        | 6,11,13     | 0.47 | 0        |
| 1   | MLY  | D     | 296 | 1    | 9,10,11      | 0.63 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | J     | 839 | 1    | 9,10,11      | 0.65 | 0        | 6,11,13     | 0.77 | 0        |
| 1   | MLY  | D     | 84  | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.81 | 0        |
| 1   | MLY  | G     | 248 | 1    | 9,10,11      | 0.80 | 0        | 6,11,13     | 0.66 | 0        |
| 1   | MLY  | G     | 19  | 1    | 9,10,11      | 1.04 | 1 (11%)  | 6,11,13     | 0.58 | 0        |
| 1   | MLY  | G     | 272 | 1    | 9,10,11      | 0.87 | 1 (11%)  | 6,11,13     | 0.53 | 0        |
| 1   | MLY  | A     | 659 | 1    | 9,10,11      | 0.85 | 1 (11%)  | 6,11,13     | 0.60 | 0        |
| 1   | MLY  | D     | 190 | 1    | 9,10,11      | 1.17 | 2 (22%)  | 6,11,13     | 0.54 | 0        |
| 1   | MLY  | J     | 35  | 1    | 9,10,11      | 0.73 | 0        | 6,11,13     | 0.38 | 0        |
| 1   | MLY  | J     | 84  | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.81 | 0        |
| 1   | MLY  | G     | 436 | 1    | 9,10,11      | 0.95 | 1 (11%)  | 6,11,13     | 0.47 | 0        |
| 1   | MLY  | D     | 764 | 1    | 9,10,11      | 0.83 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | A     | 295 | 1    | 9,10,11      | 0.80 | 0        | 6,11,13     | 0.34 | 0        |
| 1   | MLY  | A     | 55  | 1    | 9,10,11      | 0.72 | 0        | 6,11,13     | 0.80 | 0        |
| 1   | MLY  | G     | 827 | 1    | 9,10,11      | 0.68 | 0        | 6,11,13     | 0.49 | 0        |
| 1   | MLY  | J     | 827 | 1    | 9,10,11      | 0.71 | 0        | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | D     | 130 | 1    | 9,10,11      | 0.80 | 0        | 6,11,13     | 0.72 | 0        |
| 1   | MLY  | A     | 87  | 1    | 9,10,11      | 1.11 | 1 (11%)  | 6,11,13     | 0.41 | 0        |
| 1   | MLY  | A     | 768 | 1    | 9,10,11      | 0.76 | 0        | 6,11,13     | 0.41 | 0        |
| 1   | MLY  | J     | 528 | 1    | 9,10,11      | 0.88 | 0        | 6,11,13     | 0.66 | 0        |
| 1   | MLY  | A     | 504 | 1    | 9,10,11      | 0.88 | 0        | 6,11,13     | 0.24 | 0        |
| 1   | MLY  | J     | 782 | 1    | 9,10,11      | 0.81 | 0        | 6,11,13     | 0.36 | 0        |
| 1   | MLY  | A     | 833 | 1    | 9,10,11      | 1.13 | 1 (11%)  | 6,11,13     | 0.32 | 0        |
| 1   | MLY  | A     | 598 | 1    | 9,10,11      | 0.83 | 0        | 6,11,13     | 0.42 | 0        |
| 1   | MLY  | J     | 369 | 1    | 9,10,11      | 0.71 | 0        | 6,11,13     | 0.45 | 0        |
| 1   | MLY  | D     | 681 | 1    | 9,10,11      | 0.56 | 0        | 6,11,13     | 0.46 | 0        |
| 1   | MLY  | J     | 415 | 1    | 9,10,11      | 0.75 | 0        | 6,11,13     | 0.19 | 0        |
| 1   | MLY  | G     | 659 | 1    | 9,10,11      | 0.84 | 1 (11%)  | 6,11,13     | 0.59 | 0        |
| 1   | MLY  | G     | 681 | 1    | 9,10,11      | 0.58 | 0        | 6,11,13     | 0.45 | 0        |
| 1   | MLY  | D     | 385 | 1    | 9,10,11      | 0.91 | 1 (11%)  | 6,11,13     | 0.44 | 0        |
| 1   | MLY  | G     | 613 | 1    | 9,10,11      | 0.59 | 0        | 6,11,13     | 0.62 | 0        |
| 1   | MLY  | D     | 486 | 1    | 9,10,11      | 0.67 | 0        | 6,11,13     | 0.41 | 0        |
| 1   | MLY  | J     | 486 | 1    | 9,10,11      | 0.66 | 0        | 6,11,13     | 0.39 | 0        |
| 1   | MLY  | D     | 504 | 1    | 9,10,11      | 0.87 | 0        | 6,11,13     | 0.20 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | G     | 87  | 1    | 9,10,11      | 1.16 | 1 (11%)  | 6,11,13     | 0.43 | 0        |
| 1   | MLY  | G     | 59  | 1    | 9,10,11      | 0.83 | 0        | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | G     | 768 | 1    | 9,10,11      | 0.75 | 0        | 6,11,13     | 0.42 | 0        |
| 1   | MLY  | J     | 837 | 1    | 9,10,11      | 0.59 | 0        | 6,11,13     | 0.55 | 0        |
| 1   | MLY  | A     | 837 | 1    | 9,10,11      | 0.59 | 0        | 6,11,13     | 0.54 | 0        |
| 1   | MLY  | D     | 553 | 1,4  | 9,10,11      | 0.64 | 0        | 6,11,13     | 0.55 | 0        |
| 1   | MLY  | A     | 551 | 1    | 9,10,11      | 0.51 | 0        | 6,11,13     | 0.18 | 0        |
| 1   | MLY  | A     | 782 | 1    | 9,10,11      | 0.81 | 0        | 6,11,13     | 0.37 | 0        |
| 1   | MLY  | D     | 436 | 1    | 9,10,11      | 1.00 | 1 (11%)  | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | J     | 138 | 1    | 9,10,11      | 1.22 | 1 (11%)  | 6,11,13     | 0.82 | 0        |
| 1   | MLY  | G     | 348 | 1    | 9,10,11      | 0.80 | 0        | 6,11,13     | 0.47 | 0        |
| 1   | MLY  | G     | 367 | 1    | 9,10,11      | 0.60 | 0        | 6,11,13     | 0.39 | 0        |
| 1   | MLY  | D     | 63  | 1    | 9,10,11      | 0.87 | 0        | 6,11,13     | 0.46 | 0        |
| 1   | MLY  | A     | 49  | 1    | 9,10,11      | 0.94 | 1 (11%)  | 6,11,13     | 0.74 | 0        |
| 1   | MLY  | G     | 55  | 1    | 9,10,11      | 0.74 | 0        | 6,11,13     | 0.81 | 0        |
| 1   | MLY  | G     | 600 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.38 | 0        |
| 1   | MLY  | G     | 617 | 1    | 9,10,11      | 0.92 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | D     | 107 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.32 | 0        |
| 1   | MLY  | D     | 837 | 1    | 9,10,11      | 0.59 | 0        | 6,11,13     | 0.58 | 0        |
| 1   | MLY  | A     | 30  | 1    | 9,10,11      | 0.90 | 0        | 6,11,13     | 0.31 | 0        |
| 1   | MLY  | J     | 19  | 1    | 9,10,11      | 1.07 | 1 (11%)  | 6,11,13     | 0.58 | 0        |
| 1   | MLY  | D     | 551 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.19 | 0        |
| 1   | MLY  | A     | 486 | 1    | 9,10,11      | 0.68 | 0        | 6,11,13     | 0.39 | 0        |
| 1   | MLY  | G     | 833 | 1    | 9,10,11      | 1.16 | 2 (22%)  | 6,11,13     | 0.31 | 0        |
| 1   | MLY  | J     | 505 | 1    | 9,10,11      | 0.85 | 1 (11%)  | 6,11,13     | 0.34 | 0        |
| 1   | MLY  | G     | 296 | 1    | 9,10,11      | 0.62 | 0        | 6,11,13     | 0.37 | 0        |
| 1   | MLY  | D     | 236 | 1    | 9,10,11      | 0.84 | 1 (11%)  | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | J     | 598 | 1    | 9,10,11      | 0.83 | 1 (11%)  | 6,11,13     | 0.42 | 0        |
| 1   | MLY  | G     | 764 | 1    | 9,10,11      | 0.80 | 0        | 6,11,13     | 0.36 | 0        |
| 1   | MLY  | G     | 598 | 1    | 9,10,11      | 0.83 | 1 (11%)  | 6,11,13     | 0.41 | 0        |
| 1   | MLY  | D     | 55  | 1    | 9,10,11      | 0.72 | 0        | 6,11,13     | 0.81 | 0        |
| 1   | MLY  | D     | 353 | 1    | 9,10,11      | 0.85 | 0        | 6,11,13     | 0.81 | 0        |
| 1   | MLY  | D     | 87  | 1    | 9,10,11      | 1.10 | 1 (11%)  | 6,11,13     | 0.44 | 0        |
| 1   | MLY  | D     | 49  | 1    | 9,10,11      | 1.00 | 1 (11%)  | 6,11,13     | 0.74 | 0        |
| 1   | MLY  | D     | 833 | 1    | 9,10,11      | 1.11 | 1 (11%)  | 6,11,13     | 0.31 | 0        |
| 1   | MLY  | A     | 617 | 1    | 9,10,11      | 0.88 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | G     | 505 | 1    | 9,10,11      | 0.83 | 1 (11%)  | 6,11,13     | 0.34 | 0        |
| 1   | MLY  | J     | 59  | 1    | 9,10,11      | 0.84 | 0        | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | G     | 35  | 1    | 9,10,11      | 0.73 | 0        | 6,11,13     | 0.39 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | A     | 436 | 1    | 9,10,11      | 0.96 | 1 (11%)  | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | A     | 505 | 1    | 9,10,11      | 0.84 | 1 (11%)  | 6,11,13     | 0.32 | 0        |
| 1   | MLY  | J     | 613 | 1    | 9,10,11      | 0.55 | 0        | 6,11,13     | 0.62 | 0        |
| 1   | MLY  | G     | 353 | 1    | 9,10,11      | 0.85 | 0        | 6,11,13     | 0.81 | 0        |
| 1   | MLY  | D     | 348 | 1    | 9,10,11      | 0.77 | 0        | 6,11,13     | 0.47 | 0        |
| 1   | MLY  | J     | 348 | 1    | 9,10,11      | 0.78 | 0        | 6,11,13     | 0.47 | 0        |
| 1   | MLY  | D     | 367 | 1    | 9,10,11      | 0.59 | 0        | 6,11,13     | 0.38 | 0        |
| 1   | MLY  | D     | 35  | 1    | 9,10,11      | 0.73 | 0        | 6,11,13     | 0.37 | 0        |
| 1   | MLY  | J     | 768 | 1    | 9,10,11      | 0.75 | 0        | 6,11,13     | 0.42 | 0        |
| 1   | MLY  | A     | 138 | 1    | 9,10,11      | 1.23 | 1 (11%)  | 6,11,13     | 0.82 | 0        |
| 1   | MLY  | J     | 764 | 1    | 9,10,11      | 0.81 | 0        | 6,11,13     | 0.37 | 0        |
| 1   | MLY  | G     | 553 | 1,4  | 9,10,11      | 0.64 | 0        | 6,11,13     | 0.55 | 0        |
| 1   | MLY  | D     | 617 | 1    | 9,10,11      | 0.91 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | D     | 248 | 1    | 9,10,11      | 0.81 | 0        | 6,11,13     | 0.65 | 0        |
| 1   | MLY  | J     | 248 | 1    | 9,10,11      | 0.81 | 0        | 6,11,13     | 0.65 | 0        |
| 1   | MLY  | A     | 528 | 1    | 9,10,11      | 0.89 | 0        | 6,11,13     | 0.67 | 0        |
| 1   | MLY  | G     | 295 | 1    | 9,10,11      | 0.77 | 0        | 6,11,13     | 0.36 | 0        |
| 1   | MLY  | J     | 272 | 1    | 9,10,11      | 0.92 | 1 (11%)  | 6,11,13     | 0.56 | 0        |
| 1   | MLY  | D     | 782 | 1    | 9,10,11      | 0.80 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | A     | 839 | 1,2  | 9,10,11      | 0.66 | 0        | 6,11,13     | 0.82 | 0        |
| 1   | MLY  | G     | 236 | 1    | 9,10,11      | 0.82 | 1 (11%)  | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | J     | 236 | 1    | 9,10,11      | 0.83 | 1 (11%)  | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | G     | 84  | 1    | 9,10,11      | 0.50 | 0        | 6,11,13     | 0.81 | 0        |
| 1   | MLY  | J     | 681 | 1    | 9,10,11      | 0.57 | 0        | 6,11,13     | 0.46 | 0        |
| 1   | MLY  | J     | 130 | 1    | 9,10,11      | 0.76 | 0        | 6,11,13     | 0.74 | 0        |
| 1   | MLY  | G     | 190 | 1    | 9,10,11      | 1.21 | 2 (22%)  | 6,11,13     | 0.52 | 0        |
| 1   | MLY  | G     | 837 | 1    | 9,10,11      | 0.60 | 0        | 6,11,13     | 0.53 | 0        |
| 1   | MLY  | G     | 385 | 1    | 9,10,11      | 0.92 | 1 (11%)  | 6,11,13     | 0.45 | 0        |
| 1   | MLY  | A     | 348 | 1    | 9,10,11      | 0.79 | 0        | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | J     | 190 | 1    | 9,10,11      | 1.22 | 2 (22%)  | 6,11,13     | 0.52 | 0        |
| 1   | MLY  | A     | 63  | 1    | 9,10,11      | 0.88 | 0        | 6,11,13     | 0.43 | 0        |
| 1   | MLY  | D     | 30  | 1    | 9,10,11      | 0.92 | 0        | 6,11,13     | 0.31 | 0        |
| 1   | MLY  | J     | 49  | 1    | 9,10,11      | 0.99 | 1 (11%)  | 6,11,13     | 0.75 | 0        |
| 1   | MLY  | D     | 839 | 1    | 9,10,11      | 0.66 | 0        | 6,11,13     | 0.79 | 0        |
| 1   | MLY  | J     | 504 | 1    | 9,10,11      | 0.83 | 0        | 6,11,13     | 0.22 | 0        |
| 1   | MLY  | G     | 839 | 1    | 9,10,11      | 0.66 | 0        | 6,11,13     | 0.79 | 0        |
| 1   | MLY  | J     | 385 | 1    | 9,10,11      | 0.95 | 1 (11%)  | 6,11,13     | 0.45 | 0        |
| 1   | MLY  | J     | 659 | 1    | 9,10,11      | 0.82 | 1 (11%)  | 6,11,13     | 0.58 | 0        |
| 1   | MLY  | A     | 272 | 1    | 9,10,11      | 0.92 | 1 (11%)  | 6,11,13     | 0.56 | 0        |
| 1   | MLY  | D     | 431 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.46 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | D     | 505 | 1    | 9,10,11      | 0.80 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | D     | 528 | 1    | 9,10,11      | 0.92 | 0        | 6,11,13     | 0.65 | 0        |
| 1   | MLY  | G     | 30  | 1    | 9,10,11      | 0.90 | 0        | 6,11,13     | 0.30 | 0        |
| 1   | MLY  | A     | 613 | 1    | 9,10,11      | 0.56 | 0        | 6,11,13     | 0.61 | 0        |
| 1   | MLY  | A     | 415 | 1    | 9,10,11      | 0.74 | 0        | 6,11,13     | 0.20 | 0        |
| 1   | MLY  | J     | 295 | 1    | 9,10,11      | 0.76 | 0        | 6,11,13     | 0.37 | 0        |
| 1   | MLY  | A     | 130 | 1    | 9,10,11      | 0.79 | 0        | 6,11,13     | 0.73 | 0        |
| 1   | MLY  | A     | 431 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.44 | 0        |
| 1   | MLY  | A     | 107 | 1    | 9,10,11      | 0.47 | 0        | 6,11,13     | 0.32 | 0        |
| 1   | MLY  | G     | 504 | 1    | 9,10,11      | 0.88 | 0        | 6,11,13     | 0.22 | 0        |
| 1   | MLY  | G     | 551 | 1    | 9,10,11      | 0.51 | 0        | 6,11,13     | 0.19 | 0        |
| 1   | MLY  | J     | 833 | 1    | 9,10,11      | 1.15 | 2 (22%)  | 6,11,13     | 0.30 | 0        |
| 1   | MLY  | D     | 369 | 1    | 9,10,11      | 0.71 | 0        | 6,11,13     | 0.45 | 0        |
| 1   | MLY  | J     | 353 | 1    | 9,10,11      | 0.87 | 0        | 6,11,13     | 0.79 | 0        |
| 1   | MLY  | D     | 613 | 1    | 9,10,11      | 0.57 | 0        | 6,11,13     | 0.62 | 0        |
| 1   | MLY  | D     | 415 | 1    | 9,10,11      | 0.76 | 0        | 6,11,13     | 0.20 | 0        |
| 1   | MLY  | G     | 49  | 1    | 9,10,11      | 1.01 | 1 (11%)  | 6,11,13     | 0.74 | 0        |
| 1   | MLY  | J     | 553 | 1    | 9,10,11      | 0.64 | 0        | 6,11,13     | 0.53 | 0        |
| 1   | MLY  | J     | 107 | 1    | 9,10,11      | 0.48 | 0        | 6,11,13     | 0.33 | 0        |
| 1   | MLY  | A     | 190 | 1    | 9,10,11      | 1.25 | 2 (22%)  | 6,11,13     | 0.52 | 0        |
| 1   | MLY  | J     | 600 | 1    | 9,10,11      | 0.54 | 0        | 6,11,13     | 0.38 | 0        |
| 1   | MLY  | A     | 553 | 1,4  | 9,10,11      | 0.65 | 0        | 6,11,13     | 0.55 | 0        |
| 1   | MLY  | A     | 827 | 1    | 9,10,11      | 0.70 | 0        | 6,11,13     | 0.44 | 0        |
| 1   | MLY  | G     | 138 | 1    | 9,10,11      | 1.21 | 1 (11%)  | 6,11,13     | 0.82 | 0        |
| 1   | MLY  | A     | 35  | 1    | 9,10,11      | 0.74 | 0        | 6,11,13     | 0.38 | 0        |
| 1   | MLY  | D     | 138 | 1    | 9,10,11      | 1.26 | 1 (11%)  | 6,11,13     | 0.84 | 0        |
| 1   | MLY  | G     | 431 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.47 | 0        |
| 1   | MLY  | J     | 30  | 1    | 9,10,11      | 0.91 | 0        | 6,11,13     | 0.31 | 0        |
| 1   | MLY  | J     | 367 | 1    | 9,10,11      | 0.58 | 0        | 6,11,13     | 0.37 | 0        |
| 1   | MLY  | D     | 598 | 1    | 9,10,11      | 0.86 | 1 (11%)  | 6,11,13     | 0.42 | 0        |
| 1   | MLY  | G     | 415 | 1    | 9,10,11      | 0.74 | 0        | 6,11,13     | 0.19 | 0        |
| 1   | MLY  | J     | 296 | 1    | 9,10,11      | 0.67 | 0        | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | G     | 107 | 1    | 9,10,11      | 0.49 | 0        | 6,11,13     | 0.32 | 0        |
| 1   | MLY  | A     | 248 | 1    | 9,10,11      | 0.81 | 0        | 6,11,13     | 0.64 | 0        |
| 1   | MLY  | J     | 551 | 1    | 9,10,11      | 0.51 | 0        | 6,11,13     | 0.18 | 0        |
| 1   | MLY  | D     | 272 | 1    | 9,10,11      | 0.89 | 1 (11%)  | 6,11,13     | 0.58 | 0        |
| 1   | MLY  | A     | 385 | 1    | 9,10,11      | 0.93 | 1 (11%)  | 6,11,13     | 0.44 | 0        |
| 1   | MLY  | G     | 782 | 1    | 9,10,11      | 0.82 | 1 (11%)  | 6,11,13     | 0.35 | 0        |
| 1   | MLY  | G     | 528 | 1    | 9,10,11      | 0.91 | 0        | 6,11,13     | 0.66 | 0        |
| 1   | MLY  | A     | 353 | 1    | 9,10,11      | 0.87 | 0        | 6,11,13     | 0.79 | 0        |
| 1   | MLY  | D     | 295 | 1    | 9,10,11      | 0.76 | 0        | 6,11,13     | 0.37 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | A     | 600 | 1    | 9,10,11      | 0.53 | 0        | 6,11,13     | 0.39 | 0        |
| 1   | MLY  | G     | 130 | 1    | 9,10,11      | 0.78 | 0        | 6,11,13     | 0.74 | 0        |
| 1   | MLY  | D     | 827 | 1    | 9,10,11      | 0.66 | 0        | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | J     | 55  | 1    | 9,10,11      | 0.73 | 0        | 6,11,13     | 0.80 | 0        |
| 1   | MLY  | G     | 63  | 1    | 9,10,11      | 0.86 | 0        | 6,11,13     | 0.44 | 0        |
| 1   | MLY  | G     | 369 | 1    | 9,10,11      | 0.71 | 0        | 6,11,13     | 0.47 | 0        |
| 1   | MLY  | J     | 63  | 1    | 9,10,11      | 0.88 | 0        | 6,11,13     | 0.44 | 0        |
| 1   | MLY  | A     | 367 | 1    | 9,10,11      | 0.59 | 0        | 6,11,13     | 0.37 | 0        |
| 1   | MLY  | J     | 436 | 1    | 9,10,11      | 0.98 | 1 (11%)  | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | A     | 369 | 1    | 9,10,11      | 0.72 | 0        | 6,11,13     | 0.46 | 0        |
| 1   | MLY  | A     | 236 | 1    | 9,10,11      | 0.83 | 1 (11%)  | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | A     | 19  | 1    | 9,10,11      | 1.03 | 1 (11%)  | 6,11,13     | 0.57 | 0        |
| 1   | MLY  | A     | 59  | 1    | 9,10,11      | 0.85 | 0        | 6,11,13     | 0.48 | 0        |
| 1   | MLY  | A     | 296 | 1    | 9,10,11      | 0.60 | 0        | 6,11,13     | 0.34 | 0        |
| 1   | MLY  | J     | 431 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.45 | 0        |
| 1   | MLY  | D     | 768 | 1    | 9,10,11      | 0.73 | 0        | 6,11,13     | 0.41 | 0        |
| 1   | MLY  | A     | 84  | 1    | 9,10,11      | 0.50 | 0        | 6,11,13     | 0.80 | 0        |
| 1   | MLY  | D     | 659 | 1    | 9,10,11      | 0.85 | 1 (11%)  | 6,11,13     | 0.59 | 0        |
| 1   | MLY  | D     | 600 | 1    | 9,10,11      | 0.52 | 0        | 6,11,13     | 0.39 | 0        |
| 1   | MLY  | A     | 681 | 1    | 9,10,11      | 0.57 | 0        | 6,11,13     | 0.46 | 0        |
| 1   | MLY  | J     | 617 | 1    | 9,10,11      | 0.91 | 1 (11%)  | 6,11,13     | 0.34 | 0        |
| 1   | MLY  | G     | 486 | 1    | 9,10,11      | 0.67 | 0        | 6,11,13     | 0.40 | 0        |
| 1   | MLY  | J     | 87  | 1    | 9,10,11      | 1.12 | 1 (11%)  | 6,11,13     | 0.43 | 0        |
| 1   | MLY  | A     | 764 | 1    | 9,10,11      | 0.82 | 0        | 6,11,13     | 0.36 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | MLY  | D     | 19  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 59  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 296 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 839 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 84  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 248 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | G     | 19  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 272 | 1    | -       | 3/8/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | MLY  | A     | 659 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 190 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 35  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 84  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 436 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 764 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 295 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 55  | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | G     | 827 | 1    | -       | 1/8/9/11 | -     |
| 1   | MLY  | J     | 827 | 1    | -       | 1/8/9/11 | -     |
| 1   | MLY  | D     | 130 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | A     | 87  | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 768 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 528 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 504 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 782 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | A     | 833 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | A     | 598 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | J     | 369 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 681 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 415 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 659 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 681 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 385 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 613 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 486 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | J     | 486 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 504 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 87  | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 59  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 768 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 837 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | A     | 837 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | D     | 553 | 1,4  | -       | 5/8/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | MLY  | A     | 551 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 782 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | D     | 436 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 138 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 348 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | G     | 367 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 63  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 49  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 55  | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | G     | 600 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 617 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 107 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 837 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | A     | 30  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 19  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 551 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 486 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 833 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | J     | 505 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | G     | 296 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 236 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 598 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | G     | 764 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 598 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | D     | 55  | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | D     | 353 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 87  | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 49  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 833 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | A     | 617 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 505 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | J     | 59  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 35  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 436 | 1    | -       | 4/8/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | MLY  | A     | 505 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | J     | 613 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 353 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 348 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | J     | 348 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | D     | 367 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 35  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 768 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 138 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 764 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 553 | 1,4  | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 617 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | D     | 248 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | J     | 248 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | A     | 528 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 295 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | J     | 272 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 782 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | A     | 839 | 1,2  | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 236 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 236 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 84  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 681 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 130 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | G     | 190 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 837 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | G     | 385 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 348 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | J     | 190 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 63  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 30  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 49  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 839 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 504 | 1    | -       | 4/8/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | MLY  | G     | 839 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 385 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | J     | 659 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 272 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 431 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 505 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | D     | 528 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 30  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 613 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 415 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 295 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 130 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | A     | 431 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 107 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 504 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 551 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 833 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | D     | 369 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | J     | 353 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 613 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 415 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 49  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 553 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 107 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 190 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 600 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 553 | 1,4  | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 827 | 1    | -       | 1/8/9/11 | -     |
| 1   | MLY  | G     | 138 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 35  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 138 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 431 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 30  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 367 | 1    | -       | 2/8/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | MLY  | D     | 598 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | G     | 415 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | J     | 296 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 107 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 248 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | J     | 551 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 272 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 385 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 782 | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | G     | 528 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 353 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 295 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 600 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | G     | 130 | 1    | -       | 5/8/9/11 | -     |
| 1   | MLY  | D     | 827 | 1    | -       | 1/8/9/11 | -     |
| 1   | MLY  | J     | 55  | 1    | -       | 6/8/9/11 | -     |
| 1   | MLY  | G     | 63  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | G     | 369 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | J     | 63  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 367 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | J     | 436 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 369 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 236 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 19  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 59  | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 296 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 431 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 768 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | A     | 84  | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | D     | 659 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | D     | 600 | 1    | -       | 3/8/9/11 | -     |
| 1   | MLY  | A     | 681 | 1    | -       | 4/8/9/11 | -     |
| 1   | MLY  | J     | 617 | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | G     | 486 | 1    | -       | 2/8/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | MLY  | J     | 87  | 1    | -       | 2/8/9/11 | -     |
| 1   | MLY  | A     | 764 | 1    | -       | 2/8/9/11 | -     |

All (58) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 138 | MLY  | CB-CA | -3.37 | 1.48        | 1.53     |
| 1   | A     | 138 | MLY  | CB-CA | -3.23 | 1.48        | 1.53     |
| 1   | J     | 138 | MLY  | CB-CA | -3.21 | 1.48        | 1.53     |
| 1   | G     | 138 | MLY  | CB-CA | -3.20 | 1.48        | 1.53     |
| 1   | G     | 87  | MLY  | CB-CA | -2.92 | 1.49        | 1.53     |
| 1   | D     | 19  | MLY  | CB-CA | -2.89 | 1.49        | 1.53     |
| 1   | J     | 19  | MLY  | CB-CA | -2.80 | 1.49        | 1.53     |
| 1   | J     | 87  | MLY  | CB-CA | -2.74 | 1.49        | 1.53     |
| 1   | A     | 87  | MLY  | CB-CA | -2.72 | 1.49        | 1.53     |
| 1   | D     | 87  | MLY  | CB-CA | -2.72 | 1.49        | 1.53     |
| 1   | D     | 436 | MLY  | CB-CA | -2.71 | 1.49        | 1.53     |
| 1   | G     | 19  | MLY  | CB-CA | -2.68 | 1.49        | 1.53     |
| 1   | A     | 19  | MLY  | CB-CA | -2.68 | 1.49        | 1.53     |
| 1   | J     | 436 | MLY  | CB-CA | -2.64 | 1.49        | 1.53     |
| 1   | G     | 436 | MLY  | CB-CA | -2.56 | 1.49        | 1.53     |
| 1   | A     | 436 | MLY  | CB-CA | -2.54 | 1.49        | 1.53     |
| 1   | G     | 49  | MLY  | CB-CA | -2.52 | 1.49        | 1.53     |
| 1   | J     | 49  | MLY  | CB-CA | -2.51 | 1.49        | 1.53     |
| 1   | A     | 272 | MLY  | CB-CA | -2.49 | 1.49        | 1.53     |
| 1   | J     | 272 | MLY  | CB-CA | -2.49 | 1.49        | 1.53     |
| 1   | D     | 49  | MLY  | CB-CA | -2.48 | 1.49        | 1.53     |
| 1   | D     | 272 | MLY  | CB-CA | -2.36 | 1.50        | 1.53     |
| 1   | A     | 190 | MLY  | CB-CA | -2.35 | 1.50        | 1.53     |
| 1   | G     | 272 | MLY  | CB-CA | -2.34 | 1.50        | 1.53     |
| 1   | A     | 49  | MLY  | CB-CA | -2.31 | 1.50        | 1.53     |
| 1   | J     | 190 | MLY  | CB-CA | -2.30 | 1.50        | 1.53     |
| 1   | D     | 236 | MLY  | CA-N  | -2.29 | 1.41        | 1.48     |
| 1   | A     | 236 | MLY  | CA-N  | -2.28 | 1.41        | 1.48     |
| 1   | J     | 236 | MLY  | CA-N  | -2.28 | 1.41        | 1.48     |
| 1   | G     | 190 | MLY  | CB-CA | -2.27 | 1.50        | 1.53     |
| 1   | J     | 385 | MLY  | CB-CA | -2.27 | 1.50        | 1.53     |
| 1   | G     | 236 | MLY  | CA-N  | -2.23 | 1.41        | 1.48     |
| 1   | G     | 833 | MLY  | CA-N  | -2.23 | 1.41        | 1.48     |
| 1   | J     | 833 | MLY  | CB-CA | -2.22 | 1.50        | 1.53     |
| 1   | A     | 385 | MLY  | CB-CA | -2.17 | 1.50        | 1.53     |
| 1   | A     | 190 | MLY  | CA-N  | -2.14 | 1.42        | 1.48     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 385 | MLY  | CB-CA | -2.13 | 1.50        | 1.53     |
| 1   | D     | 190 | MLY  | CB-CA | -2.12 | 1.50        | 1.53     |
| 1   | D     | 833 | MLY  | CA-N  | -2.11 | 1.42        | 1.48     |
| 1   | D     | 190 | MLY  | CA-N  | -2.10 | 1.42        | 1.48     |
| 1   | A     | 833 | MLY  | CA-N  | -2.09 | 1.42        | 1.48     |
| 1   | D     | 385 | MLY  | CB-CA | -2.09 | 1.50        | 1.53     |
| 1   | J     | 190 | MLY  | CA-N  | -2.09 | 1.42        | 1.48     |
| 1   | G     | 659 | MLY  | CA-N  | -2.08 | 1.42        | 1.48     |
| 1   | A     | 659 | MLY  | CA-N  | -2.07 | 1.42        | 1.48     |
| 1   | G     | 190 | MLY  | CA-N  | -2.06 | 1.42        | 1.48     |
| 1   | D     | 659 | MLY  | CA-N  | -2.06 | 1.42        | 1.48     |
| 1   | G     | 505 | MLY  | CB-CA | -2.03 | 1.50        | 1.53     |
| 1   | A     | 505 | MLY  | CB-CA | -2.03 | 1.50        | 1.53     |
| 1   | G     | 782 | MLY  | CA-N  | -2.02 | 1.42        | 1.48     |
| 1   | G     | 833 | MLY  | CB-CA | -2.02 | 1.50        | 1.53     |
| 1   | J     | 659 | MLY  | CA-N  | -2.02 | 1.42        | 1.48     |
| 1   | J     | 598 | MLY  | CB-CA | -2.01 | 1.50        | 1.53     |
| 1   | D     | 598 | MLY  | CB-CA | -2.01 | 1.50        | 1.53     |
| 1   | J     | 505 | MLY  | CB-CA | -2.01 | 1.50        | 1.53     |
| 1   | J     | 833 | MLY  | CA-N  | -2.01 | 1.42        | 1.48     |
| 1   | J     | 617 | MLY  | CB-CA | -2.01 | 1.50        | 1.53     |
| 1   | G     | 598 | MLY  | CB-CA | -2.00 | 1.50        | 1.53     |

There are no bond angle outliers.

There are no chirality outliers.

All (645) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 1   | A     | 19  | MLY  | C-CA-CB-CG |
| 1   | A     | 49  | MLY  | N-CA-CB-CG |
| 1   | A     | 49  | MLY  | C-CA-CB-CG |
| 1   | A     | 55  | MLY  | N-CA-CB-CG |
| 1   | A     | 55  | MLY  | C-CA-CB-CG |
| 1   | A     | 84  | MLY  | C-CA-CB-CG |
| 1   | A     | 130 | MLY  | C-CA-CB-CG |
| 1   | A     | 248 | MLY  | N-CA-CB-CG |
| 1   | A     | 248 | MLY  | C-CA-CB-CG |
| 1   | A     | 348 | MLY  | C-CA-CB-CG |
| 1   | A     | 436 | MLY  | C-CA-CB-CG |
| 1   | A     | 486 | MLY  | C-CA-CB-CG |
| 1   | A     | 505 | MLY  | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 1   | A     | 505 | MLY  | C-CA-CB-CG |
| 1   | A     | 528 | MLY  | C-CA-CB-CG |
| 1   | A     | 551 | MLY  | C-CA-CB-CG |
| 1   | A     | 553 | MLY  | C-CA-CB-CG |
| 1   | A     | 598 | MLY  | N-CA-CB-CG |
| 1   | A     | 598 | MLY  | C-CA-CB-CG |
| 1   | A     | 613 | MLY  | N-CA-CB-CG |
| 1   | A     | 613 | MLY  | C-CA-CB-CG |
| 1   | A     | 681 | MLY  | C-CA-CB-CG |
| 1   | A     | 782 | MLY  | C-CA-CB-CG |
| 1   | A     | 782 | MLY  | O-C-CA-CB  |
| 1   | D     | 19  | MLY  | C-CA-CB-CG |
| 1   | D     | 49  | MLY  | N-CA-CB-CG |
| 1   | D     | 49  | MLY  | C-CA-CB-CG |
| 1   | D     | 55  | MLY  | N-CA-CB-CG |
| 1   | D     | 55  | MLY  | C-CA-CB-CG |
| 1   | D     | 84  | MLY  | C-CA-CB-CG |
| 1   | D     | 130 | MLY  | C-CA-CB-CG |
| 1   | D     | 248 | MLY  | N-CA-CB-CG |
| 1   | D     | 248 | MLY  | C-CA-CB-CG |
| 1   | D     | 348 | MLY  | C-CA-CB-CG |
| 1   | D     | 436 | MLY  | C-CA-CB-CG |
| 1   | D     | 486 | MLY  | C-CA-CB-CG |
| 1   | D     | 505 | MLY  | N-CA-CB-CG |
| 1   | D     | 505 | MLY  | C-CA-CB-CG |
| 1   | D     | 528 | MLY  | C-CA-CB-CG |
| 1   | D     | 551 | MLY  | C-CA-CB-CG |
| 1   | D     | 553 | MLY  | C-CA-CB-CG |
| 1   | D     | 553 | MLY  | O-C-CA-CB  |
| 1   | D     | 598 | MLY  | N-CA-CB-CG |
| 1   | D     | 598 | MLY  | C-CA-CB-CG |
| 1   | D     | 613 | MLY  | N-CA-CB-CG |
| 1   | D     | 613 | MLY  | C-CA-CB-CG |
| 1   | D     | 681 | MLY  | C-CA-CB-CG |
| 1   | D     | 782 | MLY  | C-CA-CB-CG |
| 1   | D     | 782 | MLY  | O-C-CA-CB  |
| 1   | G     | 19  | MLY  | C-CA-CB-CG |
| 1   | G     | 49  | MLY  | N-CA-CB-CG |
| 1   | G     | 49  | MLY  | C-CA-CB-CG |
| 1   | G     | 55  | MLY  | N-CA-CB-CG |
| 1   | G     | 55  | MLY  | C-CA-CB-CG |
| 1   | G     | 84  | MLY  | C-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 1   | G     | 130 | MLY  | C-CA-CB-CG |
| 1   | G     | 248 | MLY  | N-CA-CB-CG |
| 1   | G     | 248 | MLY  | C-CA-CB-CG |
| 1   | G     | 348 | MLY  | C-CA-CB-CG |
| 1   | G     | 436 | MLY  | C-CA-CB-CG |
| 1   | G     | 486 | MLY  | C-CA-CB-CG |
| 1   | G     | 505 | MLY  | N-CA-CB-CG |
| 1   | G     | 505 | MLY  | C-CA-CB-CG |
| 1   | G     | 528 | MLY  | C-CA-CB-CG |
| 1   | G     | 551 | MLY  | C-CA-CB-CG |
| 1   | G     | 553 | MLY  | C-CA-CB-CG |
| 1   | G     | 598 | MLY  | N-CA-CB-CG |
| 1   | G     | 598 | MLY  | C-CA-CB-CG |
| 1   | G     | 613 | MLY  | N-CA-CB-CG |
| 1   | G     | 613 | MLY  | C-CA-CB-CG |
| 1   | G     | 681 | MLY  | C-CA-CB-CG |
| 1   | G     | 782 | MLY  | C-CA-CB-CG |
| 1   | G     | 782 | MLY  | O-C-CA-CB  |
| 1   | J     | 19  | MLY  | C-CA-CB-CG |
| 1   | J     | 49  | MLY  | N-CA-CB-CG |
| 1   | J     | 49  | MLY  | C-CA-CB-CG |
| 1   | J     | 55  | MLY  | N-CA-CB-CG |
| 1   | J     | 55  | MLY  | C-CA-CB-CG |
| 1   | J     | 84  | MLY  | C-CA-CB-CG |
| 1   | J     | 130 | MLY  | C-CA-CB-CG |
| 1   | J     | 248 | MLY  | N-CA-CB-CG |
| 1   | J     | 248 | MLY  | C-CA-CB-CG |
| 1   | J     | 348 | MLY  | N-CA-CB-CG |
| 1   | J     | 348 | MLY  | C-CA-CB-CG |
| 1   | J     | 436 | MLY  | C-CA-CB-CG |
| 1   | J     | 486 | MLY  | C-CA-CB-CG |
| 1   | J     | 505 | MLY  | N-CA-CB-CG |
| 1   | J     | 505 | MLY  | C-CA-CB-CG |
| 1   | J     | 528 | MLY  | C-CA-CB-CG |
| 1   | J     | 551 | MLY  | C-CA-CB-CG |
| 1   | J     | 553 | MLY  | C-CA-CB-CG |
| 1   | J     | 598 | MLY  | N-CA-CB-CG |
| 1   | J     | 598 | MLY  | C-CA-CB-CG |
| 1   | J     | 613 | MLY  | N-CA-CB-CG |
| 1   | J     | 613 | MLY  | C-CA-CB-CG |
| 1   | J     | 681 | MLY  | C-CA-CB-CG |
| 1   | J     | 782 | MLY  | C-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | J     | 782 | MLY  | O-C-CA-CB    |
| 1   | A     | 84  | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 190 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 248 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 296 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 296 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 367 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 431 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 600 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 764 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 764 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 782 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 833 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 833 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 837 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 55  | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 84  | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 248 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 296 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 296 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 367 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 431 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 600 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 764 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 764 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 782 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 833 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 833 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 837 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 84  | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 248 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 296 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 296 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 367 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 431 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 600 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 764 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 764 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 782 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 833 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 833 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 837 | MLY  | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | J     | 55  | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 84  | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 248 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 296 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 296 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 367 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 431 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 600 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 764 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 764 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 782 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 833 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 833 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 837 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 295 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 295 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 295 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 295 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 659 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 659 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 35  | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 35  | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 35  | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 659 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 35  | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 659 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 55  | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 59  | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 59  | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 63  | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 84  | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 130 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 130 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 138 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 138 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 190 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 248 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 272 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 348 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 348 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 353 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 353 | MLY  | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 367 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 385 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 385 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 431 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 505 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 505 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 528 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 528 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 553 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 600 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 659 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 768 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 782 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 837 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 839 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 59  | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 59  | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 63  | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 84  | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 130 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 130 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 138 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 138 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 190 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 190 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 248 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 272 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 348 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 348 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 353 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 353 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 367 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 385 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 385 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 431 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 505 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 505 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 528 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 528 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 553 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 600 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 659 | MLY  | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | D     | 768 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 782 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 837 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 839 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 55  | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 59  | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 59  | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 63  | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 84  | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 130 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 130 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 138 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 138 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 190 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 190 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 248 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 272 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 348 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 348 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 353 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 353 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 367 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 385 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 385 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 431 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 505 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 505 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 528 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 528 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 553 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 600 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 659 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 768 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 782 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 837 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 839 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 59  | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 59  | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 63  | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 84  | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 130 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 130 | MLY  | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | J     | 138 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 138 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 190 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 190 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 248 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 272 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 348 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 348 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 353 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 353 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 367 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 385 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 385 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 431 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 505 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 505 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 528 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 528 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 553 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 600 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 659 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 768 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 782 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 837 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 839 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 87  | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 87  | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 87  | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 87  | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 782 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 782 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 782 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 782 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 138 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 138 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 138 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 138 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 84  | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 130 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 130 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 84  | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 130 | MLY  | CG-CD-CE-NZ  |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | J     | 84  | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 130 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 369 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 504 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 504 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 768 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 272 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 369 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 504 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 504 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 768 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 272 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 369 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 504 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 504 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 768 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 369 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 504 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 504 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 768 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 84  | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 681 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 681 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 504 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 681 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 504 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 681 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 504 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 504 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 598 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 598 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 598 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 598 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 63  | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 63  | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 87  | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 63  | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 63  | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 272 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 87  | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 272 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 415 | MLY  | CD-CE-NZ-CH1 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 415 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 553 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 55  | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 415 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 415 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 553 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 55  | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 87  | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 415 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 415 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 553 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 87  | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 415 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 415 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 553 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 295 | MLY  | CA-CB-CG-CD  |
| 1   | D     | 295 | MLY  | CA-CB-CG-CD  |
| 1   | G     | 295 | MLY  | CA-CB-CG-CD  |
| 1   | J     | 295 | MLY  | CA-CB-CG-CD  |
| 1   | A     | 551 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 551 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 551 | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 551 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 19  | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 55  | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 19  | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 107 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 19  | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 19  | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 55  | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 504 | MLY  | CA-CB-CG-CD  |
| 1   | A     | 768 | MLY  | CA-CB-CG-CD  |
| 1   | D     | 504 | MLY  | CA-CB-CG-CD  |
| 1   | D     | 768 | MLY  | CA-CB-CG-CD  |
| 1   | G     | 504 | MLY  | CA-CB-CG-CD  |
| 1   | G     | 768 | MLY  | CA-CB-CG-CD  |
| 1   | J     | 504 | MLY  | CA-CB-CG-CD  |
| 1   | J     | 768 | MLY  | CA-CB-CG-CD  |
| 1   | D     | 49  | MLY  | CE-CD-CG-CB  |
| 1   | G     | 49  | MLY  | CE-CD-CG-CB  |
| 1   | J     | 49  | MLY  | CE-CD-CG-CB  |
| 1   | A     | 49  | MLY  | CE-CD-CG-CB  |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 505 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 505 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 505 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 505 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 272 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 272 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 296 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 272 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 296 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 272 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 296 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 296 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 30  | MLY  | CE-CD-CG-CB  |
| 1   | G     | 30  | MLY  | CE-CD-CG-CB  |
| 1   | J     | 30  | MLY  | CE-CD-CG-CB  |
| 1   | J     | 353 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 30  | MLY  | CE-CD-CG-CB  |
| 1   | A     | 107 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 839 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 107 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 839 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 107 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 839 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 190 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 353 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 190 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 353 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 190 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 190 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 353 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 681 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 681 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 681 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 681 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 190 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 190 | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 768 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 190 | MLY  | CG-CD-CE-NZ  |
| 1   | G     | 768 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 768 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 190 | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 768 | MLY  | CE-CD-CG-CB  |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 369 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 369 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 782 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 782 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 369 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 782 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 369 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 107 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 659 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 839 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 659 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 107 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 782 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 415 | MLY  | CA-CB-CG-CD  |
| 1   | G     | 415 | MLY  | CA-CB-CG-CD  |
| 1   | D     | 415 | MLY  | CA-CB-CG-CD  |
| 1   | J     | 415 | MLY  | CA-CB-CG-CD  |
| 1   | A     | 236 | MLY  | CD-CE-NZ-CH1 |
| 1   | A     | 659 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 107 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 236 | MLY  | CD-CE-NZ-CH1 |
| 1   | G     | 107 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 236 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 236 | MLY  | CD-CE-NZ-CH1 |
| 1   | J     | 659 | MLY  | CD-CE-NZ-CH1 |
| 1   | D     | 55  | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 55  | MLY  | CG-CD-CE-NZ  |
| 1   | J     | 55  | MLY  | CG-CD-CE-NZ  |
| 1   | A     | 833 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 833 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 833 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 833 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 55  | MLY  | CG-CD-CE-NZ  |
| 1   | D     | 617 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 617 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 436 | MLY  | CA-CB-CG-CD  |
| 1   | D     | 436 | MLY  | CA-CB-CG-CD  |
| 1   | G     | 436 | MLY  | CA-CB-CG-CD  |
| 1   | J     | 436 | MLY  | CA-CB-CG-CD  |
| 1   | J     | 617 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 617 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 551 | MLY  | CE-CD-CG-CB  |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | D     | 551 | MLY  | CE-CD-CG-CB |
| 1   | G     | 551 | MLY  | CE-CD-CG-CB |
| 1   | J     | 551 | MLY  | CE-CD-CG-CB |
| 1   | D     | 59  | MLY  | CE-CD-CG-CB |
| 1   | A     | 55  | MLY  | CE-CD-CG-CB |
| 1   | A     | 59  | MLY  | CE-CD-CG-CB |
| 1   | D     | 55  | MLY  | CE-CD-CG-CB |
| 1   | D     | 553 | MLY  | CE-CD-CG-CB |
| 1   | G     | 59  | MLY  | CE-CD-CG-CB |
| 1   | J     | 553 | MLY  | CE-CD-CG-CB |
| 1   | D     | 528 | MLY  | CG-CD-CE-NZ |
| 1   | A     | 553 | MLY  | CE-CD-CG-CB |
| 1   | G     | 55  | MLY  | CE-CD-CG-CB |
| 1   | G     | 553 | MLY  | CE-CD-CG-CB |
| 1   | J     | 55  | MLY  | CE-CD-CG-CB |
| 1   | J     | 59  | MLY  | CE-CD-CG-CB |
| 1   | G     | 528 | MLY  | CG-CD-CE-NZ |
| 1   | J     | 528 | MLY  | CG-CD-CE-NZ |
| 1   | A     | 528 | MLY  | CG-CD-CE-NZ |
| 1   | A     | 248 | MLY  | CG-CD-CE-NZ |
| 1   | G     | 248 | MLY  | CG-CD-CE-NZ |
| 1   | J     | 248 | MLY  | CG-CD-CE-NZ |
| 1   | D     | 248 | MLY  | CG-CD-CE-NZ |
| 1   | A     | 431 | MLY  | CE-CD-CG-CB |
| 1   | D     | 431 | MLY  | CE-CD-CG-CB |
| 1   | G     | 431 | MLY  | CE-CD-CG-CB |
| 1   | J     | 431 | MLY  | CE-CD-CG-CB |
| 1   | A     | 248 | MLY  | CE-CD-CG-CB |
| 1   | D     | 248 | MLY  | CE-CD-CG-CB |
| 1   | G     | 248 | MLY  | CE-CD-CG-CB |
| 1   | J     | 248 | MLY  | CE-CD-CG-CB |
| 1   | A     | 35  | MLY  | CE-CD-CG-CB |
| 1   | D     | 35  | MLY  | CE-CD-CG-CB |
| 1   | G     | 35  | MLY  | CE-CD-CG-CB |
| 1   | J     | 35  | MLY  | CE-CD-CG-CB |
| 1   | A     | 431 | MLY  | CA-CB-CG-CD |
| 1   | D     | 431 | MLY  | CA-CB-CG-CD |
| 1   | G     | 431 | MLY  | CA-CB-CG-CD |
| 1   | J     | 431 | MLY  | CA-CB-CG-CD |
| 1   | A     | 837 | MLY  | CA-CB-CG-CD |
| 1   | D     | 837 | MLY  | CA-CB-CG-CD |
| 1   | G     | 837 | MLY  | CA-CB-CG-CD |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | J     | 837 | MLY  | CA-CB-CG-CD |
| 1   | D     | 600 | MLY  | CE-CD-CG-CB |
| 1   | A     | 436 | MLY  | CE-CD-CG-CB |
| 1   | A     | 598 | MLY  | CE-CD-CG-CB |
| 1   | A     | 600 | MLY  | CE-CD-CG-CB |
| 1   | D     | 436 | MLY  | CE-CD-CG-CB |
| 1   | D     | 598 | MLY  | CE-CD-CG-CB |
| 1   | G     | 436 | MLY  | CE-CD-CG-CB |
| 1   | G     | 598 | MLY  | CE-CD-CG-CB |
| 1   | G     | 600 | MLY  | CE-CD-CG-CB |
| 1   | J     | 436 | MLY  | CE-CD-CG-CB |
| 1   | J     | 598 | MLY  | CE-CD-CG-CB |
| 1   | J     | 600 | MLY  | CE-CD-CG-CB |
| 1   | J     | 236 | MLY  | CA-CB-CG-CD |
| 1   | A     | 486 | MLY  | CE-CD-CG-CB |
| 1   | G     | 486 | MLY  | CE-CD-CG-CB |
| 1   | J     | 486 | MLY  | CE-CD-CG-CB |
| 1   | D     | 486 | MLY  | CE-CD-CG-CB |
| 1   | A     | 236 | MLY  | CA-CB-CG-CD |
| 1   | A     | 833 | MLY  | CA-CB-CG-CD |
| 1   | D     | 236 | MLY  | CA-CB-CG-CD |
| 1   | D     | 833 | MLY  | CA-CB-CG-CD |
| 1   | G     | 236 | MLY  | CA-CB-CG-CD |
| 1   | G     | 833 | MLY  | CA-CB-CG-CD |
| 1   | J     | 833 | MLY  | CA-CB-CG-CD |
| 1   | D     | 839 | MLY  | CE-CD-CG-CB |
| 1   | G     | 839 | MLY  | CE-CD-CG-CB |
| 1   | J     | 839 | MLY  | CE-CD-CG-CB |
| 1   | A     | 839 | MLY  | CE-CD-CG-CB |
| 1   | A     | 138 | MLY  | CA-CB-CG-CD |
| 1   | A     | 296 | MLY  | CA-CB-CG-CD |
| 1   | D     | 138 | MLY  | CA-CB-CG-CD |
| 1   | D     | 296 | MLY  | CA-CB-CG-CD |
| 1   | J     | 138 | MLY  | CA-CB-CG-CD |
| 1   | J     | 296 | MLY  | CA-CB-CG-CD |
| 1   | A     | 63  | MLY  | C-CA-CB-CG  |
| 1   | A     | 353 | MLY  | C-CA-CB-CG  |
| 1   | A     | 827 | MLY  | C-CA-CB-CG  |
| 1   | A     | 833 | MLY  | C-CA-CB-CG  |
| 1   | D     | 63  | MLY  | C-CA-CB-CG  |
| 1   | D     | 353 | MLY  | C-CA-CB-CG  |
| 1   | D     | 827 | MLY  | C-CA-CB-CG  |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | D     | 833 | MLY  | C-CA-CB-CG  |
| 1   | G     | 63  | MLY  | C-CA-CB-CG  |
| 1   | G     | 353 | MLY  | C-CA-CB-CG  |
| 1   | G     | 827 | MLY  | C-CA-CB-CG  |
| 1   | G     | 833 | MLY  | C-CA-CB-CG  |
| 1   | J     | 63  | MLY  | C-CA-CB-CG  |
| 1   | J     | 353 | MLY  | C-CA-CB-CG  |
| 1   | J     | 827 | MLY  | C-CA-CB-CG  |
| 1   | J     | 833 | MLY  | C-CA-CB-CG  |
| 1   | G     | 138 | MLY  | CA-CB-CG-CD |
| 1   | G     | 296 | MLY  | CA-CB-CG-CD |
| 1   | A     | 35  | MLY  | N-CA-CB-CG  |
| 1   | A     | 63  | MLY  | N-CA-CB-CG  |
| 1   | A     | 130 | MLY  | N-CA-CB-CG  |
| 1   | A     | 348 | MLY  | N-CA-CB-CG  |
| 1   | A     | 436 | MLY  | N-CA-CB-CG  |
| 1   | A     | 681 | MLY  | N-CA-CB-CG  |
| 1   | A     | 833 | MLY  | N-CA-CB-CG  |
| 1   | A     | 837 | MLY  | N-CA-CB-CG  |
| 1   | D     | 35  | MLY  | N-CA-CB-CG  |
| 1   | D     | 63  | MLY  | N-CA-CB-CG  |
| 1   | D     | 130 | MLY  | N-CA-CB-CG  |
| 1   | D     | 348 | MLY  | N-CA-CB-CG  |
| 1   | D     | 436 | MLY  | N-CA-CB-CG  |
| 1   | D     | 681 | MLY  | N-CA-CB-CG  |
| 1   | D     | 833 | MLY  | N-CA-CB-CG  |
| 1   | D     | 837 | MLY  | N-CA-CB-CG  |
| 1   | G     | 35  | MLY  | N-CA-CB-CG  |
| 1   | G     | 63  | MLY  | N-CA-CB-CG  |
| 1   | G     | 130 | MLY  | N-CA-CB-CG  |
| 1   | G     | 348 | MLY  | N-CA-CB-CG  |
| 1   | G     | 436 | MLY  | N-CA-CB-CG  |
| 1   | G     | 681 | MLY  | N-CA-CB-CG  |
| 1   | G     | 833 | MLY  | N-CA-CB-CG  |
| 1   | G     | 837 | MLY  | N-CA-CB-CG  |
| 1   | J     | 35  | MLY  | N-CA-CB-CG  |
| 1   | J     | 63  | MLY  | N-CA-CB-CG  |
| 1   | J     | 130 | MLY  | N-CA-CB-CG  |
| 1   | J     | 436 | MLY  | N-CA-CB-CG  |
| 1   | J     | 681 | MLY  | N-CA-CB-CG  |
| 1   | J     | 833 | MLY  | N-CA-CB-CG  |
| 1   | J     | 837 | MLY  | N-CA-CB-CG  |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 19  | MLY  | CA-CB-CG-CD  |
| 1   | D     | 19  | MLY  | CA-CB-CG-CD  |
| 1   | G     | 19  | MLY  | CA-CB-CG-CD  |
| 1   | J     | 19  | MLY  | CA-CB-CG-CD  |
| 1   | D     | 837 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 837 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 19  | MLY  | CE-CD-CG-CB  |
| 1   | A     | 837 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 837 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 19  | MLY  | CE-CD-CG-CB  |
| 1   | J     | 19  | MLY  | CE-CD-CG-CB  |
| 1   | G     | 19  | MLY  | CE-CD-CG-CB  |
| 1   | G     | 613 | MLY  | CE-CD-CG-CB  |
| 1   | J     | 613 | MLY  | CE-CD-CG-CB  |
| 1   | D     | 613 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 613 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 236 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 236 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 236 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 236 | MLY  | CD-CE-NZ-CH2 |
| 1   | A     | 598 | MLY  | CD-CE-NZ-CH2 |
| 1   | D     | 598 | MLY  | CD-CE-NZ-CH2 |
| 1   | G     | 598 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 598 | MLY  | CD-CE-NZ-CH2 |
| 1   | J     | 348 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 30  | MLY  | C-CA-CB-CG   |
| 1   | A     | 617 | MLY  | C-CA-CB-CG   |
| 1   | A     | 837 | MLY  | C-CA-CB-CG   |
| 1   | D     | 30  | MLY  | C-CA-CB-CG   |
| 1   | D     | 617 | MLY  | C-CA-CB-CG   |
| 1   | D     | 837 | MLY  | C-CA-CB-CG   |
| 1   | G     | 30  | MLY  | C-CA-CB-CG   |
| 1   | G     | 617 | MLY  | C-CA-CB-CG   |
| 1   | G     | 837 | MLY  | C-CA-CB-CG   |
| 1   | J     | 30  | MLY  | C-CA-CB-CG   |
| 1   | J     | 617 | MLY  | C-CA-CB-CG   |
| 1   | J     | 837 | MLY  | C-CA-CB-CG   |
| 1   | D     | 348 | MLY  | CE-CD-CG-CB  |
| 1   | G     | 348 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 348 | MLY  | CE-CD-CG-CB  |
| 1   | A     | 30  | MLY  | CA-CB-CG-CD  |
| 1   | D     | 30  | MLY  | CA-CB-CG-CD  |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | G     | 30  | MLY  | CA-CB-CG-CD |
| 1   | J     | 30  | MLY  | CA-CB-CG-CD |

There are no ring outliers.

125 monomers are involved in 534 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | D     | 59  | MLY  | 2       | 0            |
| 1   | D     | 296 | MLY  | 3       | 0            |
| 1   | J     | 839 | MLY  | 5       | 0            |
| 1   | G     | 248 | MLY  | 2       | 0            |
| 1   | G     | 272 | MLY  | 1       | 0            |
| 1   | A     | 659 | MLY  | 2       | 0            |
| 1   | D     | 190 | MLY  | 2       | 0            |
| 1   | J     | 84  | MLY  | 25      | 0            |
| 1   | G     | 436 | MLY  | 2       | 0            |
| 1   | D     | 764 | MLY  | 2       | 0            |
| 1   | A     | 295 | MLY  | 6       | 0            |
| 1   | A     | 55  | MLY  | 1       | 0            |
| 1   | G     | 827 | MLY  | 1       | 0            |
| 1   | J     | 827 | MLY  | 1       | 0            |
| 1   | A     | 87  | MLY  | 3       | 0            |
| 1   | A     | 768 | MLY  | 14      | 0            |
| 1   | J     | 528 | MLY  | 3       | 0            |
| 1   | A     | 504 | MLY  | 5       | 0            |
| 1   | J     | 782 | MLY  | 1       | 0            |
| 1   | A     | 598 | MLY  | 1       | 0            |
| 1   | J     | 415 | MLY  | 1       | 0            |
| 1   | G     | 659 | MLY  | 2       | 0            |
| 1   | D     | 486 | MLY  | 3       | 0            |
| 1   | J     | 486 | MLY  | 3       | 0            |
| 1   | D     | 504 | MLY  | 1       | 0            |
| 1   | G     | 87  | MLY  | 2       | 0            |
| 1   | G     | 59  | MLY  | 3       | 0            |
| 1   | G     | 768 | MLY  | 13      | 0            |
| 1   | J     | 837 | MLY  | 1       | 0            |
| 1   | A     | 837 | MLY  | 1       | 0            |
| 1   | D     | 553 | MLY  | 16      | 0            |
| 1   | A     | 551 | MLY  | 2       | 0            |
| 1   | A     | 782 | MLY  | 1       | 0            |
| 1   | D     | 436 | MLY  | 2       | 0            |
| 1   | J     | 138 | MLY  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | G     | 348 | MLY  | 4       | 0            |
| 1   | D     | 63  | MLY  | 3       | 0            |
| 1   | A     | 49  | MLY  | 3       | 0            |
| 1   | G     | 55  | MLY  | 1       | 0            |
| 1   | G     | 600 | MLY  | 1       | 0            |
| 1   | G     | 617 | MLY  | 1       | 0            |
| 1   | D     | 107 | MLY  | 3       | 0            |
| 1   | D     | 837 | MLY  | 1       | 0            |
| 1   | A     | 30  | MLY  | 1       | 0            |
| 1   | D     | 551 | MLY  | 1       | 0            |
| 1   | A     | 486 | MLY  | 3       | 0            |
| 1   | G     | 296 | MLY  | 2       | 0            |
| 1   | J     | 598 | MLY  | 1       | 0            |
| 1   | G     | 764 | MLY  | 13      | 0            |
| 1   | G     | 598 | MLY  | 1       | 0            |
| 1   | D     | 55  | MLY  | 1       | 0            |
| 1   | D     | 87  | MLY  | 3       | 0            |
| 1   | D     | 49  | MLY  | 4       | 0            |
| 1   | A     | 617 | MLY  | 1       | 0            |
| 1   | J     | 59  | MLY  | 3       | 0            |
| 1   | A     | 436 | MLY  | 2       | 0            |
| 1   | A     | 505 | MLY  | 11      | 0            |
| 1   | D     | 348 | MLY  | 6       | 0            |
| 1   | J     | 348 | MLY  | 5       | 0            |
| 1   | J     | 768 | MLY  | 40      | 0            |
| 1   | A     | 138 | MLY  | 2       | 0            |
| 1   | J     | 764 | MLY  | 22      | 0            |
| 1   | G     | 553 | MLY  | 27      | 0            |
| 1   | D     | 617 | MLY  | 1       | 0            |
| 1   | D     | 248 | MLY  | 2       | 0            |
| 1   | J     | 248 | MLY  | 2       | 0            |
| 1   | A     | 528 | MLY  | 2       | 0            |
| 1   | G     | 295 | MLY  | 6       | 0            |
| 1   | J     | 272 | MLY  | 1       | 0            |
| 1   | D     | 782 | MLY  | 31      | 0            |
| 1   | A     | 839 | MLY  | 15      | 0            |
| 1   | G     | 84  | MLY  | 18      | 0            |
| 1   | G     | 190 | MLY  | 2       | 0            |
| 1   | G     | 837 | MLY  | 1       | 0            |
| 1   | A     | 348 | MLY  | 5       | 0            |
| 1   | J     | 190 | MLY  | 2       | 0            |
| 1   | A     | 63  | MLY  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | D     | 30  | MLY  | 1       | 0            |
| 1   | J     | 49  | MLY  | 3       | 0            |
| 1   | D     | 839 | MLY  | 16      | 0            |
| 1   | J     | 504 | MLY  | 1       | 0            |
| 1   | G     | 839 | MLY  | 4       | 0            |
| 1   | J     | 659 | MLY  | 2       | 0            |
| 1   | A     | 272 | MLY  | 1       | 0            |
| 1   | D     | 528 | MLY  | 3       | 0            |
| 1   | G     | 30  | MLY  | 1       | 0            |
| 1   | A     | 415 | MLY  | 1       | 0            |
| 1   | J     | 295 | MLY  | 6       | 0            |
| 1   | A     | 107 | MLY  | 3       | 0            |
| 1   | G     | 504 | MLY  | 1       | 0            |
| 1   | D     | 415 | MLY  | 1       | 0            |
| 1   | G     | 49  | MLY  | 3       | 0            |
| 1   | J     | 553 | MLY  | 11      | 0            |
| 1   | J     | 107 | MLY  | 3       | 0            |
| 1   | A     | 190 | MLY  | 2       | 0            |
| 1   | J     | 600 | MLY  | 1       | 0            |
| 1   | A     | 553 | MLY  | 17      | 0            |
| 1   | G     | 138 | MLY  | 2       | 0            |
| 1   | D     | 138 | MLY  | 2       | 0            |
| 1   | J     | 30  | MLY  | 1       | 0            |
| 1   | D     | 598 | MLY  | 1       | 0            |
| 1   | G     | 415 | MLY  | 1       | 0            |
| 1   | J     | 296 | MLY  | 3       | 0            |
| 1   | G     | 107 | MLY  | 3       | 0            |
| 1   | A     | 248 | MLY  | 2       | 0            |
| 1   | D     | 272 | MLY  | 1       | 0            |
| 1   | G     | 782 | MLY  | 1       | 0            |
| 1   | G     | 528 | MLY  | 3       | 0            |
| 1   | D     | 295 | MLY  | 6       | 0            |
| 1   | A     | 600 | MLY  | 1       | 0            |
| 1   | J     | 55  | MLY  | 1       | 0            |
| 1   | G     | 63  | MLY  | 3       | 0            |
| 1   | G     | 369 | MLY  | 1       | 0            |
| 1   | J     | 63  | MLY  | 4       | 0            |
| 1   | J     | 436 | MLY  | 2       | 0            |
| 1   | A     | 369 | MLY  | 1       | 0            |
| 1   | A     | 59  | MLY  | 2       | 0            |
| 1   | A     | 296 | MLY  | 2       | 0            |
| 1   | D     | 768 | MLY  | 7       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | D     | 659 | MLY  | 2       | 0            |
| 1   | D     | 600 | MLY  | 1       | 0            |
| 1   | J     | 617 | MLY  | 1       | 0            |
| 1   | G     | 486 | MLY  | 3       | 0            |
| 1   | J     | 87  | MLY  | 3       | 0            |
| 1   | A     | 764 | MLY  | 7       | 0            |

## 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 |
|-----|-------|------------------|
| 1   | G     | 4                |
| 1   | J     | 4                |
| 1   | D     | 4                |
| 1   | A     | 4                |
| 3   | C     | 1                |
| 3   | F     | 1                |
| 3   | I     | 1                |
| 3   | L     | 1                |
| 2   | B     | 1                |
| 2   | E     | 1                |
| 2   | H     | 1                |
| 2   | K     | 1                |

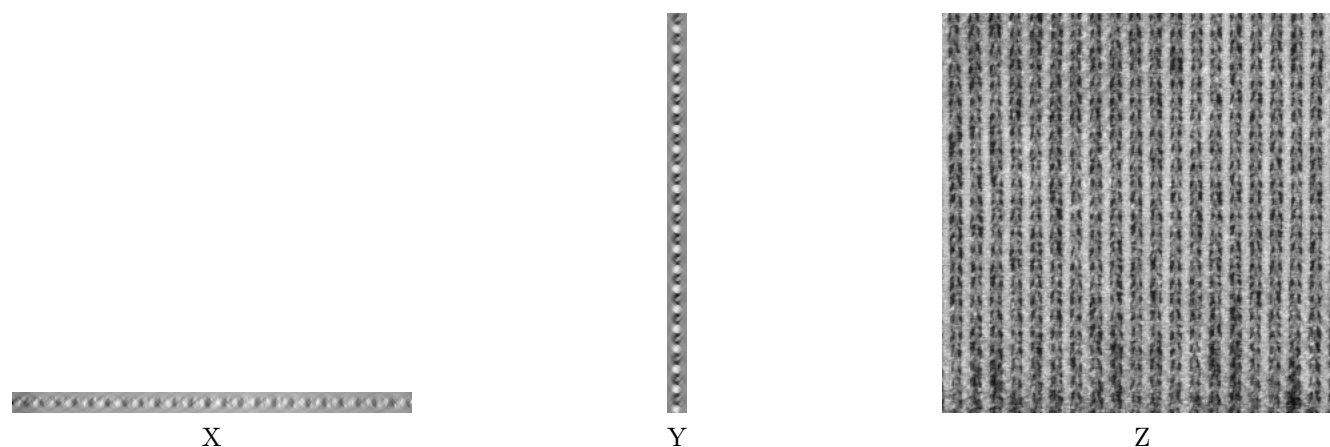
All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | G     | 769:ALA   | C      | 770:GLY   | N      | 4.88         |
| 1     | J     | 769:ALA   | C      | 770:GLY   | N      | 4.64         |
| 1     | D     | 769:ALA   | C      | 770:GLY   | N      | 4.52         |
| 1     | D     | 709:LYS   | C      | 710:GLY   | N      | 3.32         |
| 1     | A     | 709:LYS   | C      | 710:GLY   | N      | 3.27         |
| 1     | A     | 769:ALA   | C      | 770:GLY   | N      | 2.77         |
| 1     | C     | 4:LYS     | C      | 5:ALA     | N      | 2.61         |
| 1     | F     | 4:LYS     | C      | 5:ALA     | N      | 2.61         |
| 1     | I     | 4:LYS     | C      | 5:ALA     | N      | 2.61         |
| 1     | L     | 4:LYS     | C      | 5:ALA     | N      | 2.61         |
| 1     | G     | 709:LYS   | C      | 710:GLY   | N      | 2.16         |
| 1     | B     | 140:PHE   | C      | 141:PRO   | N      | 1.09         |
| 1     | E     | 140:PHE   | C      | 141:PRO   | N      | 1.09         |
| 1     | H     | 140:PHE   | C      | 141:PRO   | N      | 1.09         |
| 1     | K     | 140:PHE   | C      | 141:PRO   | N      | 1.09         |
| 1     | A     | 637:LYS   | C      | 638:GLY   | N      | 1.06         |
| 1     | D     | 637:LYS   | C      | 638:GLY   | N      | 1.06         |
| 1     | G     | 637:LYS   | C      | 638:GLY   | N      | 1.06         |
| 1     | J     | 637:LYS   | C      | 638:GLY   | N      | 1.06         |
| 1     | D     | 649:VAL   | C      | 650:SER   | N      | 1.03         |
| 1     | J     | 649:VAL   | C      | 650:SER   | N      | 1.03         |
| 1     | A     | 649:VAL   | C      | 650:SER   | N      | 1.02         |
| 1     | G     | 649:VAL   | C      | 650:SER   | N      | 1.02         |
| 1     | J     | 709:LYS   | C      | 710:GLY   | N      | 0.33         |

## 6 Tomogram visualisation [i](#)

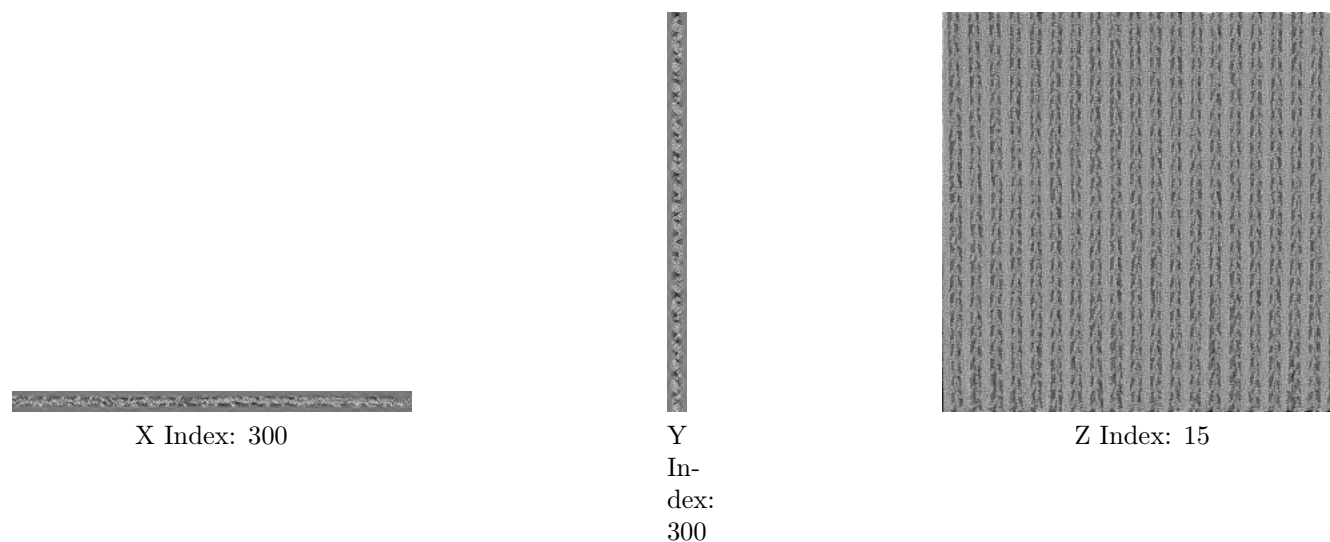
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

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



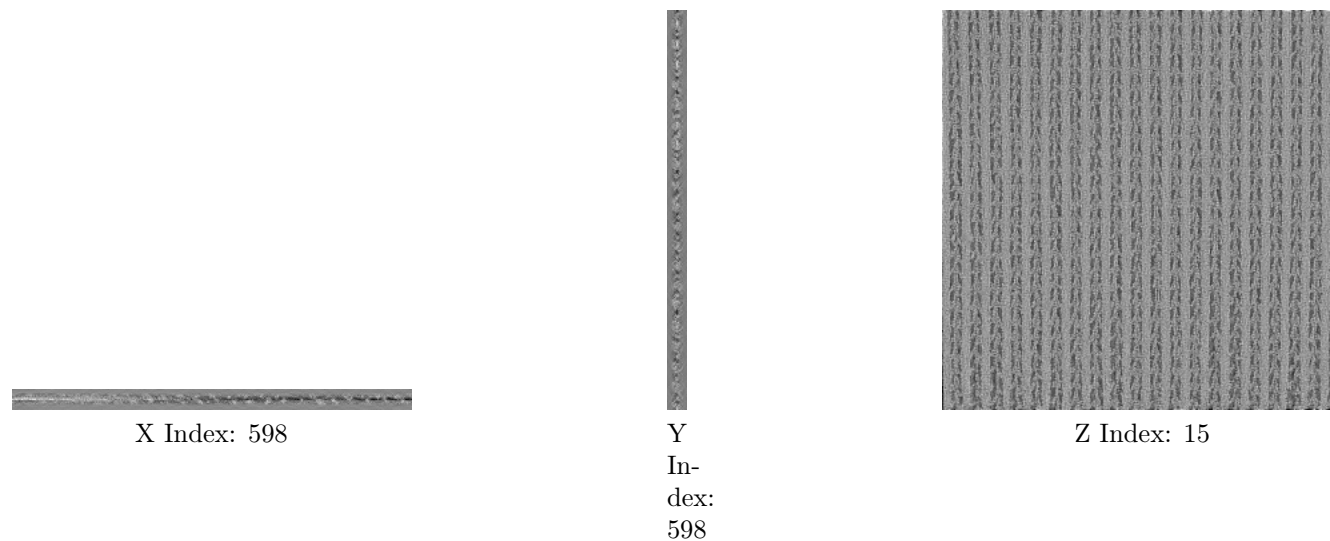
The images above show the tomogram projected in three orthogonal directions.

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



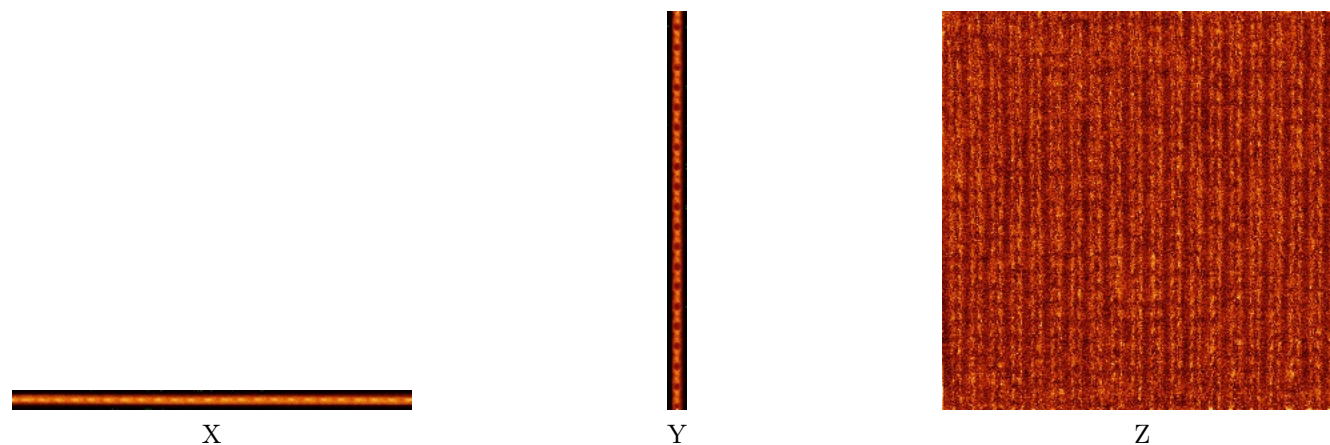
The images above show central slices of the tomogram in three orthogonal directions.

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



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

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



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

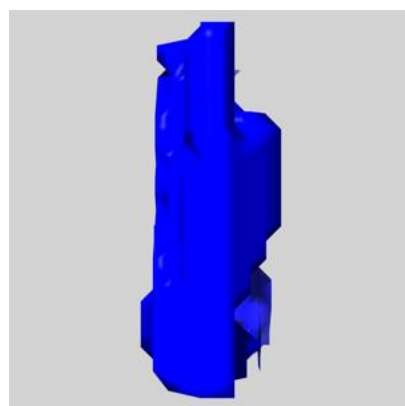
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

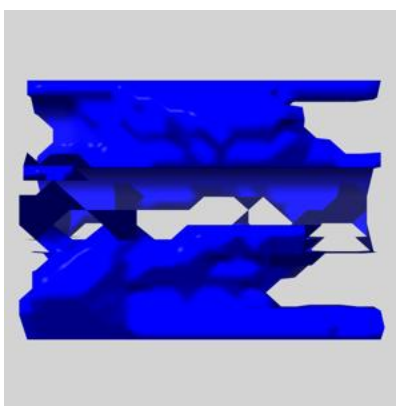
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

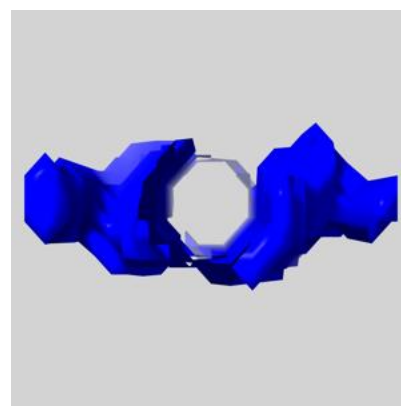
### 6.5.1 emd\_1001\_msk\_25.map [i](#)



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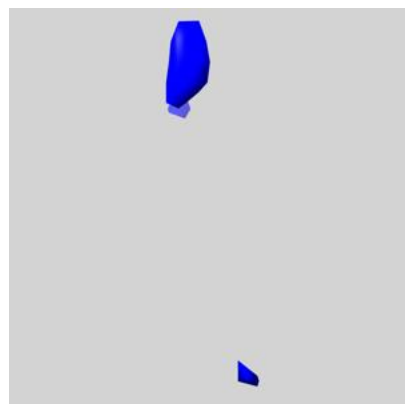


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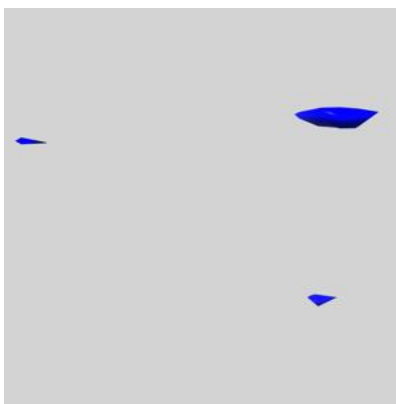


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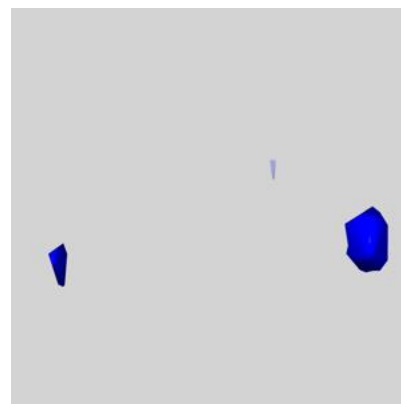
### 6.5.2 emd\_1001\_msk\_24.map [i](#)



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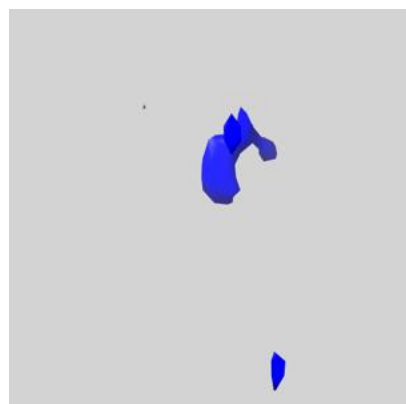


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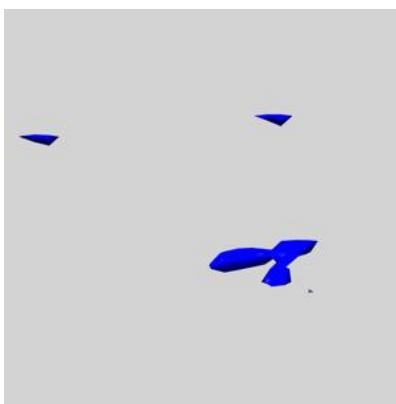


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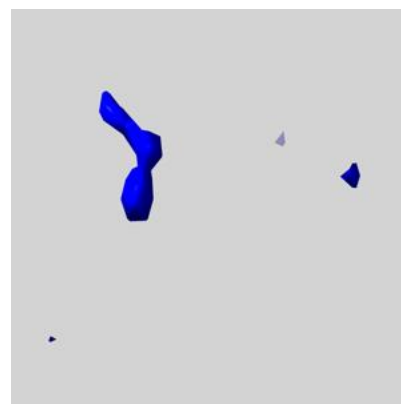
### 6.5.3 emd\_1001\_msk\_23.map [i](#)



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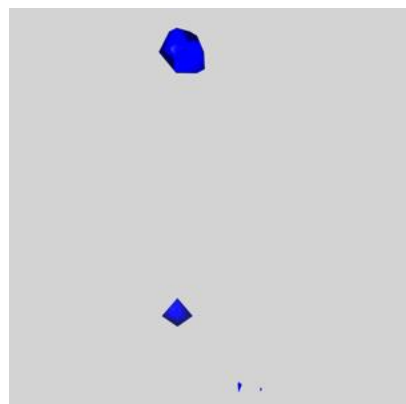


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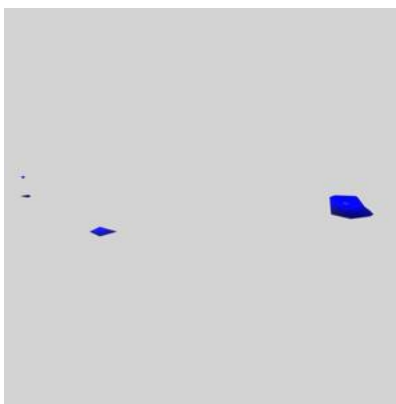


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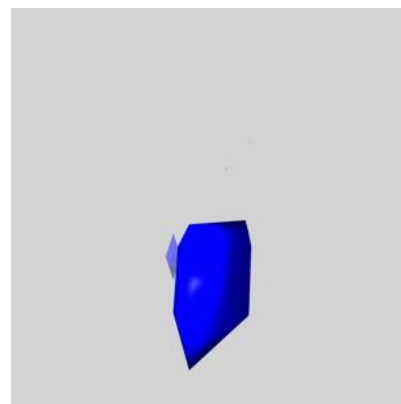
### 6.5.4 emd\_1001\_msk\_22.map [i](#)



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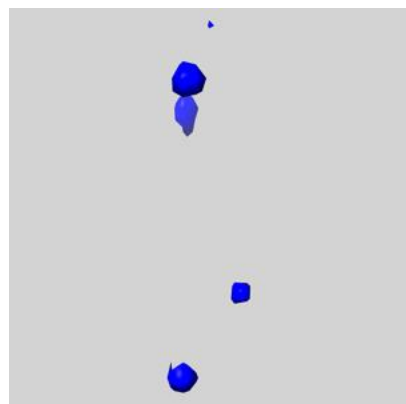


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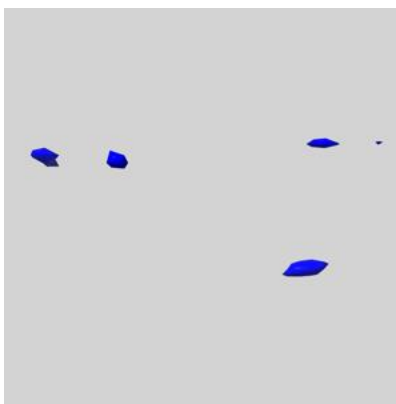


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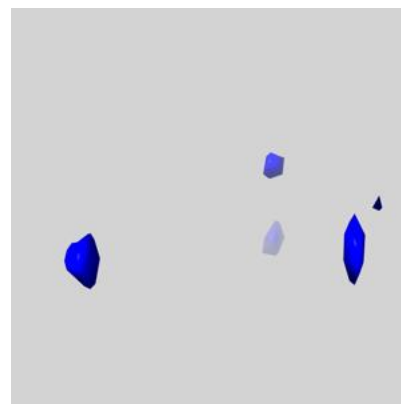
### 6.5.5 emd\_1001\_msk\_21.map [i](#)



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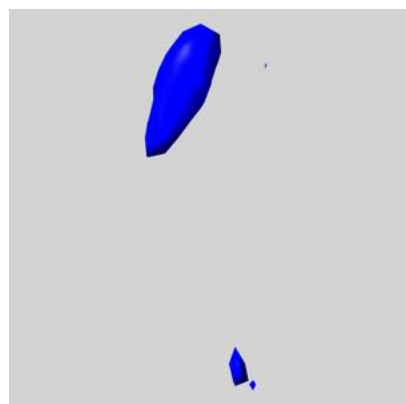


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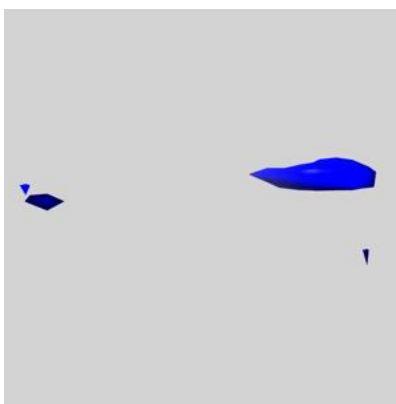


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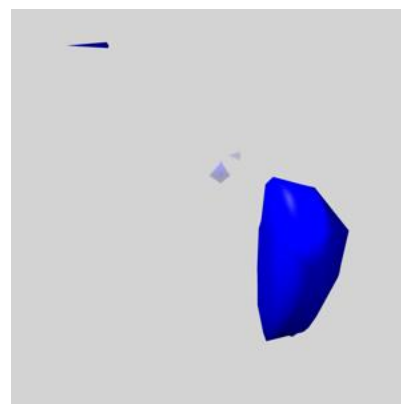
### 6.5.6 emd\_1001\_msk\_20.map [i](#)



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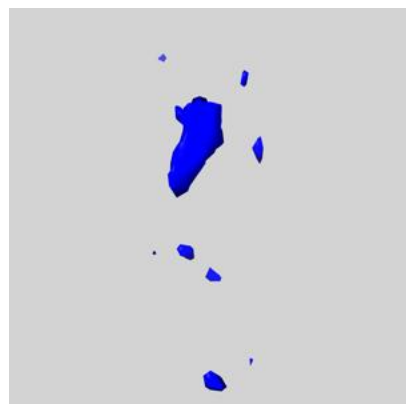


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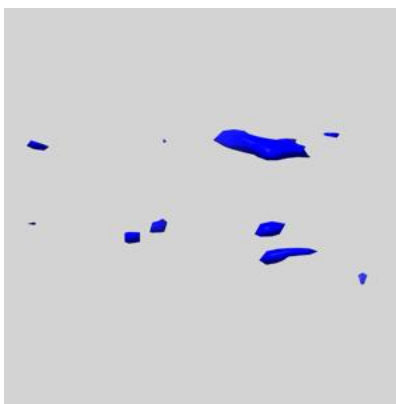


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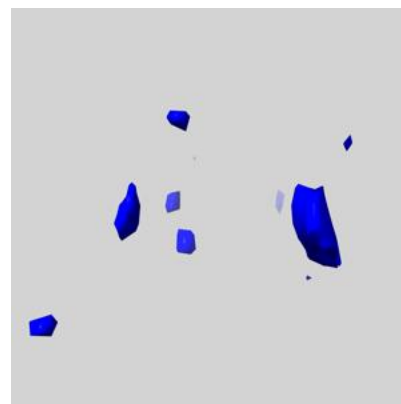
### 6.5.7 emd\_1001\_msk\_19.map [i](#)



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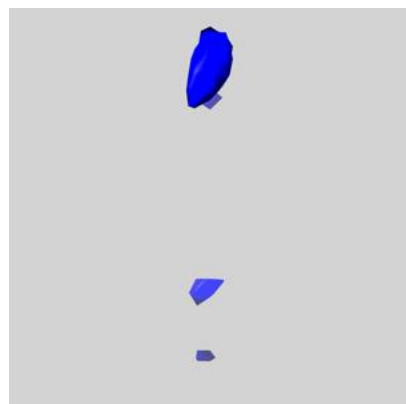


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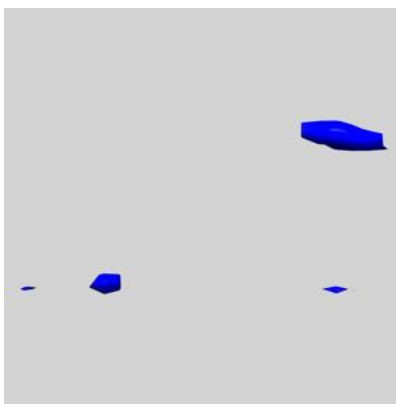


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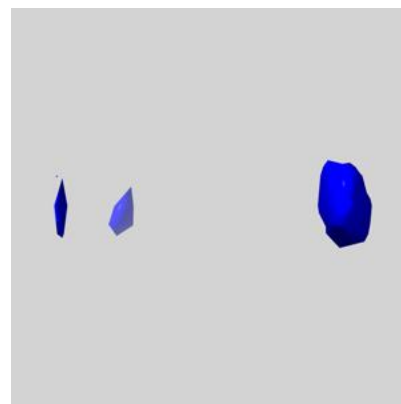
### 6.5.8 emd\_1001\_msk\_18.map [i](#)



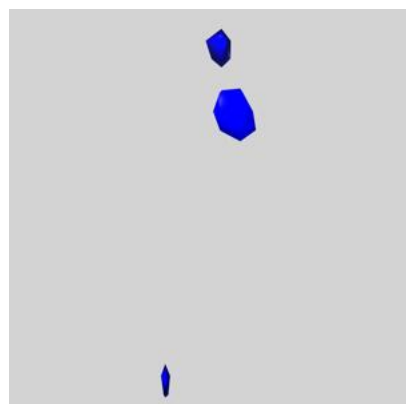
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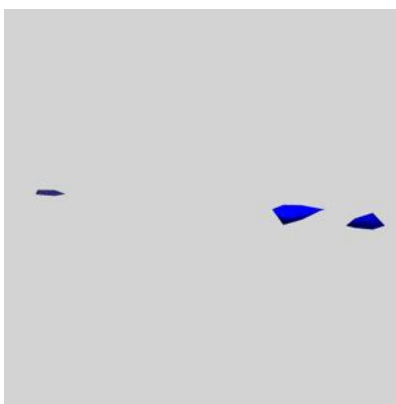
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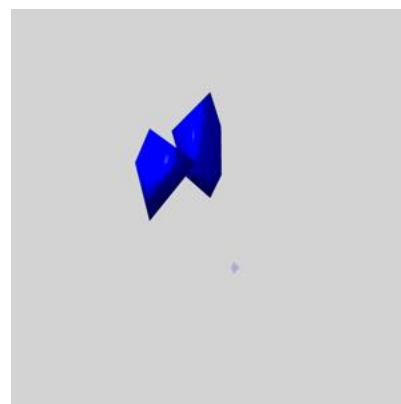
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6.5.9 emd\_1001\_msk\_17.map [i](#)

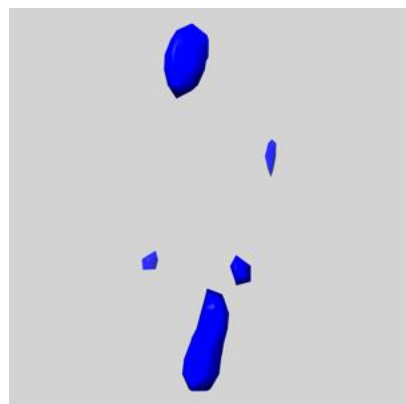
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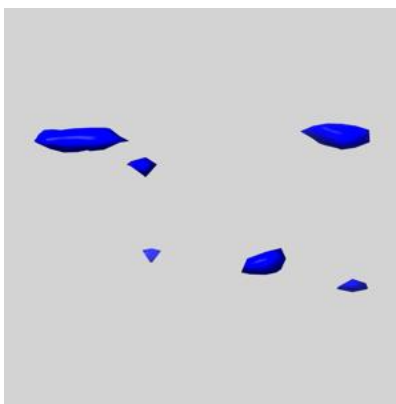
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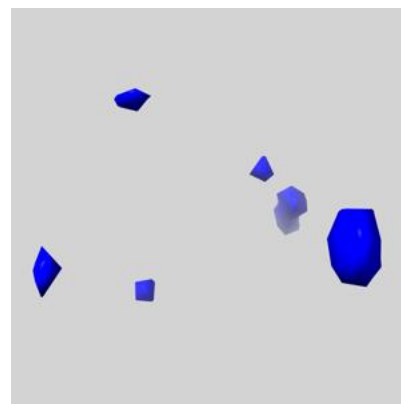
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6.5.10 emd\_1001\_msk\_16.map [i](#)

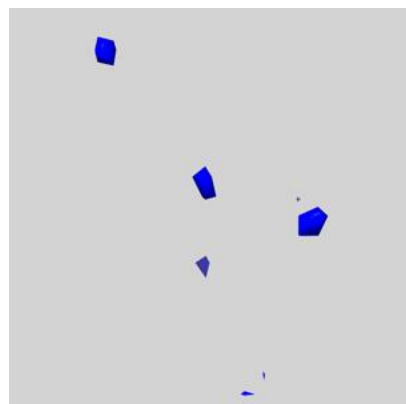
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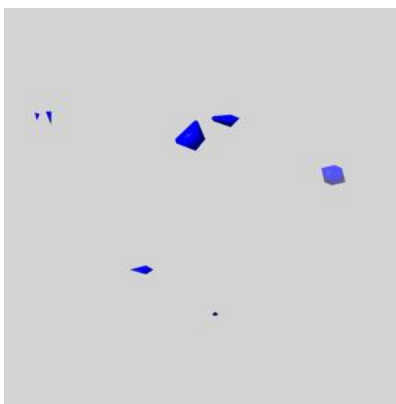
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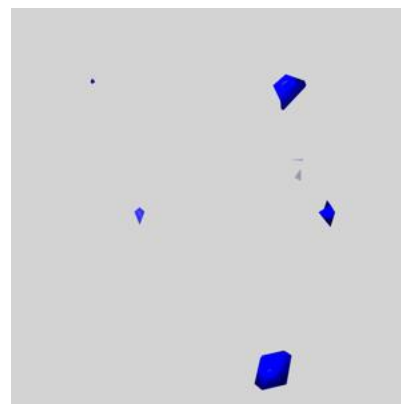
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6.5.11 emd\_1001\_msk\_15.map [i](#)

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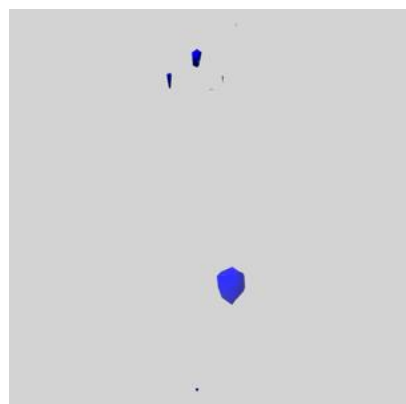


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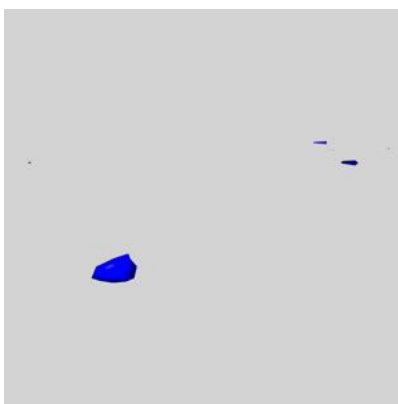


Z

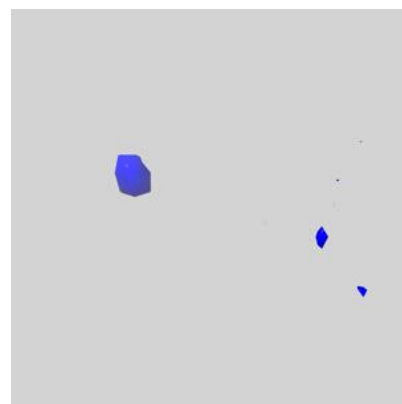
### 6.5.12 emd\_1001\_msk\_14.map [i](#)



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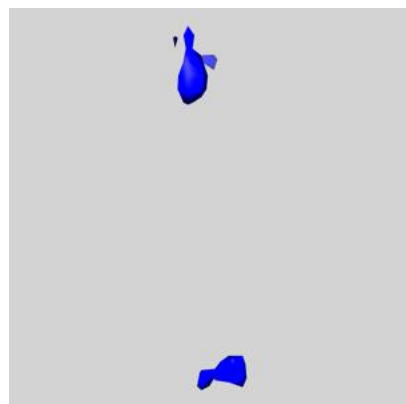


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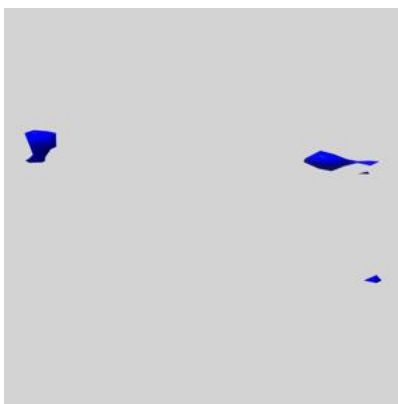


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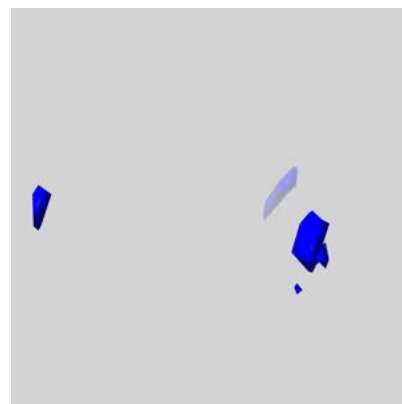
### 6.5.13 emd\_1001\_msk\_13.map [i](#)



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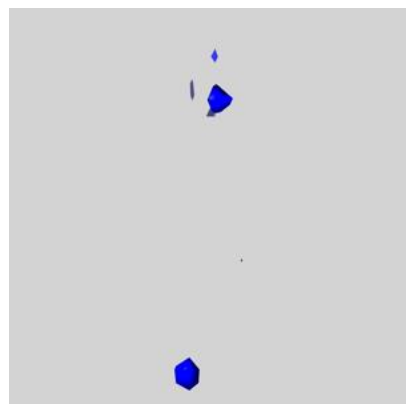


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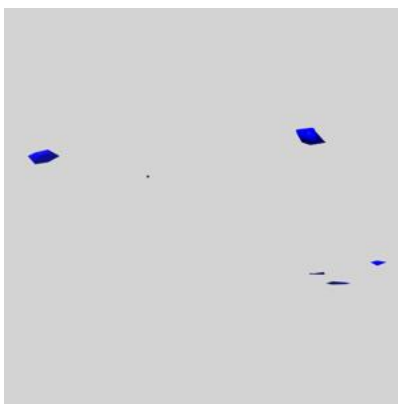


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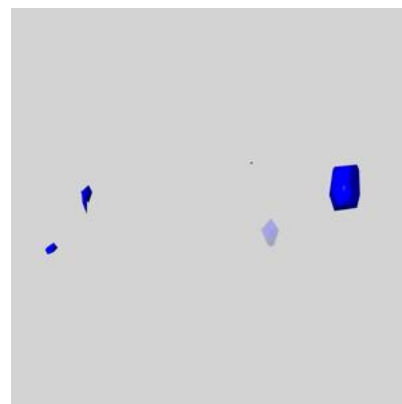
### 6.5.14 emd\_1001\_msk\_12.map [i](#)



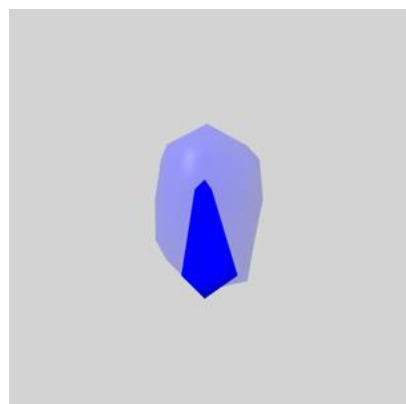
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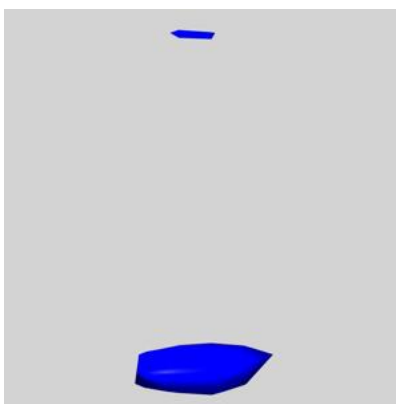
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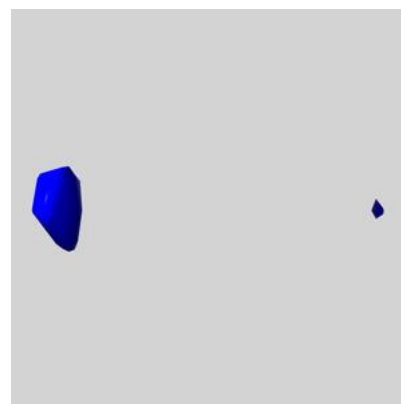
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6.5.15 emd\_1001\_msk\_11.map [i](#)

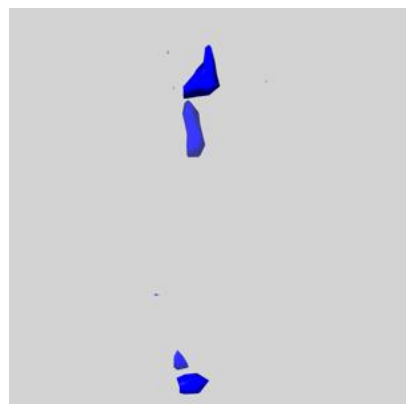
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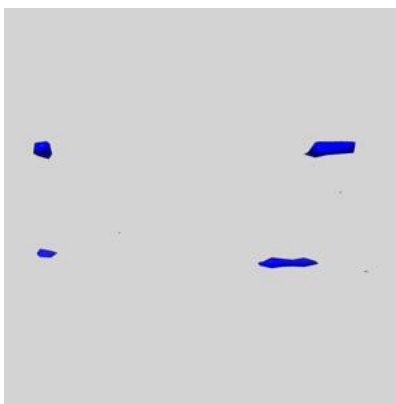
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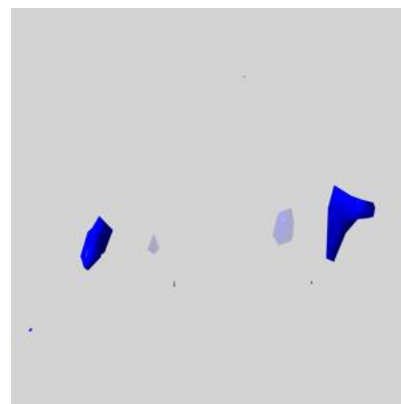
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6.5.16 emd\_1001\_msk\_10.map [i](#)

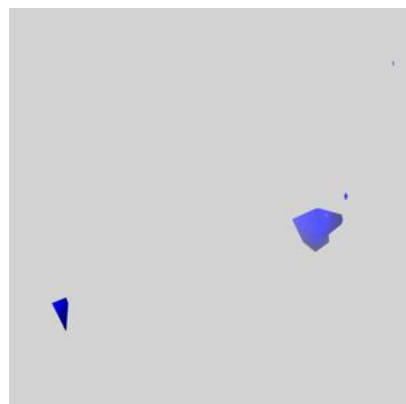
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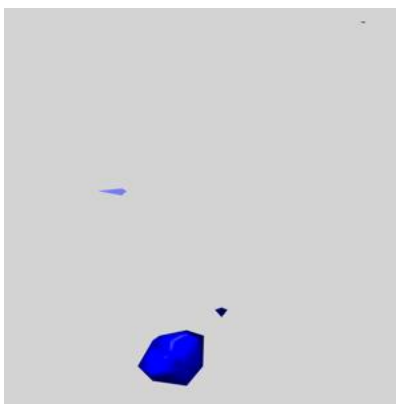
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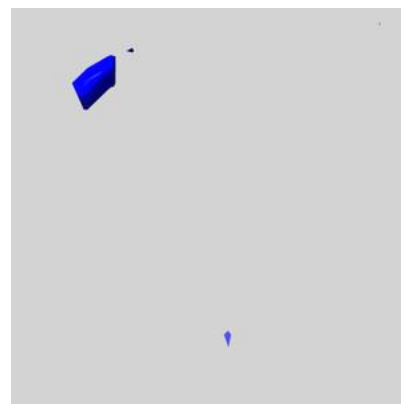
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6.5.17 emd\_1001\_msk\_9.map [i](#)

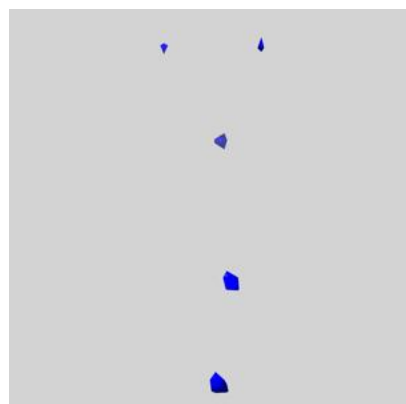
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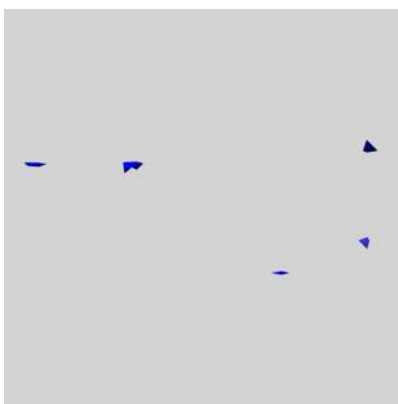
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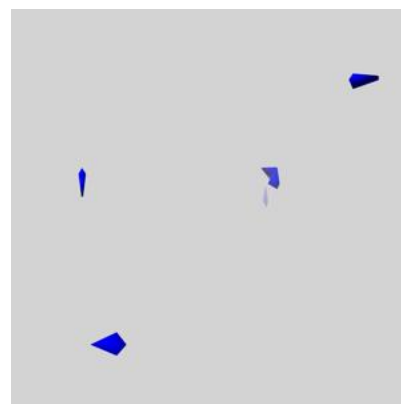
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6.5.18 emd\_1001\_msk\_8.map [i](#)

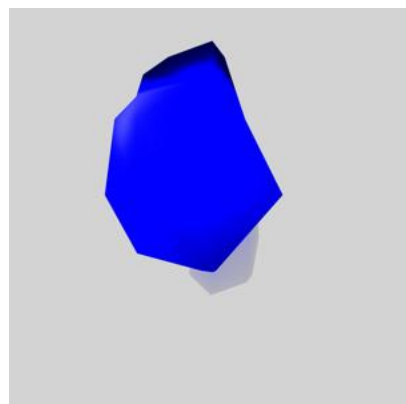
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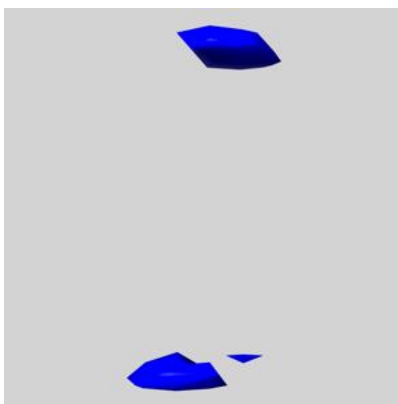
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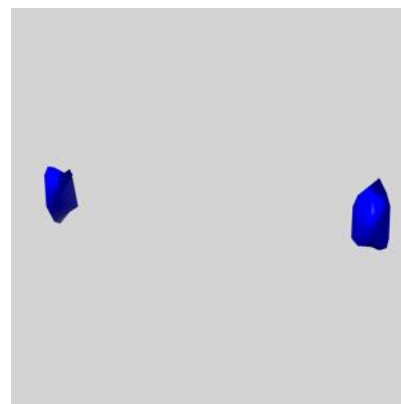
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6.5.19 emd\_1001\_msk\_7.map [i](#)

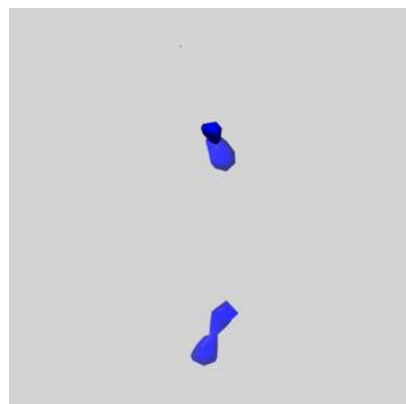
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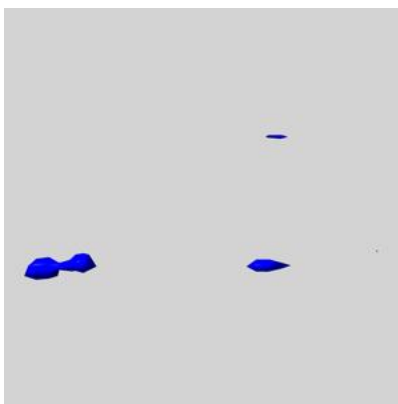
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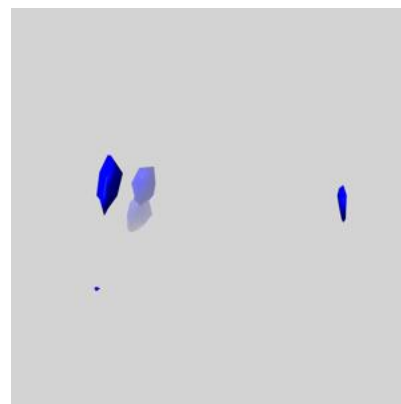
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6.5.20 emd\_1001\_msk\_6.map [i](#)

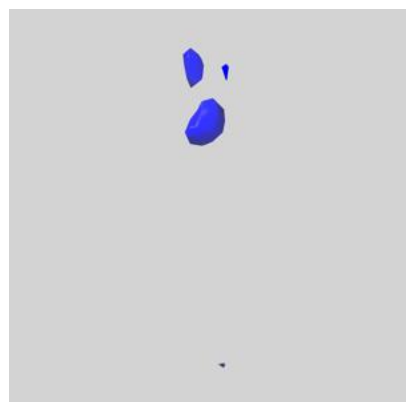
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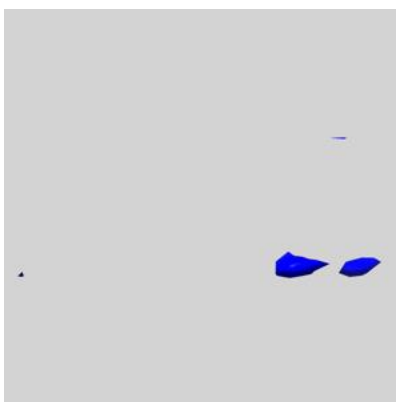
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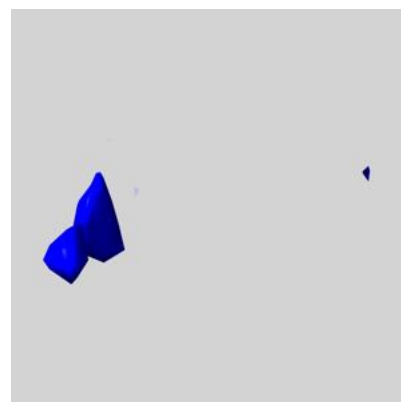
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6.5.21 emd\_1001\_msk\_5.map [i](#)

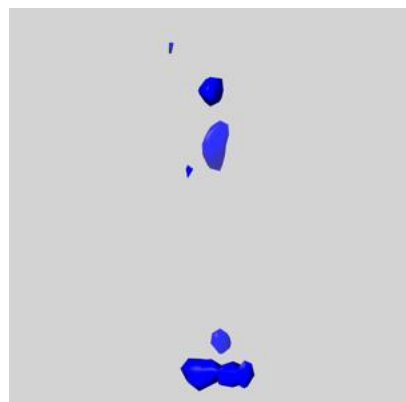
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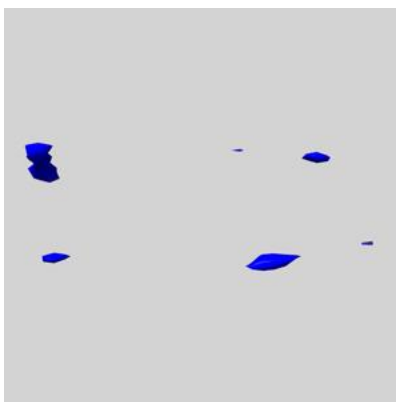
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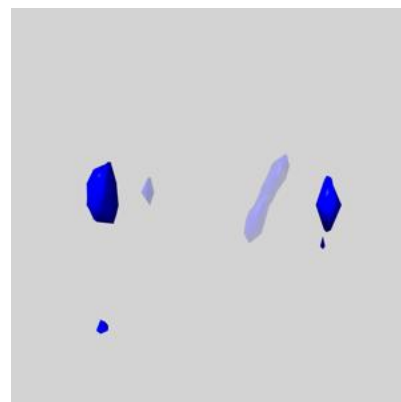
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6.5.22 emd\_1001\_msk\_4.map [i](#)

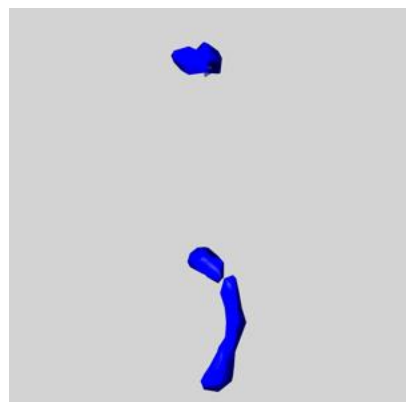
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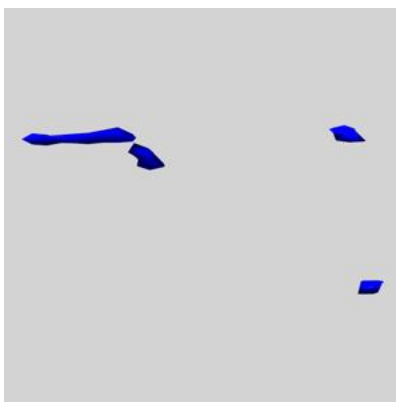
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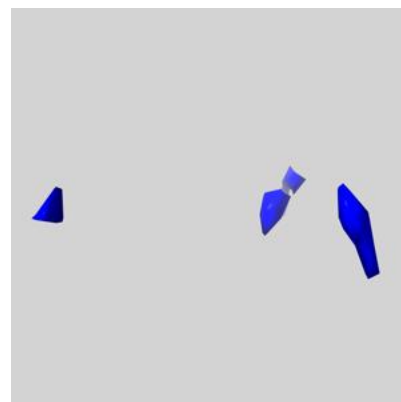
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6.5.23 emd\_1001\_msk\_3.map [i](#)

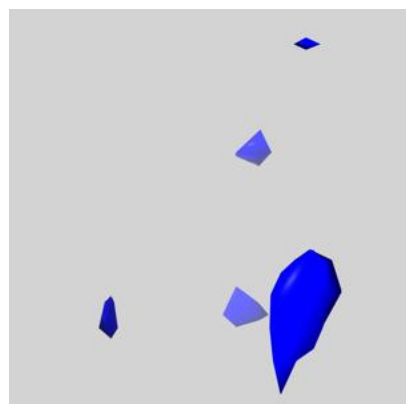
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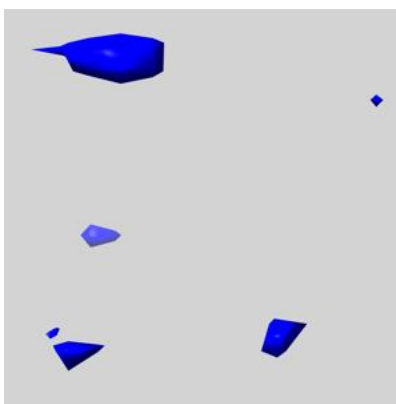
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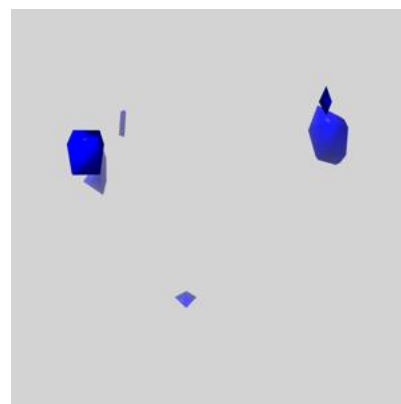
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6.5.24 emd\_1001\_msk\_2.map [i](#)

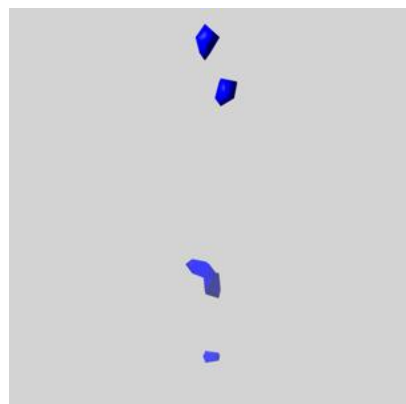
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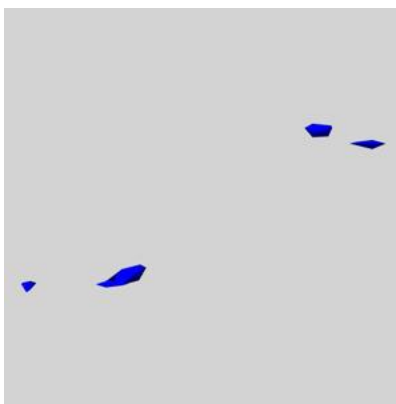
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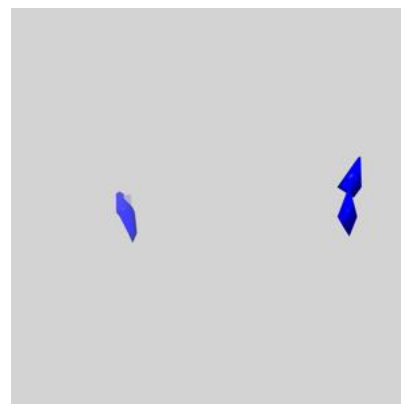
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6.5.25 emd\_1001\_msk\_1.map [i](#)

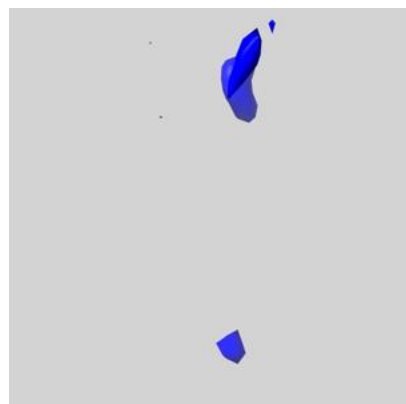
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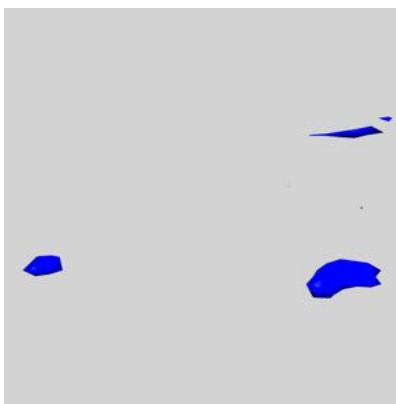
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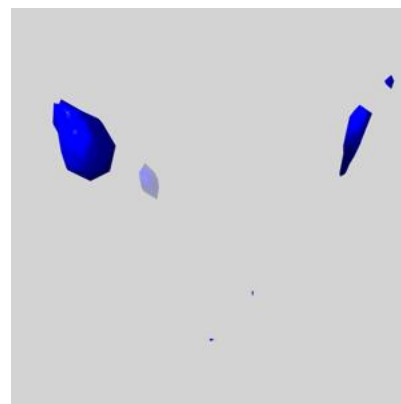
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6.5.26 emd\_1001\_msk\_26.map [i](#)

X



Y

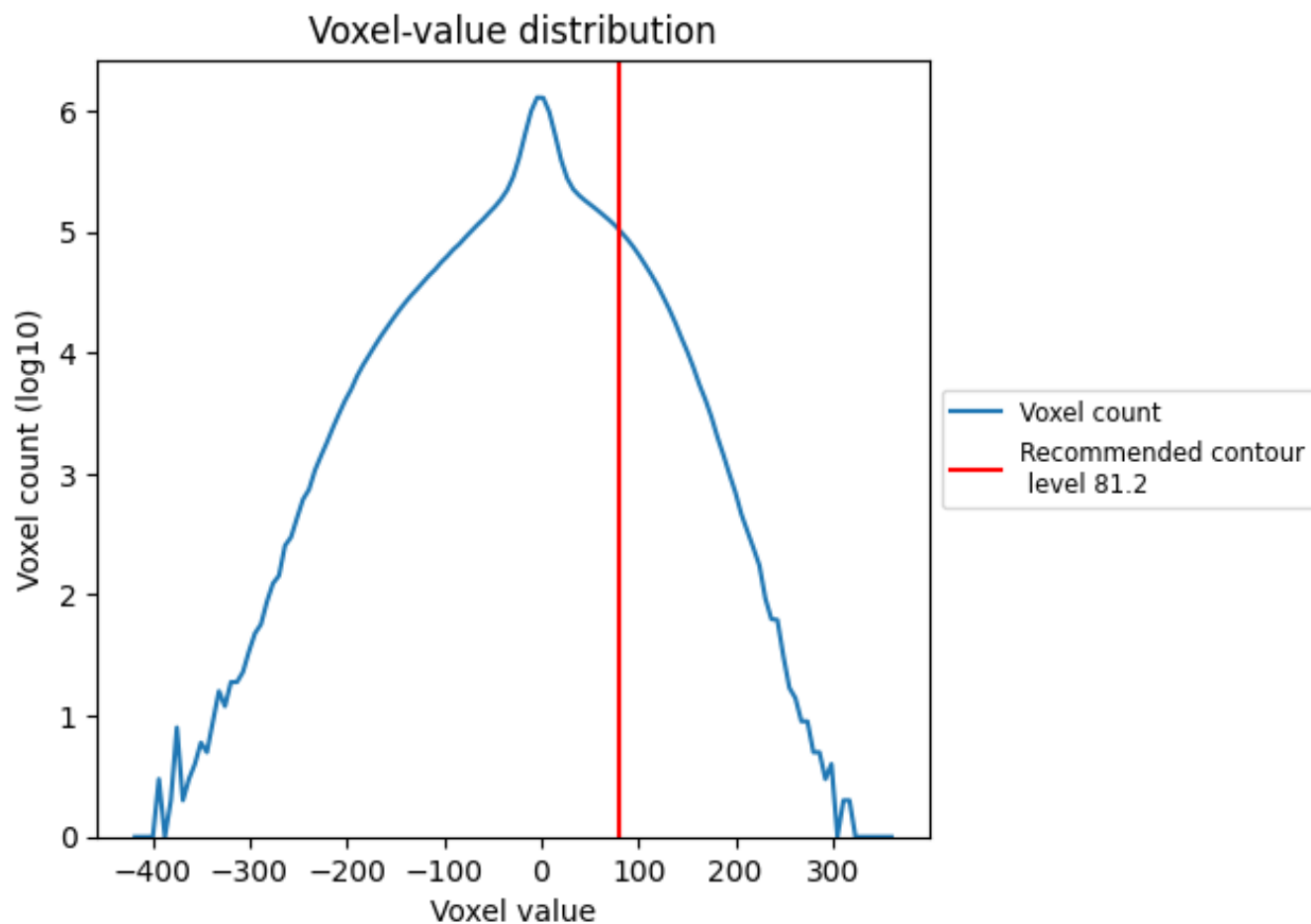


Z

## 7 Tomogram analysis [i](#)

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

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



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

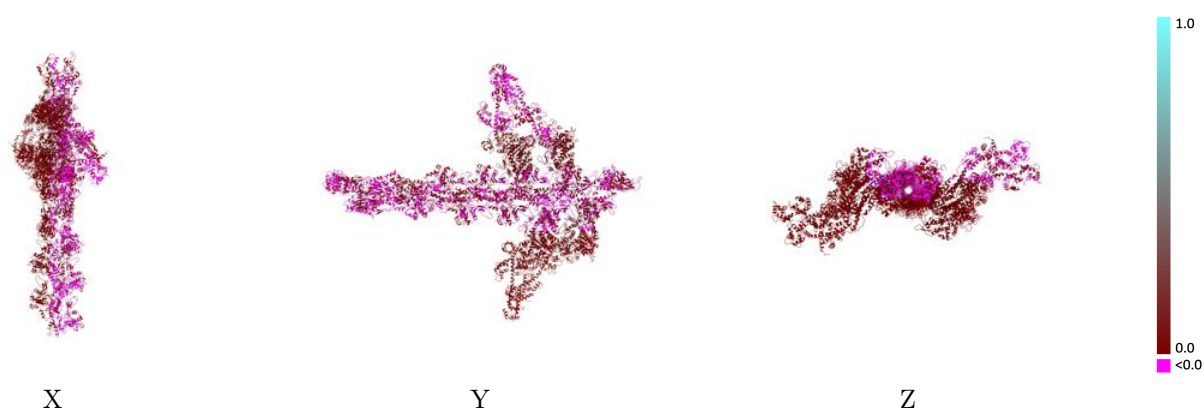
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1B. Per-residue inclusion information can be found in section 3 on page 7.

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

This section was not generated.

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

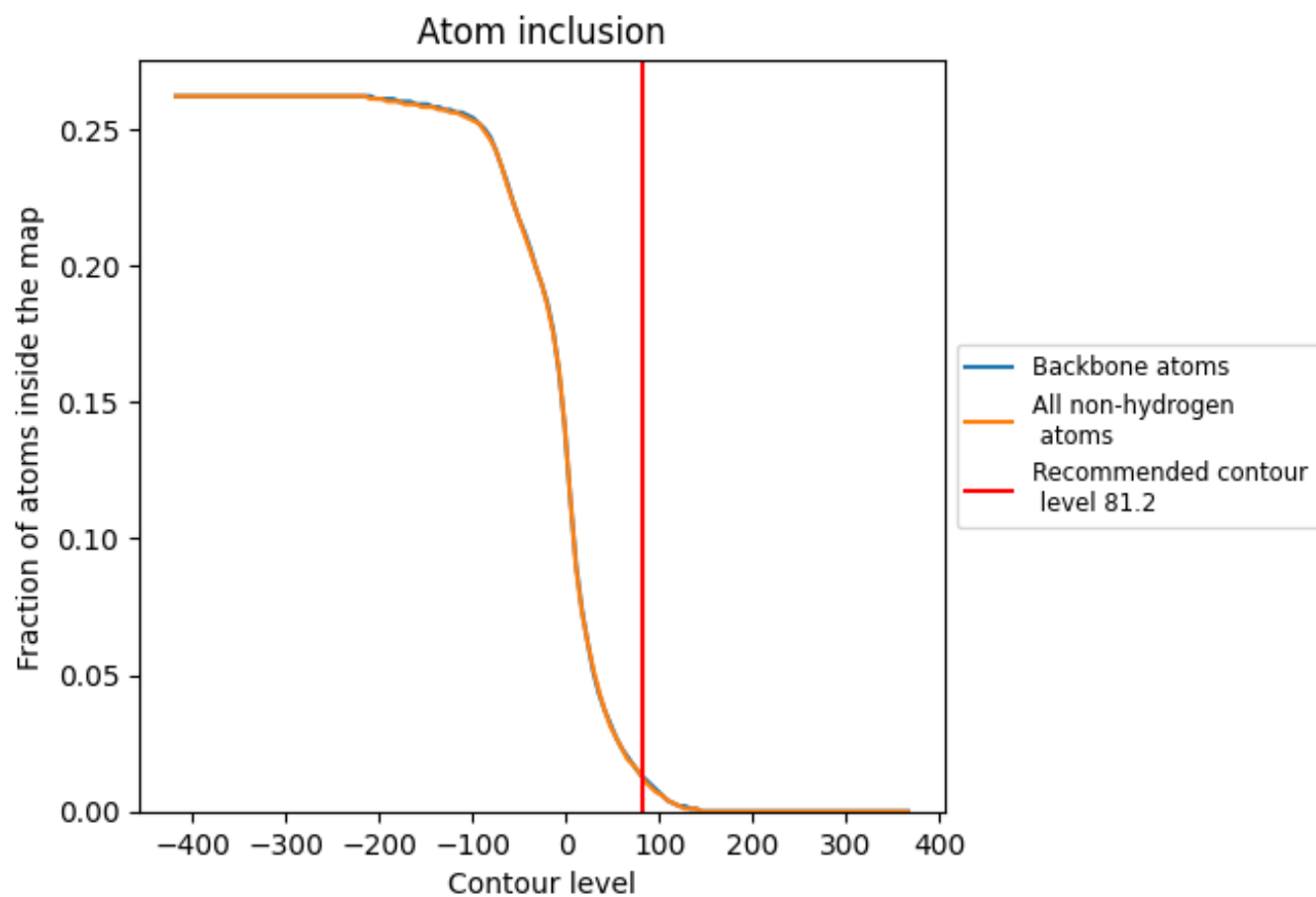


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 1% of all backbone atoms, 1% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| All   |  0.0130   |  -0.0010   |
| 0     |  0.0000   |  -0.0040   |
| 1     |  0.0000   |  -0.0070   |
| 2     |  0.0000   |  -0.0100   |
| 3     |  0.0000   |  -0.0110   |
| 4     |  0.0000   |  -0.0080   |
| 5     |  0.0000   |  0.0020    |
| 7     |  0.0000   |  0.0040    |
| 8     |  0.0000   |  0.0080    |
| 9     |  0.0000   |  0.0100    |
| A     |  0.0000   |  -0.0020   |
| B     |  0.0000   |  0.0000    |
| C     |  0.0000   |  0.0000    |
| D     |  0.0000   |  0.0070    |
| E     |  0.0000  |  -0.0440  |
| F     |  0.2030 |  0.0400  |
| G     |  0.0000 |  -0.0050 |
| H     |  0.0000 |  0.0000  |
| I     |  0.0000 |  0.0000  |
| J     |  0.0090 |  -0.0010 |
| K     |  0.0620 |  0.0150  |
| L     |  0.0780 |  -0.0100 |
| V     |  0.0000 |  -0.0260 |
| W     |  0.0000 |  0.0030  |
| X     |  0.0610 |  0.0140  |
| Y     |  0.0000 |  0.0000  |
| Z     |  0.1200 |  0.0110  |

