



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:50 PM EDT

PDB ID : 3IAS / pdb\_00003ias  
Title : Crystal structure of the hydrophilic domain of respiratory complex I from *Thermus thermophilus*, oxidized, 4 mol/ASU, re-refined to 3.15 angstrom resolution  
Authors : Sazanov, L.A.; Berrisford, J.M.  
Deposited on : 2009-07-14  
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

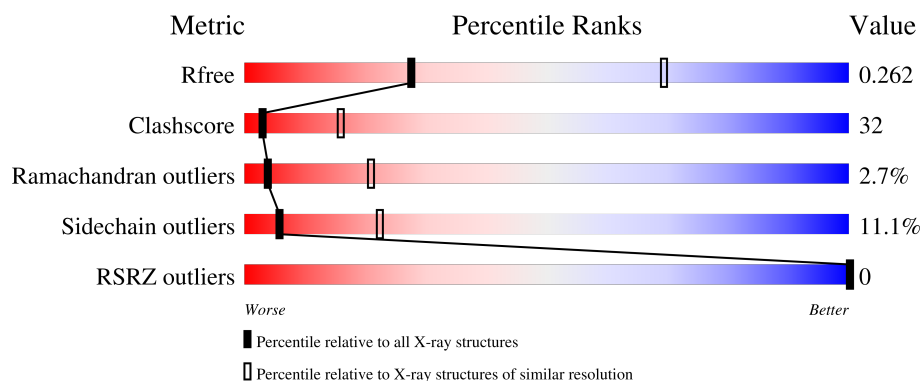
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 Å.

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



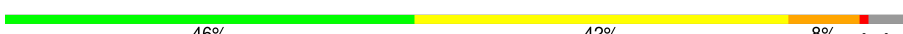
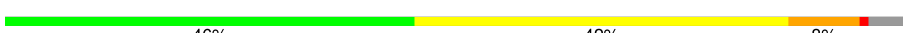
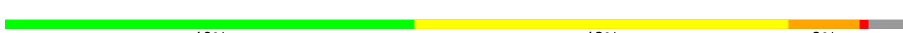
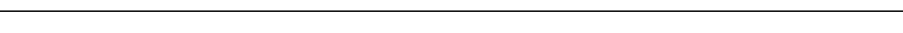
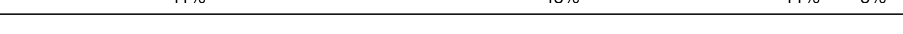
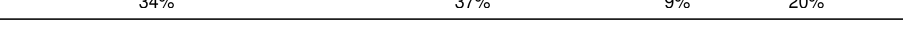
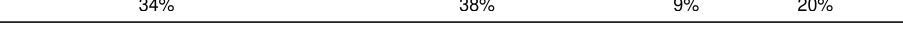
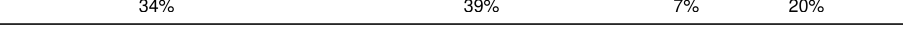
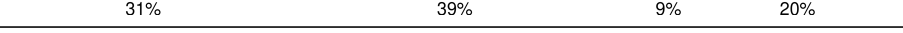
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2361 (3.20-3.12)                                      |
| Clashscore            | 190562                      | 2486 (3.20-3.12)                                      |
| Ramachandran outliers | 187476                      | 2405 (3.20-3.12)                                      |
| Sidechain outliers    | 187428                      | 2404 (3.20-3.12)                                      |
| RSRZ outliers         | 180081                      | 2361 (3.20-3.12)                                      |

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

| Mol | Chain | Length | Quality of chain                                         |
|-----|-------|--------|----------------------------------------------------------|
| 1   | 1     | 438    | <div> <div>49%</div> <div>42%</div> <div>8%</div> </div> |
| 1   | A     | 438    | <div> <div>49%</div> <div>43%</div> <div>8%</div> </div> |
| 1   | J     | 438    | <div> <div>48%</div> <div>43%</div> <div>8%</div> </div> |
| 1   | S     | 438    | <div> <div>49%</div> <div>42%</div> <div>8%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | 2     | 181    |    |
| 2   | B     | 181    |    |
| 2   | K     | 181    |    |
| 2   | T     | 181    |    |
| 3   | 3     | 783    |    |
| 3   | C     | 783    |    |
| 3   | L     | 783    |    |
| 3   | U     | 783    |    |
| 4   | 4     | 409    |    |
| 4   | D     | 409    |    |
| 4   | M     | 409    |    |
| 4   | V     | 409    |    |
| 5   | 5     | 207    |  |
| 5   | E     | 207    |  |
| 5   | N     | 207    |  |
| 5   | W     | 207    |  |
| 6   | 6     | 181    |  |
| 6   | F     | 181    |  |
| 6   | O     | 181    |  |
| 6   | X     | 181    |  |
| 7   | 9     | 182    |  |
| 7   | G     | 182    |  |
| 7   | P     | 182    |  |
| 7   | Y     | 182    |  |
| 8   | 7     | 129    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 8   | H     | 129    |  |
| 8   | Q     | 129    |  |
| 8   | Z     | 129    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 9   | SF4  | 6     | 182 | -         | -        | X       | -                |
| 9   | SF4  | F     | 182 | -         | -        | X       | -                |
| 9   | SF4  | O     | 182 | -         | -        | X       | -                |
| 9   | SF4  | X     | 182 | -         | -        | X       | -                |

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 75028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | 1     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2180 | 595 | 624 | 18 |         |         |       |
| 1   | A     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2180 | 595 | 624 | 18 |         |         |       |
| 1   | J     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2180 | 595 | 624 | 18 |         |         |       |
| 1   | S     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2180 | 595 | 624 | 18 |         |         |       |

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | 2     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 895 | 238 | 265 | 8 |         |         |       |
| 2   | B     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 895 | 238 | 265 | 8 |         |         |       |
| 2   | K     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 895 | 238 | 265 | 8 |         |         |       |
| 2   | T     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 895 | 238 | 265 | 8 |         |         |       |

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | 3     | 754      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 5880  | 3743 | 1055 | 1051 | 31 |         |         |       |
| 3   | C     | 754      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 5880  | 3743 | 1055 | 1051 | 31 |         |         |       |
| 3   | L     | 754      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 5880  | 3743 | 1055 | 1051 | 31 |         |         |       |
| 3   | U     | 754      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 5880  | 3743 | 1055 | 1051 | 31 |         |         |       |

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | 4     | 377      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3011  | 1941 | 510 | 549 | 11 |         |         |       |
| 4   | D     | 377      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3011  | 1941 | 510 | 549 | 11 |         |         |       |
| 4   | M     | 377      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3011  | 1941 | 510 | 549 | 11 |         |         |       |
| 4   | V     | 377      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3011  | 1941 | 510 | 549 | 11 |         |         |       |

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | 5     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1607  | 1043 | 273 | 288 | 3 |         |         |       |
| 5   | E     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1607  | 1043 | 273 | 288 | 3 |         |         |       |
| 5   | N     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1607  | 1043 | 273 | 288 | 3 |         |         |       |
| 5   | W     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1607  | 1043 | 273 | 288 | 3 |         |         |       |

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 6   | 6     | 145      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1113  | 706 | 196 | 198 | 13 |         |         |       |
| 6   | F     | 145      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1113  | 706 | 196 | 198 | 13 |         |         |       |
| 6   | O     | 145      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1113  | 706 | 196 | 198 | 13 |         |         |       |
| 6   | X     | 145      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1113  | 706 | 196 | 198 | 13 |         |         |       |

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | 9     | 154      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1193  | 759 | 201 | 222 | 11 |         |         |       |
| 7   | G     | 154      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1193  | 759 | 201 | 222 | 11 |         |         |       |
| 7   | P     | 154      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1193  | 759 | 201 | 222 | 11 |         |         |       |

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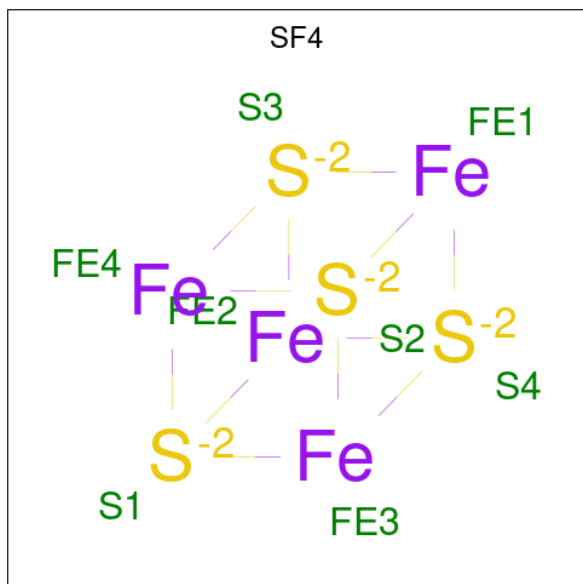
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| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | Y     | 154      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1193  | 759 | 201 | 222 | 11 |         |         |       |

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 7     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1031  | 664 | 183 | 181 | 3 |         |         |       |
| 8   | H     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1031  | 664 | 183 | 181 | 3 |         |         |       |
| 8   | Q     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1031  | 664 | 183 | 181 | 3 |         |         |       |
| 8   | Z     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1031  | 664 | 183 | 181 | 3 |         |         |       |

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | 1     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 3     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 3     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 3     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

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| Mol | Chain | Residues | Atoms      |         |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 9   | 6     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | 9     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | 9     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | A     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | C     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | C     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | C     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | F     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | G     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | G     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | J     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | L     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | L     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | L     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | O     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | P     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | P     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | S     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | U     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | U     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 9   | U     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |

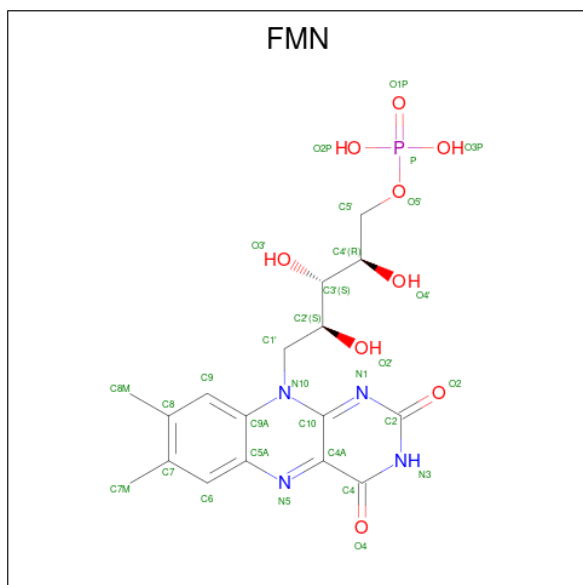
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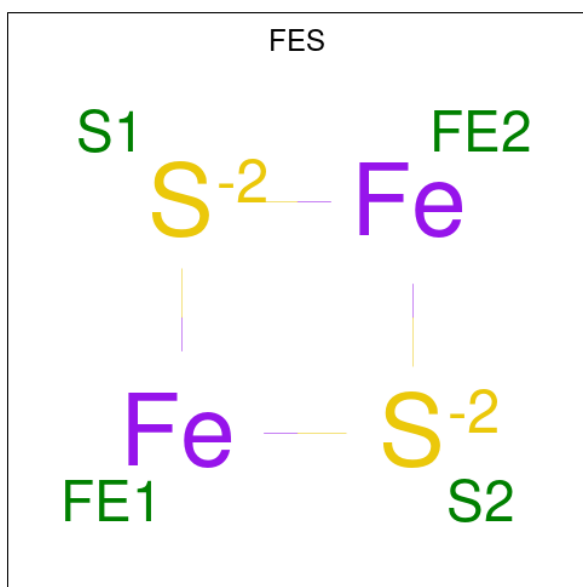
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | X     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | Y     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | Y     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 10  | 1     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |         |
| 10  | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |         |
| 10  | J     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |         |
| 10  | S     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |         |

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11  | 2     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 11  | 3     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 11  | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 11  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 11  | K     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 11  | L     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 11  | T     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 11  | U     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 12  | 2     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 12  | 3     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 12  | 9     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 12  | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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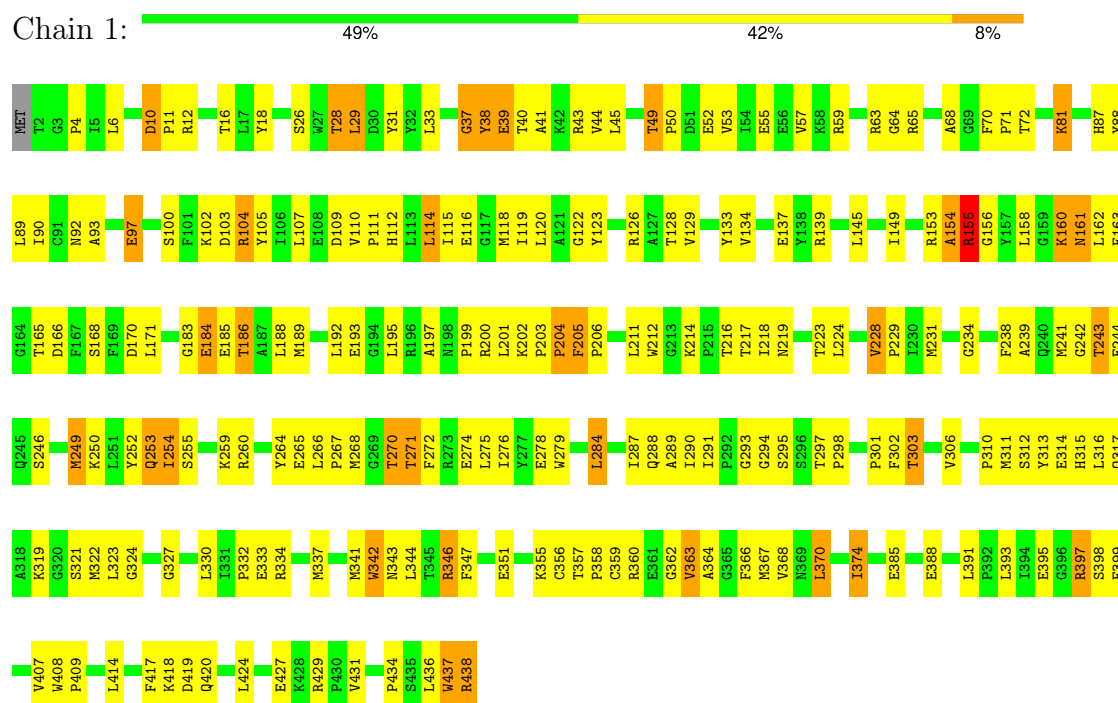
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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 12  | C     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | G     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | H     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | K     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | L     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 12  | P     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | T     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | U     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | Y     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 12  | Z     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

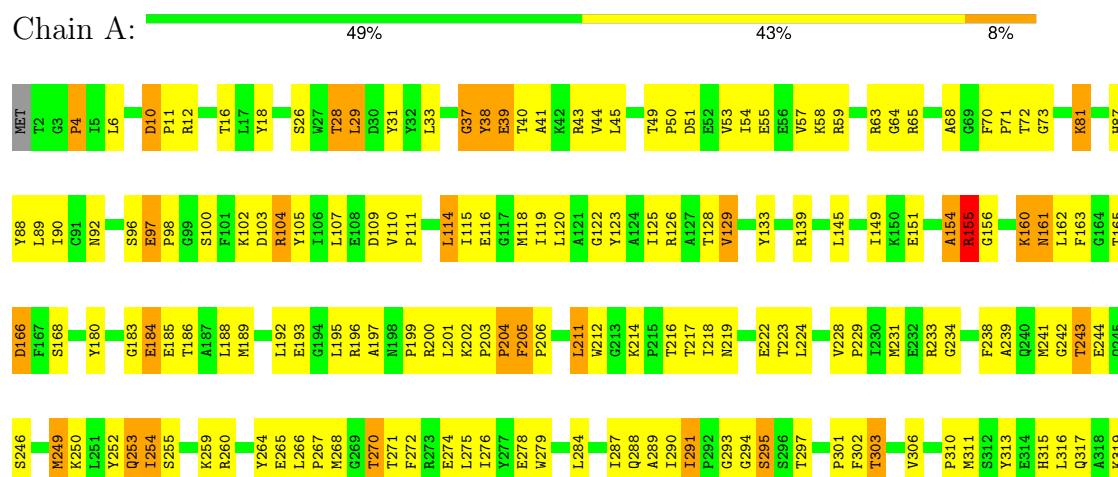
### 3 Residue-property plots

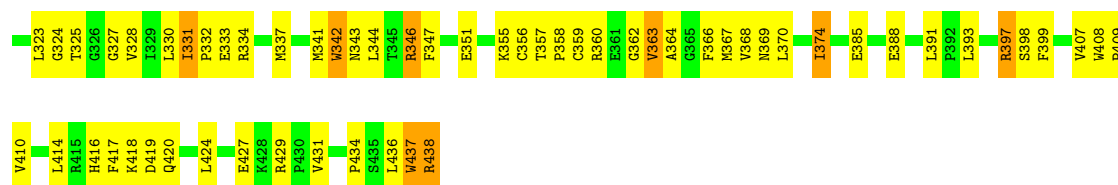
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: NADH-quinone oxidoreductase subunit 1

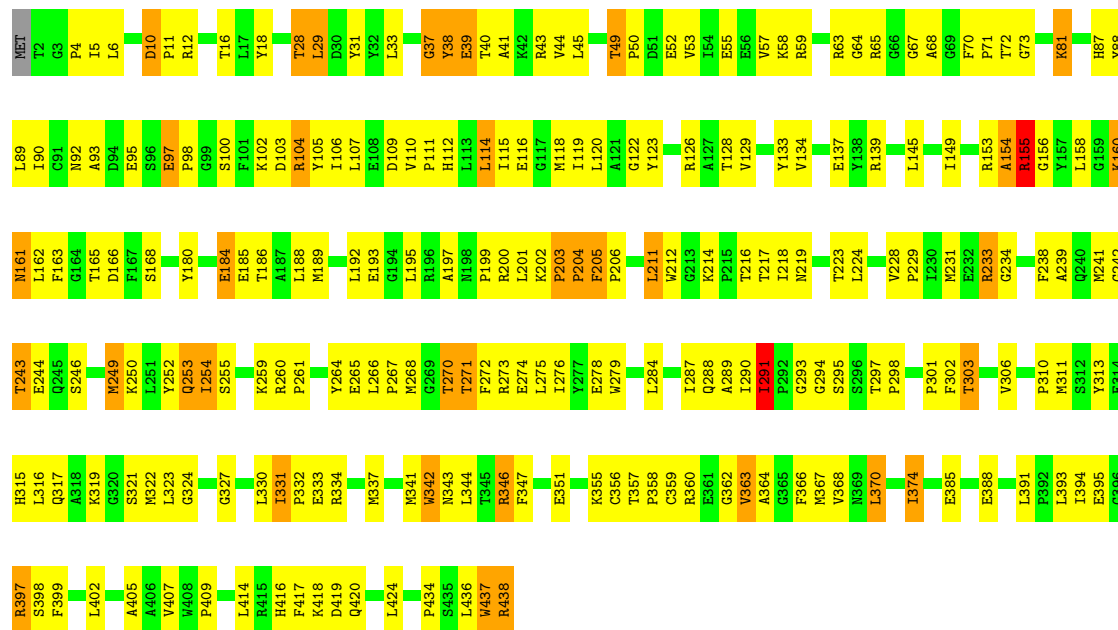


#### • Molecule 1: NADH-quinone oxidoreductase subunit 1

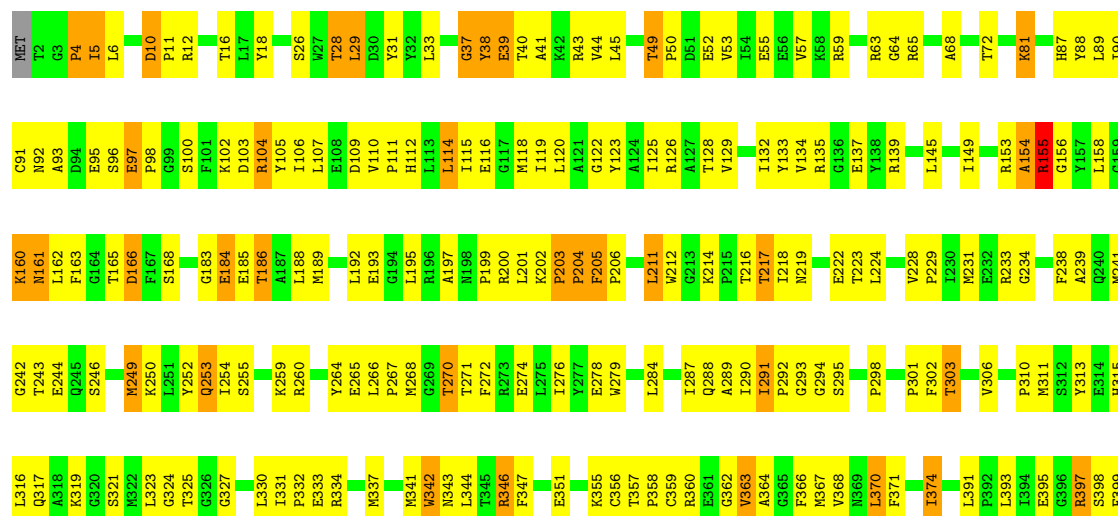




• Molecule 1: NADH-quinone oxidoreductase subunit 1



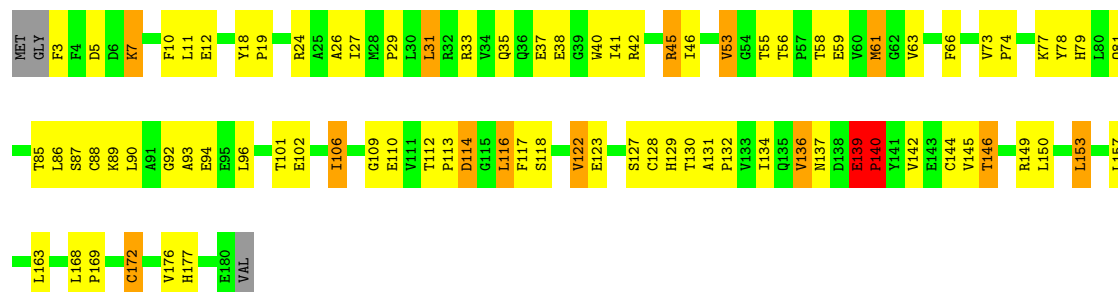
• Molecule 1: NADH-quinone oxidoreductase subunit 1





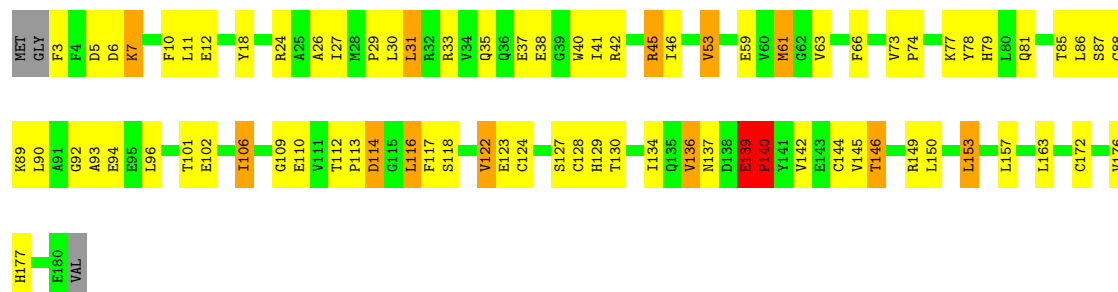
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 52% 38% 7% ..



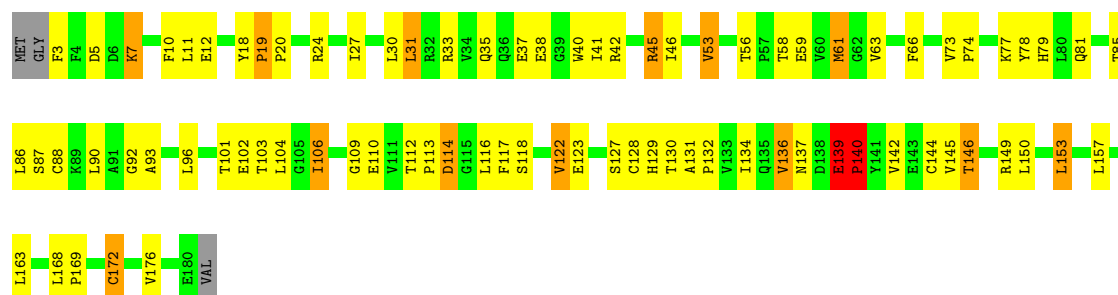
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain B: 55% 36% 7% ..



• Molecule 2: NADH-quinone oxidoreductase subunit 2

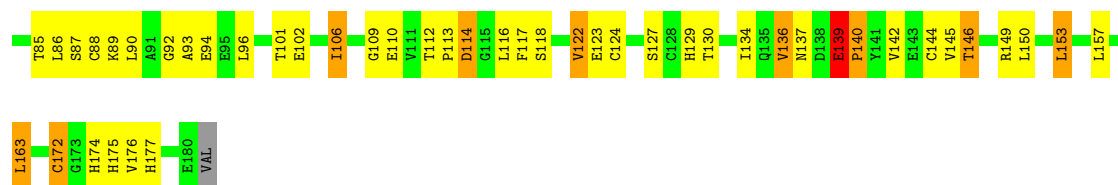
Chain K: 53% 37% 7% ..



• Molecule 2: NADH-quinone oxidoreductase subunit 2

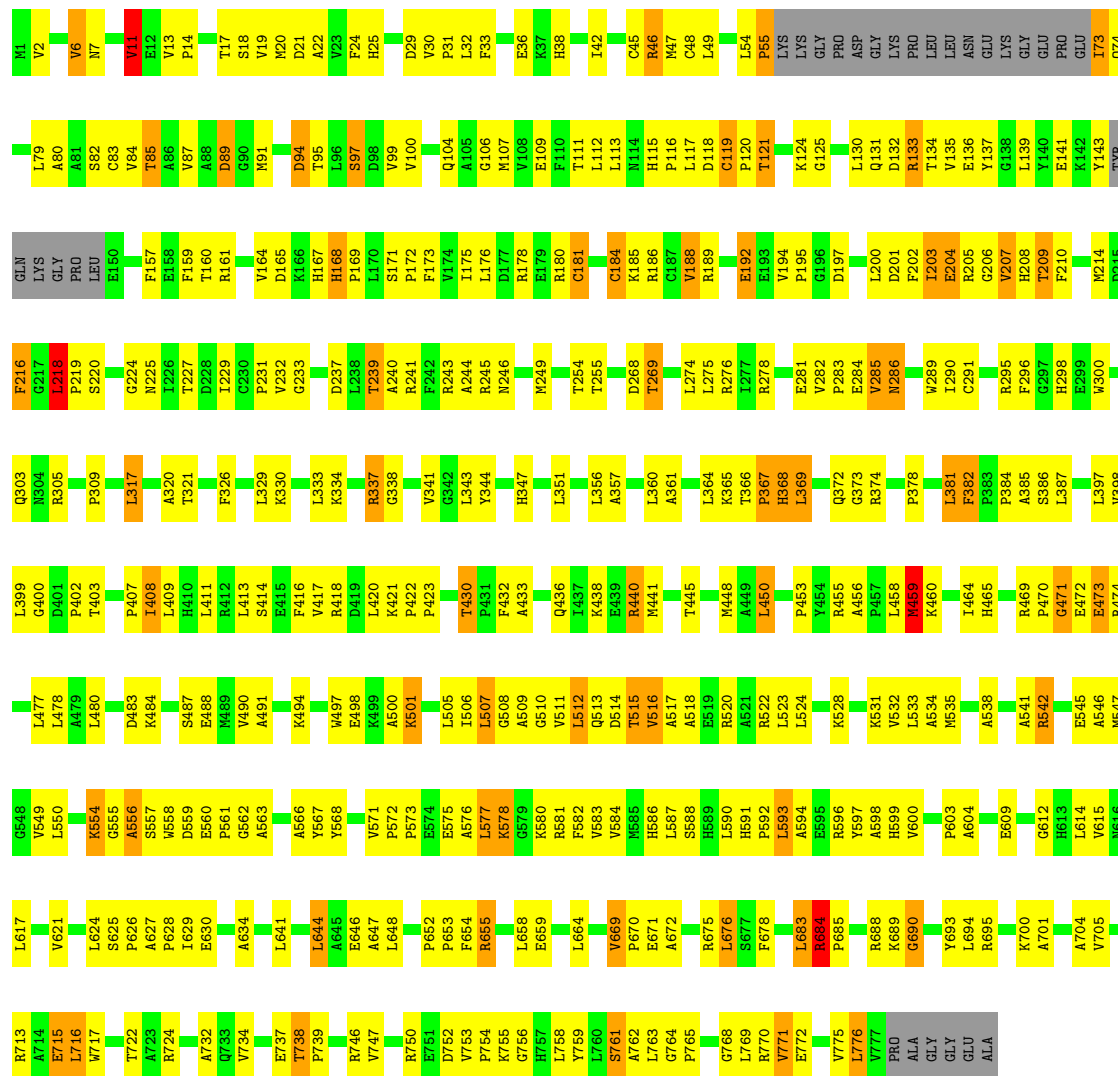
Chain T: 52% 38% 8% ..





• Molecule 3: NADH-quinone oxidoreductase subunit 3

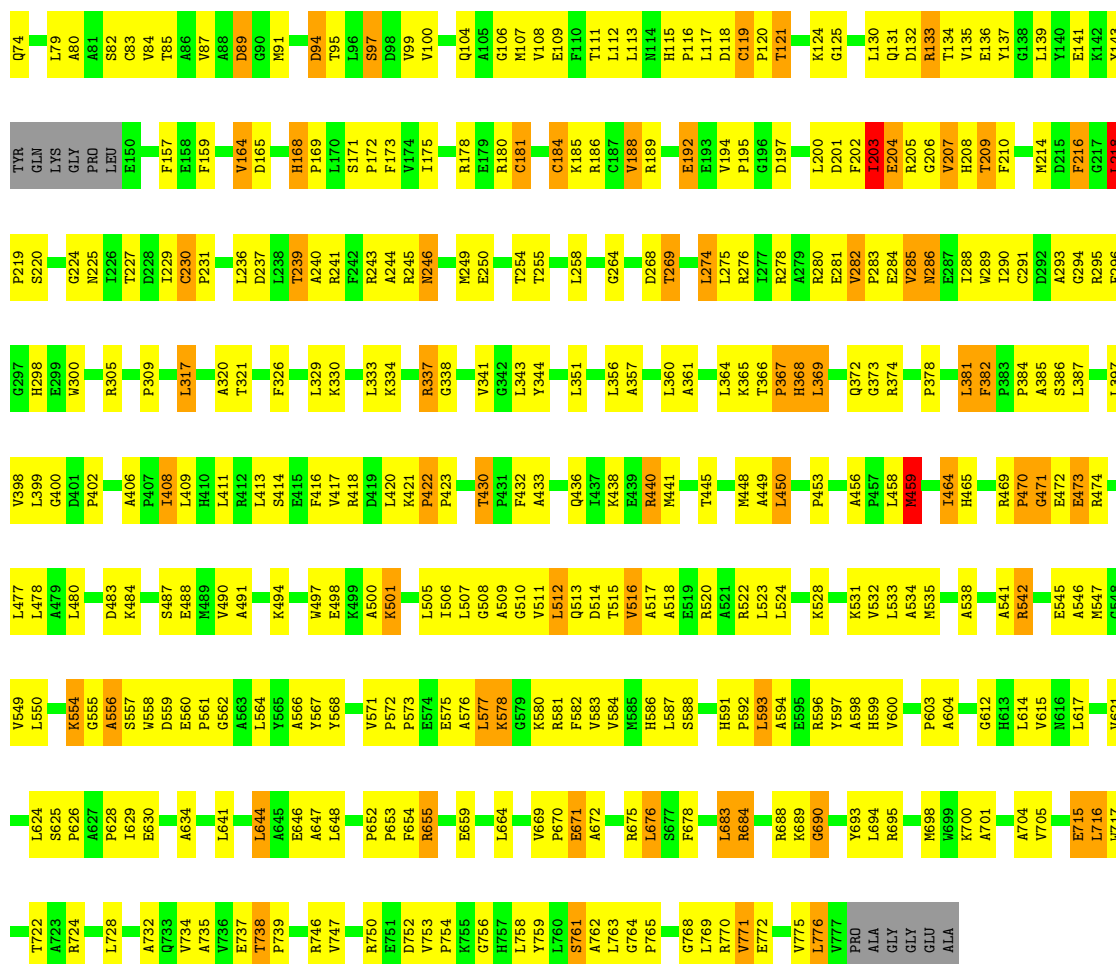
Chain 3: 46% 42% 8% . .



• Molecule 3: NADH-quinone oxidoreductase subunit 3

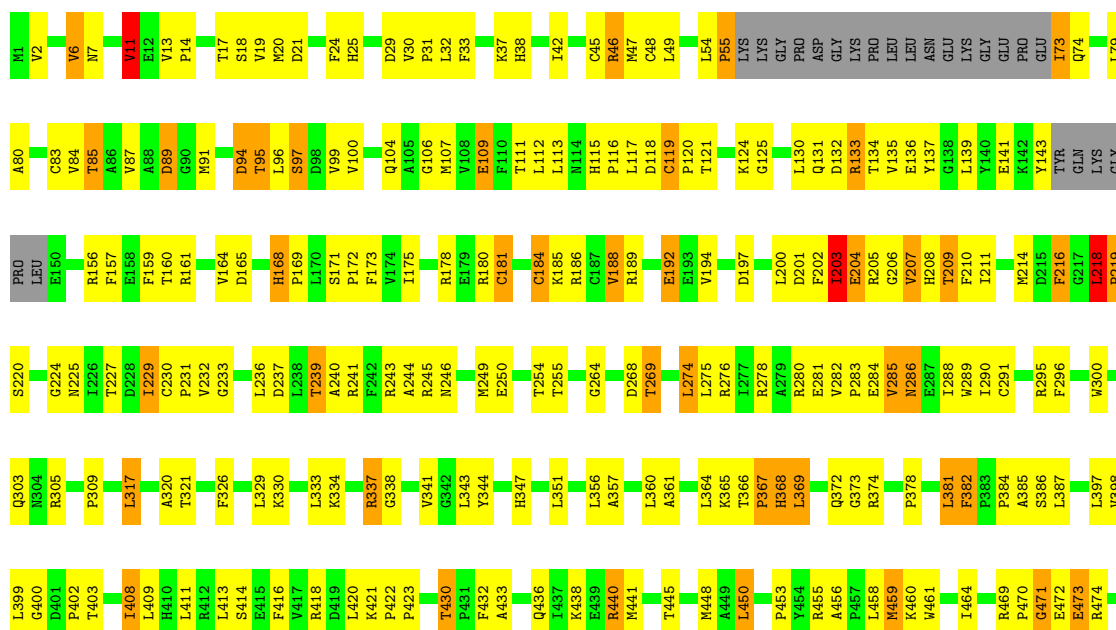
Chain C: 46% 42% 8% . .



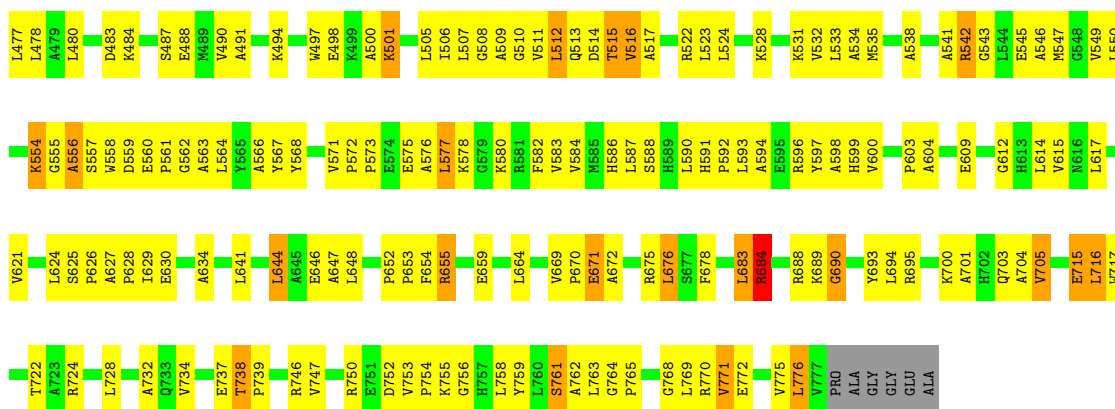


### • Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain L: 46% 42% 8%

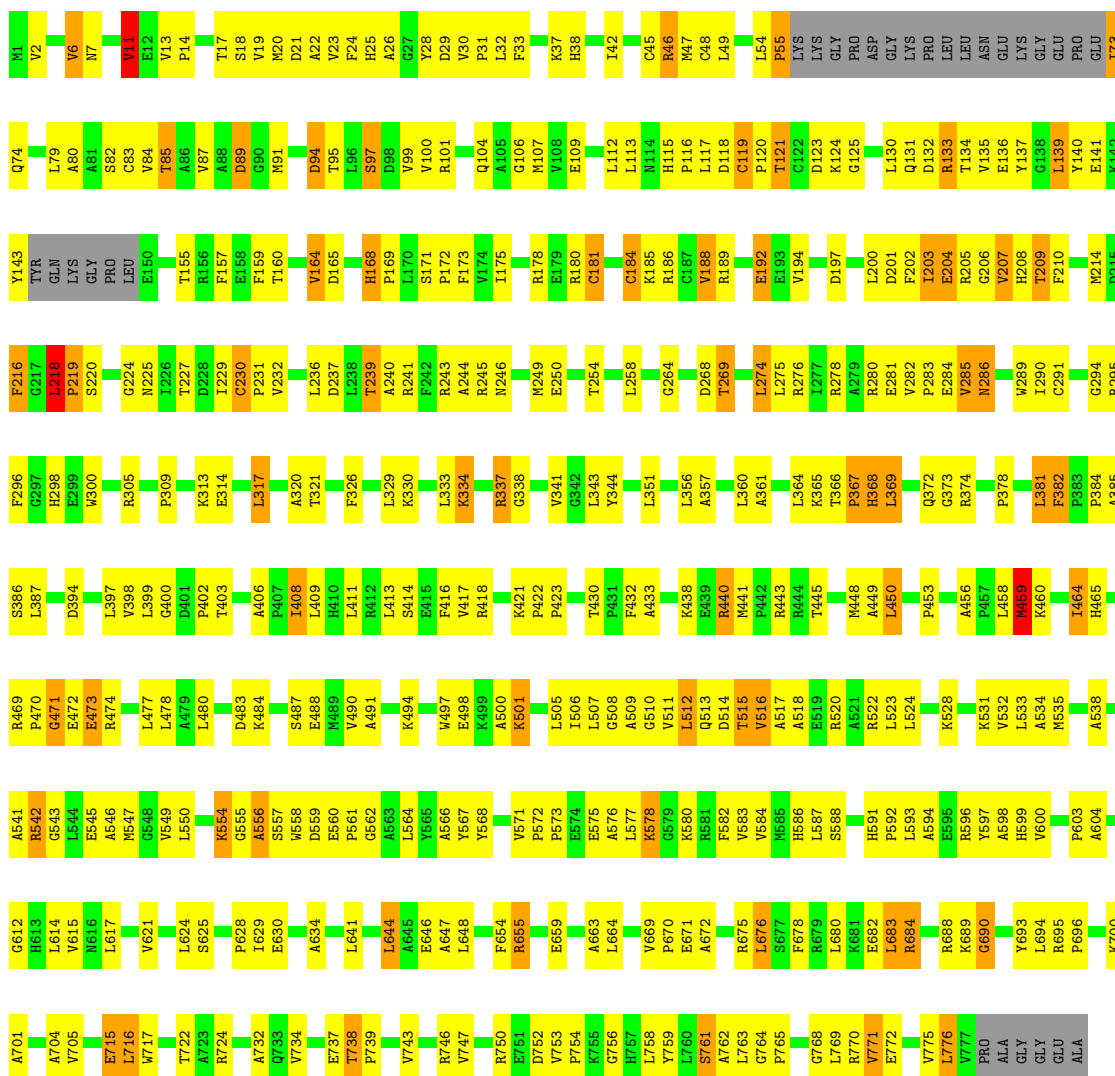




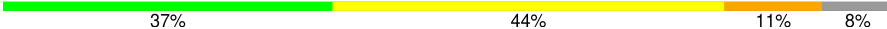


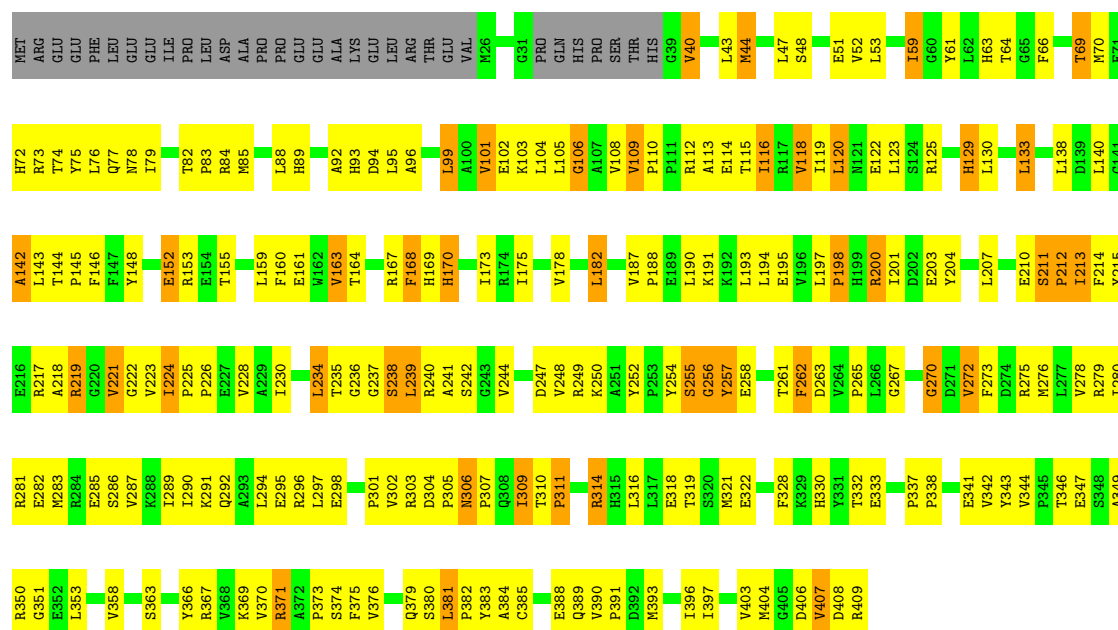
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain U: 45% 42% 8% .



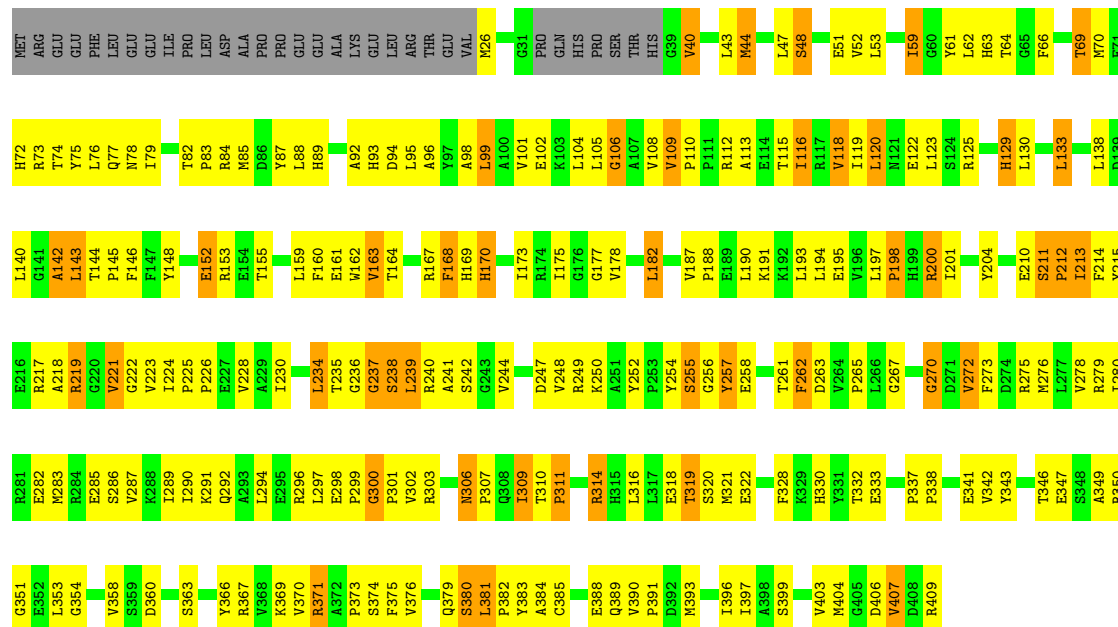
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4: 

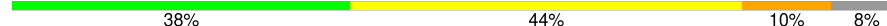


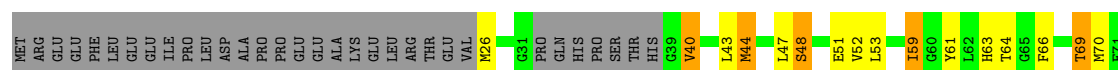
• Molecule 4: NADH-quinone oxidoreductase subunit 4

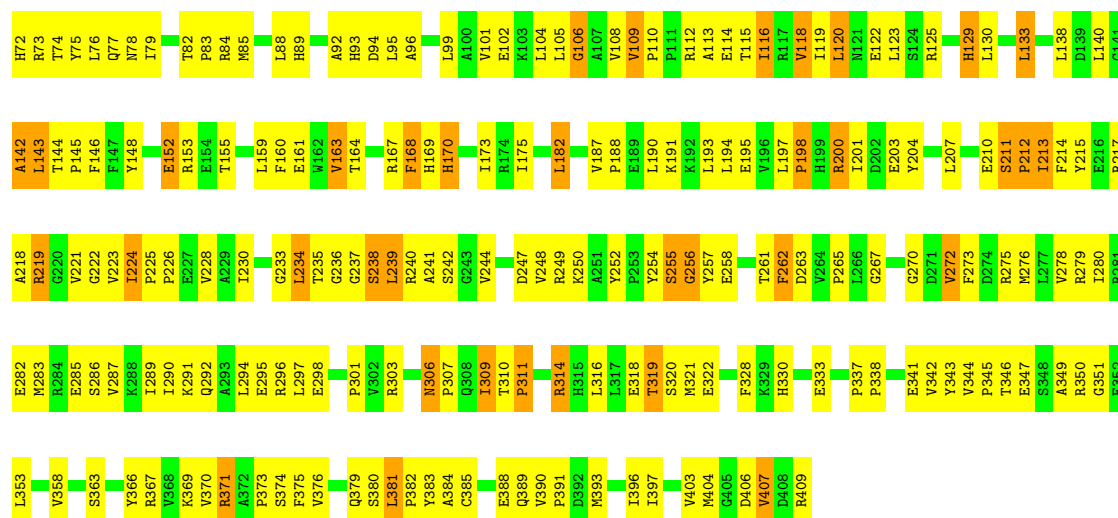
Chain D: 



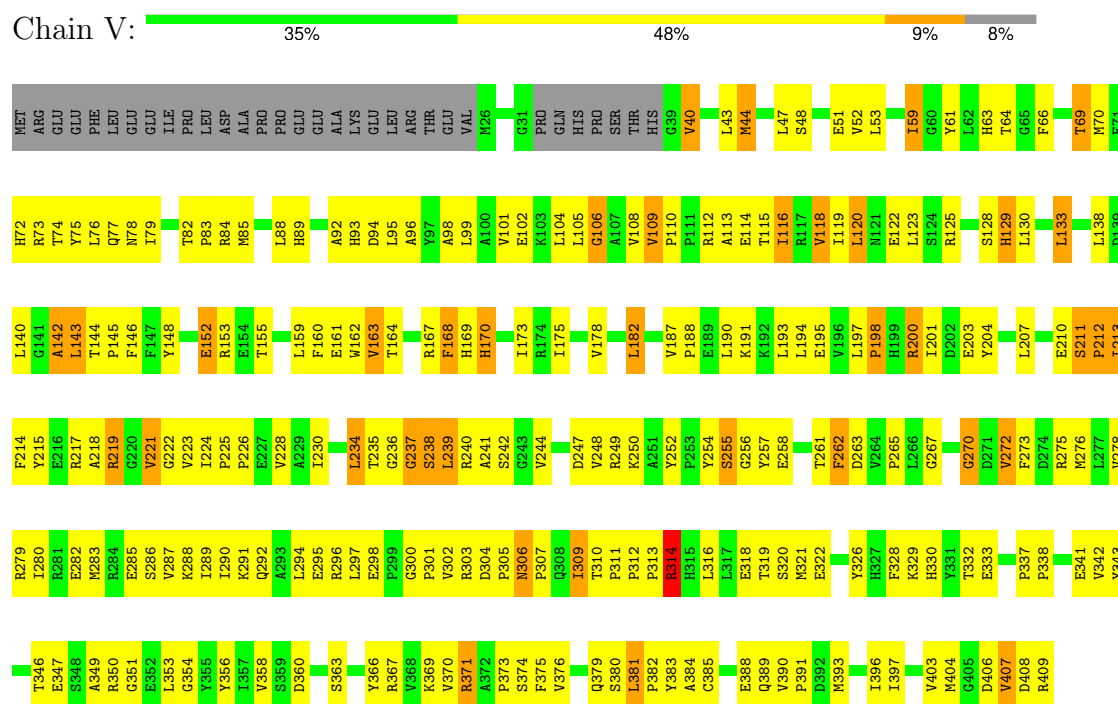
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain M: 

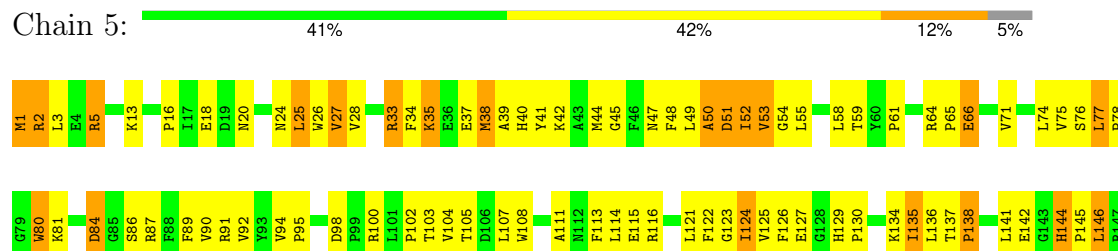


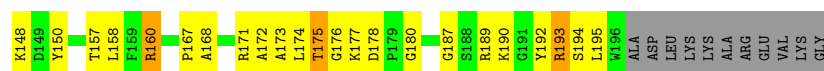


• Molecule 4: NADH-quinone oxidoreductase subunit 4



• Molecule 5: NADH-quinone oxidoreductase subunit 5





• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain E: 40% 43% 12% 5%



• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain N: 41% 43% 11% 5%



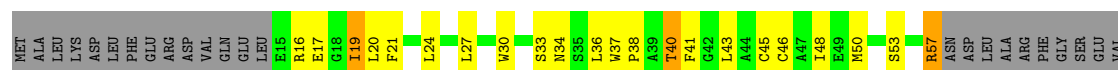
• Molecule 5: NADH-quinone oxidoreductase subunit 5

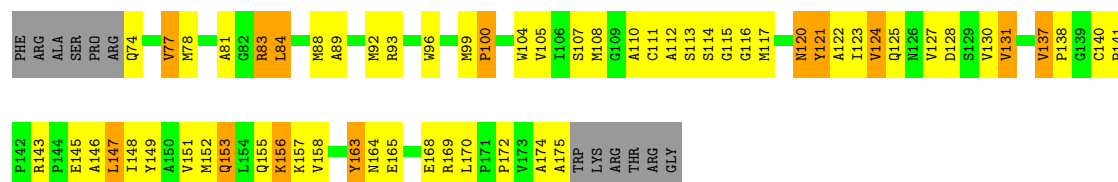
Chain W: 38% 45% 12% 5%



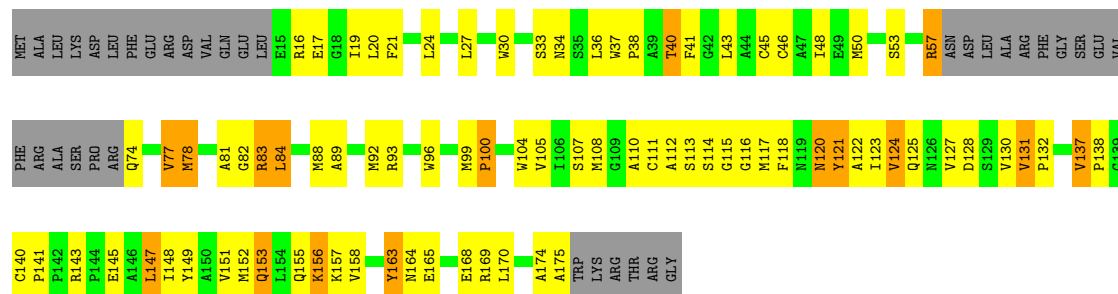
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6: 34% 37% 9% 20%





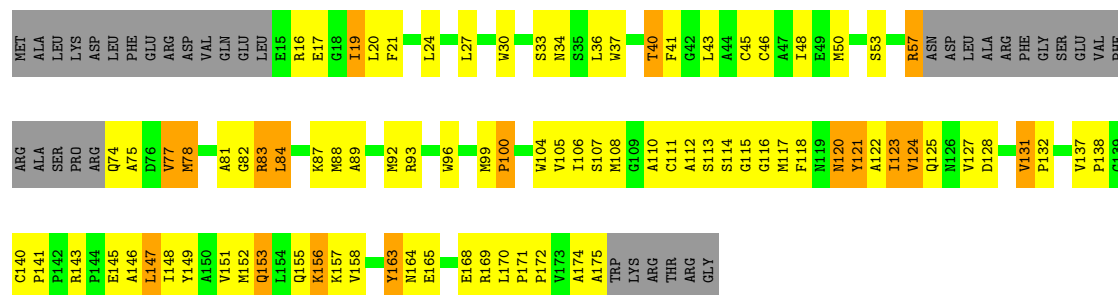
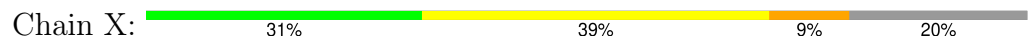
- Molecule 6: NADH-quinone oxidoreductase subunit 6



- Molecule 6: NADH-quinone oxidoreductase subunit 6

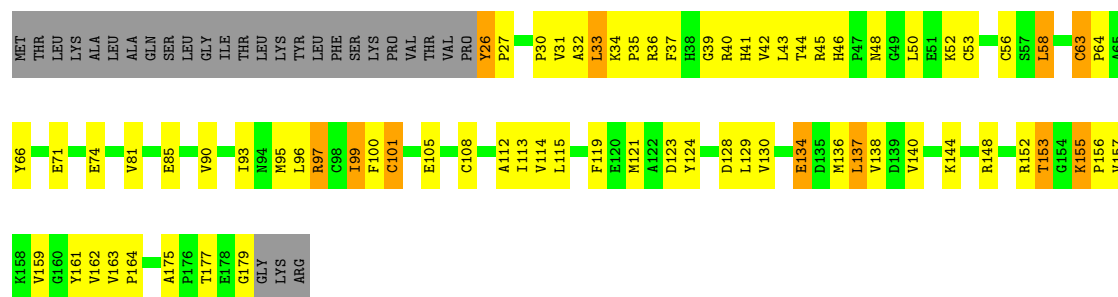


- Molecule 6: NADH-quinone oxidoreductase subunit 6

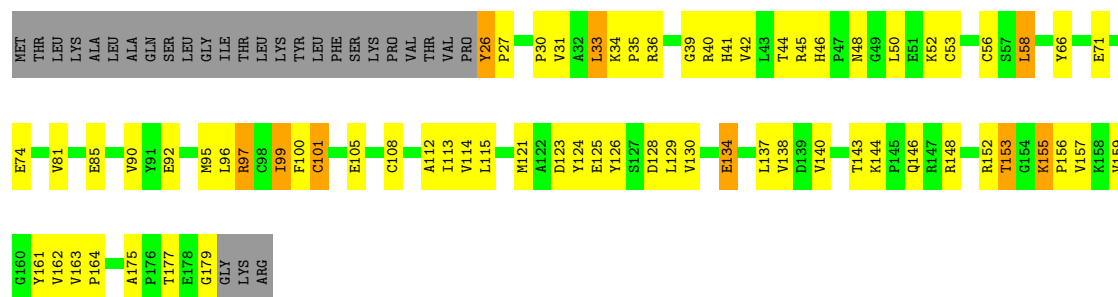


- Molecule 7: NADH-quinone oxidoreductase subunit 9

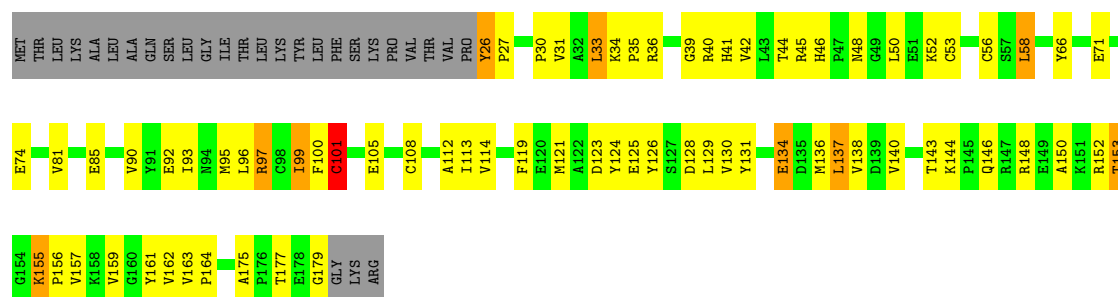




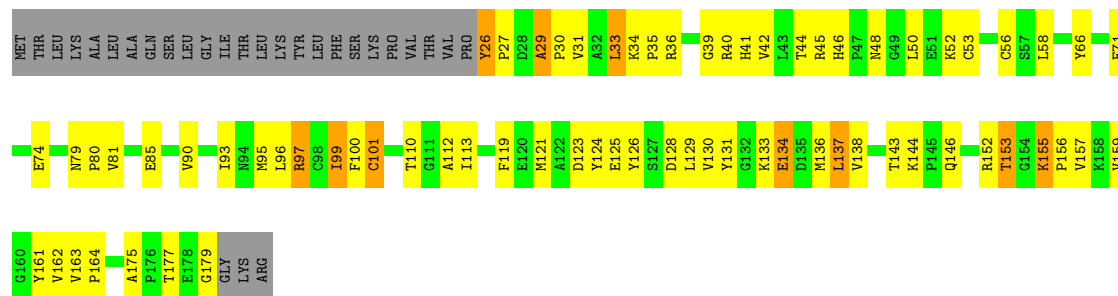
- Molecule 7: NADH-quinone oxidoreductase subunit 9



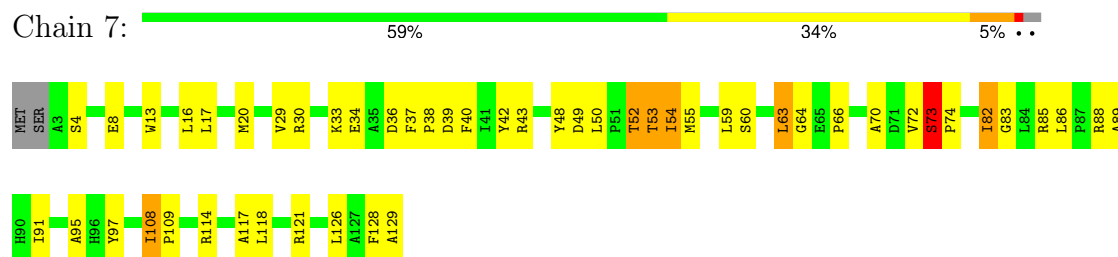
- Molecule 7: NADH-quinone oxidoreductase subunit 9



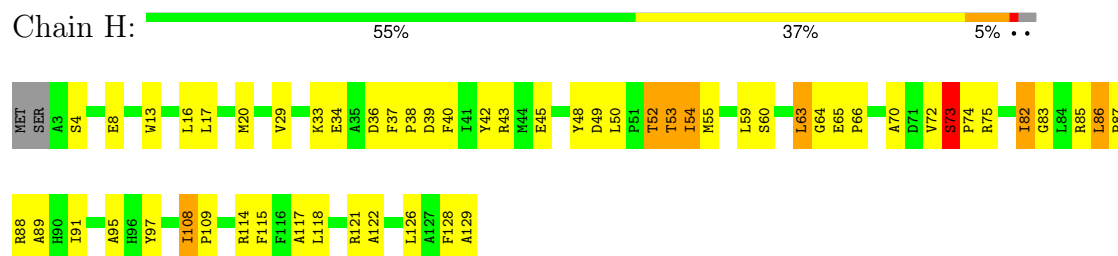
- Molecule 7: NADH-quinone oxidoreductase subunit 9



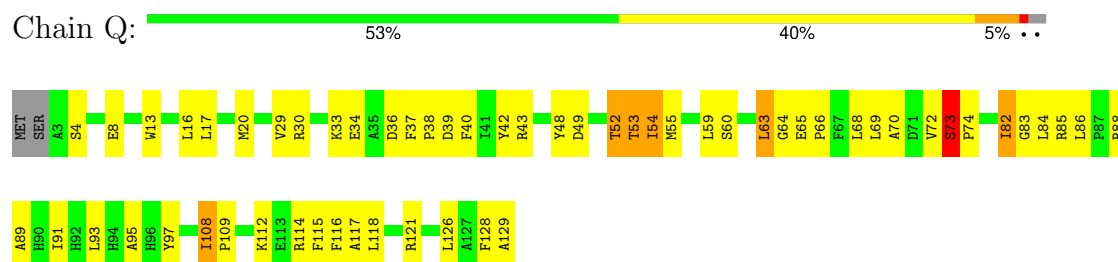
- Molecule 8: NADH-quinone oxidoreductase subunit 15



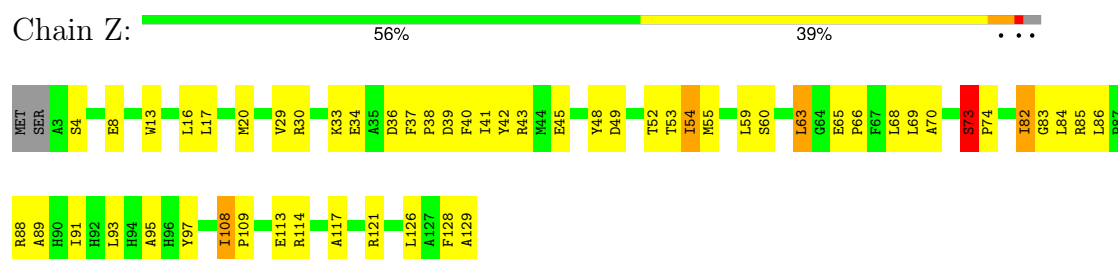
• Molecule 8: NADH-quinone oxidoreductase subunit 15



• Molecule 8: NADH-quinone oxidoreductase subunit 15



• Molecule 8: NADH-quinone oxidoreductase subunit 15



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 135.08Å 266.11Å 201.73Å<br>90.00° 104.71° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 29.98 – 3.15<br>29.98 – 3.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 82.5 (29.98-3.15)<br>82.5 (29.98-3.15)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.18                                                        | Depositor        |
| $R_{sym}$                                                               | 0.18                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.72 (at 3.18Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.237 , 0.270<br>0.232 , 0.262                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4194 reflections (2.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 69.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.027                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 39.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 75028                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 72.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CA, SF4, FMN

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   | 1     | 0.55         | 0/3506      | 0.93        | 6/4745 (0.1%)  |
| 1   | A     | 0.51         | 0/3506      | 0.94        | 8/4745 (0.2%)  |
| 1   | J     | 0.57         | 0/3506      | 0.93        | 9/4745 (0.2%)  |
| 1   | S     | 0.50         | 0/3506      | 0.94        | 6/4745 (0.1%)  |
| 2   | 2     | 0.55         | 0/1439      | 0.97        | 9/1953 (0.5%)  |
| 2   | B     | 0.49         | 0/1439      | 0.95        | 6/1953 (0.3%)  |
| 2   | K     | 0.55         | 0/1439      | 0.95        | 11/1953 (0.6%) |
| 2   | T     | 0.52         | 0/1439      | 0.95        | 9/1953 (0.5%)  |
| 3   | 3     | 0.54         | 0/6019      | 0.98        | 24/8163 (0.3%) |
| 3   | C     | 0.51         | 0/6019      | 0.98        | 27/8163 (0.3%) |
| 3   | L     | 0.50         | 0/6019      | 0.97        | 21/8163 (0.3%) |
| 3   | U     | 0.51         | 0/6019      | 0.97        | 22/8163 (0.3%) |
| 4   | 4     | 0.52         | 0/3089      | 0.94        | 12/4197 (0.3%) |
| 4   | D     | 0.52         | 0/3089      | 0.94        | 9/4197 (0.2%)  |
| 4   | M     | 0.56         | 0/3089      | 0.95        | 11/4197 (0.3%) |
| 4   | V     | 0.50         | 0/3089      | 0.94        | 8/4197 (0.2%)  |
| 5   | 5     | 0.50         | 0/1656      | 1.00        | 11/2246 (0.5%) |
| 5   | E     | 0.48         | 0/1656      | 1.03        | 12/2246 (0.5%) |
| 5   | N     | 0.51         | 0/1656      | 1.03        | 13/2246 (0.6%) |
| 5   | W     | 0.46         | 0/1656      | 1.01        | 13/2246 (0.6%) |
| 6   | 6     | 0.57         | 0/1137      | 1.01        | 5/1542 (0.3%)  |
| 6   | F     | 0.59         | 0/1137      | 1.01        | 5/1542 (0.3%)  |
| 6   | O     | 0.55         | 0/1137      | 0.99        | 3/1542 (0.2%)  |
| 6   | X     | 0.53         | 0/1137      | 0.99        | 3/1542 (0.2%)  |
| 7   | 9     | 0.57         | 0/1224      | 0.96        | 4/1663 (0.2%)  |
| 7   | G     | 0.57         | 0/1224      | 0.97        | 2/1663 (0.1%)  |
| 7   | P     | 0.55         | 0/1224      | 0.97        | 3/1663 (0.2%)  |
| 7   | Y     | 0.52         | 0/1224      | 0.97        | 4/1663 (0.2%)  |
| 8   | 7     | 0.51         | 0/1059      | 0.97        | 5/1429 (0.3%)  |
| 8   | H     | 0.50         | 0/1059      | 0.96        | 7/1429 (0.5%)  |
| 8   | Q     | 0.51         | 0/1059      | 0.96        | 5/1429 (0.3%)  |
| 8   | Z     | 0.48         | 0/1059      | 0.94        | 6/1429 (0.4%)  |

| Mol | Chain | Bond lengths |         | Bond angles |                   |
|-----|-------|--------------|---------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5           |
| All | All   | 0.52         | 0/76516 | 0.96        | 299/103752 (0.3%) |

There are no bond length outliers.

All (299) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | U     | 184 | CYS  | N-CA-C | -10.00 | 98.11       | 110.41   |
| 3   | 3     | 184 | CYS  | N-CA-C | -9.44  | 98.80       | 110.41   |
| 3   | L     | 184 | CYS  | N-CA-C | -9.39  | 98.86       | 110.41   |
| 3   | C     | 430 | THR  | CA-C-N | 9.35   | 129.11      | 119.76   |
| 3   | C     | 430 | THR  | C-N-CA | 9.35   | 129.11      | 119.76   |
| 3   | 3     | 430 | THR  | CA-C-N | 9.35   | 129.11      | 119.76   |
| 3   | 3     | 430 | THR  | C-N-CA | 9.35   | 129.11      | 119.76   |
| 3   | 3     | 216 | PHE  | N-CA-C | 9.23   | 121.34      | 111.28   |
| 3   | C     | 184 | CYS  | N-CA-C | -9.22  | 99.07       | 110.41   |
| 3   | L     | 430 | THR  | CA-C-N | 9.12   | 128.88      | 119.76   |
| 3   | L     | 430 | THR  | C-N-CA | 9.12   | 128.88      | 119.76   |
| 3   | L     | 14  | PRO  | CA-C-N | 8.98   | 128.31      | 118.97   |
| 3   | L     | 14  | PRO  | C-N-CA | 8.98   | 128.31      | 118.97   |
| 3   | C     | 14  | PRO  | CA-C-N | 8.96   | 128.29      | 118.97   |
| 3   | C     | 14  | PRO  | C-N-CA | 8.96   | 128.29      | 118.97   |
| 3   | 3     | 14  | PRO  | CA-C-N | 8.94   | 128.27      | 118.97   |
| 3   | 3     | 14  | PRO  | C-N-CA | 8.94   | 128.27      | 118.97   |
| 3   | U     | 430 | THR  | CA-C-N | 8.91   | 128.67      | 119.76   |
| 3   | U     | 430 | THR  | C-N-CA | 8.91   | 128.67      | 119.76   |
| 3   | U     | 216 | PHE  | N-CA-C | 8.72   | 120.78      | 111.28   |
| 3   | L     | 216 | PHE  | N-CA-C | 8.60   | 120.65      | 111.28   |
| 3   | C     | 216 | PHE  | N-CA-C | 8.58   | 120.63      | 111.28   |
| 5   | N     | 190 | LYS  | N-CA-C | -8.33  | 102.14      | 113.30   |
| 3   | U     | 14  | PRO  | CA-C-N | 8.26   | 127.56      | 118.97   |
| 3   | U     | 14  | PRO  | C-N-CA | 8.26   | 127.56      | 118.97   |
| 3   | U     | 168 | HIS  | CA-C-N | 8.25   | 128.74      | 119.83   |
| 3   | U     | 168 | HIS  | C-N-CA | 8.25   | 128.74      | 119.83   |
| 3   | L     | 168 | HIS  | CA-C-N | 8.19   | 128.67      | 119.83   |
| 3   | L     | 168 | HIS  | C-N-CA | 8.19   | 128.67      | 119.83   |
| 5   | E     | 190 | LYS  | N-CA-C | -8.05  | 102.51      | 113.30   |
| 5   | W     | 77  | LEU  | CA-C-N | 7.98   | 128.17      | 119.87   |
| 5   | W     | 77  | LEU  | C-N-CA | 7.98   | 128.17      | 119.87   |
| 5   | N     | 144 | HIS  | CA-C-N | 7.96   | 127.24      | 118.97   |
| 5   | N     | 144 | HIS  | C-N-CA | 7.96   | 127.24      | 118.97   |
| 2   | 2     | 139 | GLU  | CA-C-N | 7.88   | 129.68      | 119.84   |
| 2   | 2     | 139 | GLU  | C-N-CA | 7.88   | 129.68      | 119.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | 5     | 190 | LYS  | N-CA-C  | -7.81 | 102.83      | 113.30   |
| 3   | L     | 55  | PRO  | CB-CA-C | -7.64 | 95.58       | 110.10   |
| 4   | M     | 306 | ASN  | CA-C-N  | 7.50  | 127.54      | 119.28   |
| 4   | M     | 306 | ASN  | C-N-CA  | 7.50  | 127.54      | 119.28   |
| 4   | M     | 309 | ILE  | CB-CA-C | -7.46 | 102.56      | 110.62   |
| 4   | M     | 238 | SER  | N-CA-C  | -7.43 | 103.34      | 113.30   |
| 5   | 5     | 144 | HIS  | CA-C-N  | 7.34  | 126.61      | 118.97   |
| 5   | 5     | 144 | HIS  | C-N-CA  | 7.34  | 126.61      | 118.97   |
| 4   | D     | 306 | ASN  | CA-C-N  | 7.34  | 127.36      | 119.28   |
| 4   | D     | 306 | ASN  | C-N-CA  | 7.34  | 127.36      | 119.28   |
| 2   | K     | 139 | GLU  | CA-C-N  | 7.33  | 129.00      | 119.84   |
| 2   | K     | 139 | GLU  | C-N-CA  | 7.33  | 129.00      | 119.84   |
| 5   | N     | 77  | LEU  | CA-C-N  | 7.32  | 127.95      | 120.04   |
| 5   | N     | 77  | LEU  | C-N-CA  | 7.32  | 127.95      | 120.04   |
| 3   | C     | 55  | PRO  | CB-CA-C | -7.29 | 96.24       | 110.10   |
| 5   | E     | 144 | HIS  | CA-C-N  | 7.29  | 126.55      | 118.97   |
| 5   | E     | 144 | HIS  | C-N-CA  | 7.29  | 126.55      | 118.97   |
| 3   | U     | 55  | PRO  | CB-CA-C | -7.27 | 96.28       | 110.10   |
| 3   | 3     | 55  | PRO  | CB-CA-C | -7.27 | 96.28       | 110.10   |
| 2   | T     | 139 | GLU  | CA-C-N  | 7.26  | 128.92      | 119.84   |
| 2   | T     | 139 | GLU  | C-N-CA  | 7.26  | 128.92      | 119.84   |
| 5   | N     | 94  | VAL  | CA-C-N  | 7.26  | 128.91      | 119.84   |
| 5   | N     | 94  | VAL  | C-N-CA  | 7.26  | 128.91      | 119.84   |
| 4   | V     | 238 | SER  | N-CA-C  | -7.23 | 104.06      | 113.17   |
| 3   | 3     | 168 | HIS  | CA-C-N  | 7.19  | 128.32      | 119.98   |
| 3   | 3     | 168 | HIS  | C-N-CA  | 7.19  | 128.32      | 119.98   |
| 5   | E     | 77  | LEU  | CA-C-N  | 7.19  | 127.80      | 120.04   |
| 5   | E     | 77  | LEU  | C-N-CA  | 7.19  | 127.80      | 120.04   |
| 5   | W     | 190 | LYS  | N-CA-C  | -7.17 | 103.69      | 113.30   |
| 4   | 4     | 306 | ASN  | CA-C-N  | 7.16  | 127.16      | 119.28   |
| 4   | 4     | 306 | ASN  | C-N-CA  | 7.16  | 127.16      | 119.28   |
| 8   | 7     | 4   | SER  | N-CA-C  | -7.15 | 104.17      | 113.17   |
| 3   | C     | 168 | HIS  | CA-C-N  | 7.12  | 127.52      | 119.83   |
| 3   | C     | 168 | HIS  | C-N-CA  | 7.12  | 127.52      | 119.83   |
| 2   | B     | 139 | GLU  | CA-C-N  | 7.10  | 128.72      | 119.84   |
| 2   | B     | 139 | GLU  | C-N-CA  | 7.10  | 128.72      | 119.84   |
| 4   | 4     | 238 | SER  | N-CA-C  | -7.07 | 104.26      | 113.17   |
| 8   | Q     | 4   | SER  | N-CA-C  | -6.98 | 104.38      | 113.17   |
| 5   | 5     | 77  | LEU  | CA-C-N  | 6.90  | 127.50      | 120.04   |
| 5   | 5     | 77  | LEU  | C-N-CA  | 6.90  | 127.50      | 120.04   |
| 1   | 1     | 97  | GLU  | CA-C-N  | 6.89  | 127.30      | 119.93   |
| 1   | 1     | 97  | GLU  | C-N-CA  | 6.89  | 127.30      | 119.93   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 291 | ILE  | CA-C-N  | 6.84  | 128.39      | 119.84   |
| 1   | A     | 291 | ILE  | C-N-CA  | 6.84  | 128.39      | 119.84   |
| 4   | D     | 238 | SER  | N-CA-C  | -6.82 | 104.58      | 113.17   |
| 4   | V     | 306 | ASN  | CA-C-N  | 6.73  | 126.68      | 119.28   |
| 4   | V     | 306 | ASN  | C-N-CA  | 6.73  | 126.68      | 119.28   |
| 8   | H     | 4   | SER  | N-CA-C  | -6.71 | 104.72      | 113.17   |
| 5   | E     | 94  | VAL  | CA-C-N  | 6.71  | 128.22      | 119.84   |
| 5   | E     | 94  | VAL  | C-N-CA  | 6.71  | 128.22      | 119.84   |
| 5   | W     | 94  | VAL  | CA-C-N  | 6.65  | 128.15      | 119.84   |
| 5   | W     | 94  | VAL  | C-N-CA  | 6.65  | 128.15      | 119.84   |
| 1   | S     | 291 | ILE  | CA-C-N  | 6.49  | 127.95      | 119.84   |
| 1   | S     | 291 | ILE  | C-N-CA  | 6.49  | 127.95      | 119.84   |
| 5   | E     | 64  | ARG  | CA-C-N  | 6.41  | 127.86      | 119.84   |
| 5   | E     | 64  | ARG  | C-N-CA  | 6.41  | 127.86      | 119.84   |
| 1   | S     | 97  | GLU  | CA-C-N  | 6.41  | 126.79      | 119.93   |
| 1   | S     | 97  | GLU  | C-N-CA  | 6.41  | 126.79      | 119.93   |
| 8   | Z     | 4   | SER  | N-CA-C  | -6.40 | 105.11      | 113.17   |
| 3   | 3     | 218 | LEU  | CA-C-N  | 6.39  | 127.83      | 119.84   |
| 3   | 3     | 218 | LEU  | C-N-CA  | 6.39  | 127.83      | 119.84   |
| 5   | 5     | 94  | VAL  | CA-C-N  | 6.38  | 127.81      | 119.84   |
| 5   | 5     | 94  | VAL  | C-N-CA  | 6.38  | 127.81      | 119.84   |
| 8   | 7     | 108 | ILE  | N-CA-C  | 6.38  | 114.12      | 108.63   |
| 3   | L     | 421 | LYS  | CA-C-N  | 6.31  | 126.88      | 120.38   |
| 3   | L     | 421 | LYS  | C-N-CA  | 6.31  | 126.88      | 120.38   |
| 4   | D     | 300 | GLY  | CA-C-N  | 6.27  | 126.45      | 120.31   |
| 4   | D     | 300 | GLY  | C-N-CA  | 6.27  | 126.45      | 120.31   |
| 2   | B     | 18  | TYR  | CA-C-N  | 6.26  | 126.83      | 120.38   |
| 2   | B     | 18  | TYR  | C-N-CA  | 6.26  | 126.83      | 120.38   |
| 4   | 4     | 309 | ILE  | CB-CA-C | -6.24 | 103.88      | 110.62   |
| 2   | 2     | 19  | PRO  | CA-C-N  | 6.20  | 125.76      | 119.19   |
| 2   | 2     | 19  | PRO  | C-N-CA  | 6.20  | 125.76      | 119.19   |
| 3   | C     | 459 | MET  | N-CA-C  | -6.18 | 105.70      | 113.18   |
| 5   | W     | 64  | ARG  | CA-C-N  | 6.18  | 127.57      | 119.84   |
| 5   | W     | 64  | ARG  | C-N-CA  | 6.18  | 127.57      | 119.84   |
| 6   | O     | 120 | ASN  | N-CA-C  | 6.15  | 116.39      | 108.34   |
| 1   | 1     | 205 | PHE  | N-CA-C  | 6.14  | 118.91      | 110.01   |
| 1   | J     | 291 | ILE  | CA-C-N  | 6.10  | 127.47      | 119.84   |
| 1   | J     | 291 | ILE  | C-N-CA  | 6.10  | 127.47      | 119.84   |
| 6   | X     | 170 | LEU  | CA-C-N  | 6.09  | 126.65      | 120.38   |
| 6   | X     | 170 | LEU  | C-N-CA  | 6.09  | 126.65      | 120.38   |
| 2   | 2     | 18  | TYR  | CA-C-N  | 6.08  | 126.64      | 120.38   |
| 2   | 2     | 18  | TYR  | C-N-CA  | 6.08  | 126.64      | 120.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | T     | 18  | TYR  | CA-C-N  | 6.04  | 126.61      | 120.38   |
| 2   | T     | 18  | TYR  | C-N-CA  | 6.04  | 126.61      | 120.38   |
| 1   | J     | 205 | PHE  | N-CA-C  | 6.00  | 118.71      | 110.01   |
| 6   | 6     | 120 | ASN  | N-CA-C  | 5.99  | 116.18      | 108.34   |
| 3   | U     | 421 | LYS  | CA-C-N  | 5.94  | 126.50      | 120.38   |
| 3   | U     | 421 | LYS  | C-N-CA  | 5.94  | 126.50      | 120.38   |
| 3   | 3     | 421 | LYS  | CA-C-N  | 5.93  | 126.49      | 120.38   |
| 3   | 3     | 421 | LYS  | C-N-CA  | 5.93  | 126.49      | 120.38   |
| 3   | C     | 421 | LYS  | CA-C-N  | 5.92  | 126.48      | 120.38   |
| 3   | C     | 421 | LYS  | C-N-CA  | 5.92  | 126.48      | 120.38   |
| 3   | U     | 459 | MET  | N-CA-C  | -5.86 | 106.09      | 113.18   |
| 1   | A     | 205 | PHE  | N-CA-C  | 5.86  | 118.50      | 110.01   |
| 5   | N     | 64  | ARG  | CA-C-N  | 5.86  | 127.16      | 119.84   |
| 5   | N     | 64  | ARG  | C-N-CA  | 5.86  | 127.16      | 119.84   |
| 5   | 5     | 64  | ARG  | CA-C-N  | 5.85  | 127.15      | 119.84   |
| 5   | 5     | 64  | ARG  | C-N-CA  | 5.85  | 127.15      | 119.84   |
| 4   | M     | 256 | GLY  | N-CA-C  | -5.84 | 107.11      | 115.64   |
| 4   | 4     | 311 | PRO  | CA-C-N  | 5.83  | 126.39      | 120.38   |
| 4   | 4     | 311 | PRO  | C-N-CA  | 5.83  | 126.39      | 120.38   |
| 3   | C     | 218 | LEU  | CA-C-N  | 5.81  | 127.10      | 119.84   |
| 3   | C     | 218 | LEU  | C-N-CA  | 5.81  | 127.10      | 119.84   |
| 5   | 5     | 124 | ILE  | N-CA-C  | 5.80  | 116.50      | 108.84   |
| 1   | S     | 205 | PHE  | N-CA-C  | 5.80  | 118.42      | 110.01   |
| 5   | N     | 124 | ILE  | N-CA-C  | 5.78  | 116.46      | 108.84   |
| 5   | 5     | 94  | VAL  | N-CA-C  | 5.76  | 113.25      | 107.55   |
| 1   | A     | 331 | ILE  | CA-C-N  | 5.74  | 126.22      | 120.14   |
| 1   | A     | 331 | ILE  | C-N-CA  | 5.74  | 126.22      | 120.14   |
| 5   | E     | 124 | ILE  | N-CA-C  | 5.73  | 116.41      | 108.84   |
| 4   | D     | 309 | ILE  | CB-CA-C | -5.73 | 104.43      | 110.62   |
| 8   | Z     | 73  | SER  | CA-C-N  | 5.73  | 125.73      | 119.89   |
| 8   | Z     | 73  | SER  | C-N-CA  | 5.73  | 125.73      | 119.89   |
| 3   | C     | 422 | PRO  | CA-C-N  | 5.68  | 126.00      | 119.92   |
| 3   | C     | 422 | PRO  | C-N-CA  | 5.68  | 126.00      | 119.92   |
| 3   | C     | 230 | CYS  | CA-C-N  | 5.67  | 126.05      | 119.47   |
| 3   | C     | 230 | CYS  | C-N-CA  | 5.67  | 126.05      | 119.47   |
| 4   | V     | 309 | ILE  | CB-CA-C | -5.67 | 104.49      | 110.62   |
| 6   | F     | 170 | LEU  | CA-C-N  | 5.67  | 126.22      | 120.38   |
| 6   | F     | 170 | LEU  | C-N-CA  | 5.67  | 126.22      | 120.38   |
| 8   | H     | 73  | SER  | CA-C-N  | 5.66  | 125.67      | 119.90   |
| 8   | H     | 73  | SER  | C-N-CA  | 5.66  | 125.67      | 119.90   |
| 3   | U     | 218 | LEU  | CA-C-N  | 5.62  | 126.86      | 119.84   |
| 3   | U     | 218 | LEU  | C-N-CA  | 5.62  | 126.86      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1     | 291 | ILE  | CA-C-N | 5.61  | 126.86      | 119.84   |
| 1   | 1     | 291 | ILE  | C-N-CA | 5.61  | 126.86      | 119.84   |
| 8   | Q     | 73  | SER  | CA-C-N | 5.61  | 125.61      | 119.89   |
| 8   | Q     | 73  | SER  | C-N-CA | 5.61  | 125.61      | 119.89   |
| 6   | X     | 120 | ASN  | N-CA-C | 5.60  | 115.67      | 108.34   |
| 3   | L     | 218 | LEU  | CA-C-N | 5.59  | 126.83      | 119.84   |
| 3   | L     | 218 | LEU  | C-N-CA | 5.59  | 126.83      | 119.84   |
| 3   | 3     | 459 | MET  | N-CA-C | -5.59 | 106.42      | 113.18   |
| 5   | E     | 94  | VAL  | N-CA-C | 5.58  | 113.08      | 107.55   |
| 6   | F     | 120 | ASN  | N-CA-C | 5.58  | 115.64      | 108.34   |
| 2   | K     | 18  | TYR  | CA-C-N | 5.57  | 126.12      | 120.38   |
| 2   | K     | 18  | TYR  | C-N-CA | 5.57  | 126.12      | 120.38   |
| 2   | 2     | 172 | CYS  | N-CA-C | 5.56  | 117.48      | 108.26   |
| 2   | T     | 73  | VAL  | CA-C-N | 5.56  | 126.78      | 119.84   |
| 2   | T     | 73  | VAL  | C-N-CA | 5.56  | 126.78      | 119.84   |
| 3   | L     | 764 | GLY  | CA-C-N | 5.55  | 126.78      | 119.84   |
| 3   | L     | 764 | GLY  | C-N-CA | 5.55  | 126.78      | 119.84   |
| 4   | 4     | 298 | GLU  | CA-C-N | 5.54  | 126.76      | 119.84   |
| 4   | 4     | 298 | GLU  | C-N-CA | 5.54  | 126.76      | 119.84   |
| 5   | N     | 104 | VAL  | N-CA-C | -5.52 | 107.35      | 112.43   |
| 7   | Y     | 29  | ALA  | CA-C-N | 5.49  | 125.49      | 119.89   |
| 7   | Y     | 29  | ALA  | C-N-CA | 5.49  | 125.49      | 119.89   |
| 2   | 2     | 73  | VAL  | CA-C-N | 5.47  | 126.68      | 119.84   |
| 2   | 2     | 73  | VAL  | C-N-CA | 5.47  | 126.68      | 119.84   |
| 4   | M     | 311 | PRO  | CA-C-N | 5.47  | 126.01      | 120.38   |
| 4   | M     | 311 | PRO  | C-N-CA | 5.47  | 126.01      | 120.38   |
| 1   | A     | 97  | GLU  | CA-C-N | 5.45  | 125.77      | 119.93   |
| 1   | A     | 97  | GLU  | C-N-CA | 5.45  | 125.77      | 119.93   |
| 5   | W     | 94  | VAL  | N-CA-C | 5.45  | 112.94      | 107.55   |
| 3   | 3     | 184 | CYS  | CA-C-N | -5.44 | 113.94      | 122.65   |
| 3   | 3     | 184 | CYS  | C-N-CA | -5.44 | 113.94      | 122.65   |
| 7   | 9     | 155 | LYS  | CA-C-N | 5.43  | 126.63      | 119.84   |
| 7   | 9     | 155 | LYS  | C-N-CA | 5.43  | 126.63      | 119.84   |
| 6   | 6     | 170 | LEU  | CA-C-N | 5.41  | 125.95      | 120.38   |
| 6   | 6     | 170 | LEU  | C-N-CA | 5.41  | 125.95      | 120.38   |
| 4   | V     | 298 | GLU  | CA-C-N | 5.41  | 126.61      | 119.84   |
| 4   | V     | 298 | GLU  | C-N-CA | 5.41  | 126.61      | 119.84   |
| 4   | D     | 257 | TYR  | N-CA-C | -5.41 | 105.78      | 112.38   |
| 4   | D     | 311 | PRO  | CA-C-N | 5.41  | 125.95      | 120.38   |
| 4   | D     | 311 | PRO  | C-N-CA | 5.41  | 125.95      | 120.38   |
| 5   | E     | 104 | VAL  | N-CA-C | -5.39 | 107.47      | 112.43   |
| 3   | U     | 764 | GLY  | CA-C-N | 5.39  | 126.58      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | U     | 764 | GLY  | C-N-CA | 5.39  | 126.58      | 119.84   |
| 3   | 3     | 566 | ALA  | N-CA-C | 5.38  | 117.58      | 109.23   |
| 7   | P     | 155 | LYS  | CA-C-N | 5.38  | 126.57      | 119.84   |
| 7   | P     | 155 | LYS  | C-N-CA | 5.38  | 126.57      | 119.84   |
| 2   | K     | 73  | VAL  | CA-C-N | 5.38  | 126.56      | 119.84   |
| 2   | K     | 73  | VAL  | C-N-CA | 5.38  | 126.56      | 119.84   |
| 1   | J     | 331 | ILE  | CA-C-N | 5.36  | 125.82      | 120.14   |
| 1   | J     | 331 | ILE  | C-N-CA | 5.36  | 125.82      | 120.14   |
| 5   | W     | 104 | VAL  | N-CA-C | -5.36 | 107.50      | 112.43   |
| 3   | C     | 246 | ASN  | N-CA-C | 5.35  | 117.87      | 111.71   |
| 4   | M     | 298 | GLU  | CA-C-N | 5.33  | 126.51      | 119.84   |
| 4   | M     | 298 | GLU  | C-N-CA | 5.33  | 126.51      | 119.84   |
| 2   | T     | 19  | PRO  | CA-C-N | 5.33  | 124.84      | 119.19   |
| 2   | T     | 19  | PRO  | C-N-CA | 5.33  | 124.84      | 119.19   |
| 8   | Z     | 30  | ARG  | N-CA-C | 5.32  | 117.94      | 109.96   |
| 3   | C     | 11  | VAL  | N-CA-C | 5.32  | 116.32      | 108.45   |
| 3   | U     | 566 | ALA  | N-CA-C | 5.31  | 117.47      | 109.23   |
| 7   | G     | 155 | LYS  | CA-C-N | 5.31  | 126.48      | 119.84   |
| 7   | G     | 155 | LYS  | C-N-CA | 5.31  | 126.48      | 119.84   |
| 1   | J     | 97  | GLU  | CA-C-N | 5.30  | 126.47      | 119.84   |
| 1   | J     | 97  | GLU  | C-N-CA | 5.30  | 126.47      | 119.84   |
| 5   | W     | 62  | ASP  | CA-C-N | 5.30  | 125.29      | 119.89   |
| 5   | W     | 62  | ASP  | C-N-CA | 5.30  | 125.29      | 119.89   |
| 8   | H     | 108 | ILE  | N-CA-C | 5.29  | 113.18      | 108.63   |
| 4   | M     | 224 | ILE  | CA-C-N | 5.29  | 125.83      | 120.38   |
| 4   | M     | 224 | ILE  | C-N-CA | 5.29  | 125.83      | 120.38   |
| 3   | C     | 764 | GLY  | CA-C-N | 5.29  | 126.45      | 119.84   |
| 3   | C     | 764 | GLY  | C-N-CA | 5.29  | 126.45      | 119.84   |
| 6   | F     | 137 | VAL  | CA-C-N | 5.27  | 125.25      | 120.03   |
| 6   | F     | 137 | VAL  | C-N-CA | 5.27  | 125.25      | 120.03   |
| 6   | O     | 137 | VAL  | CA-C-N | 5.26  | 125.55      | 119.92   |
| 6   | O     | 137 | VAL  | C-N-CA | 5.26  | 125.55      | 119.92   |
| 3   | 3     | 684 | ARG  | CA-C-N | 5.25  | 125.25      | 120.21   |
| 3   | 3     | 684 | ARG  | C-N-CA | 5.25  | 125.25      | 120.21   |
| 2   | K     | 19  | PRO  | CA-C-N | 5.25  | 124.76      | 119.19   |
| 2   | K     | 19  | PRO  | C-N-CA | 5.25  | 124.76      | 119.19   |
| 3   | 3     | 11  | VAL  | N-CA-C | 5.25  | 116.22      | 108.45   |
| 1   | J     | 137 | GLU  | N-CA-C | -5.23 | 107.27      | 113.97   |
| 6   | 6     | 137 | VAL  | CA-C-N | 5.22  | 125.51      | 119.92   |
| 6   | 6     | 137 | VAL  | C-N-CA | 5.22  | 125.51      | 119.92   |
| 8   | 7     | 73  | SER  | CA-C-N | 5.22  | 125.22      | 119.89   |
| 8   | 7     | 73  | SER  | C-N-CA | 5.22  | 125.22      | 119.89   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | L     | 11  | VAL  | N-CA-C | 5.21  | 116.16      | 108.45   |
| 4   | 4     | 224 | ILE  | CA-C-N | 5.20  | 125.74      | 120.38   |
| 4   | 4     | 224 | ILE  | C-N-CA | 5.20  | 125.74      | 120.38   |
| 3   | L     | 566 | ALA  | N-CA-C | 5.20  | 117.29      | 109.23   |
| 1   | 1     | 137 | GLU  | N-CA-C | -5.20 | 107.32      | 113.97   |
| 1   | S     | 5   | ILE  | N-CA-C | 5.20  | 116.20      | 108.46   |
| 4   | V     | 300 | GLY  | CA-C-N | 5.20  | 125.40      | 120.31   |
| 4   | V     | 300 | GLY  | C-N-CA | 5.20  | 125.40      | 120.31   |
| 7   | 9     | 63  | CYS  | CA-C-N | 5.19  | 125.65      | 120.04   |
| 7   | 9     | 63  | CYS  | C-N-CA | 5.19  | 125.65      | 120.04   |
| 2   | T     | 172 | CYS  | N-CA-C | 5.17  | 116.84      | 108.26   |
| 7   | Y     | 155 | LYS  | CA-C-N | 5.17  | 126.30      | 119.84   |
| 7   | Y     | 155 | LYS  | C-N-CA | 5.17  | 126.30      | 119.84   |
| 3   | U     | 406 | ALA  | CA-C-N | 5.17  | 126.30      | 119.84   |
| 3   | U     | 406 | ALA  | C-N-CA | 5.17  | 126.30      | 119.84   |
| 2   | K     | 56  | THR  | CA-C-N | 5.16  | 124.95      | 119.28   |
| 2   | K     | 56  | THR  | C-N-CA | 5.16  | 124.95      | 119.28   |
| 1   | A     | 129 | VAL  | N-CA-C | 5.15  | 115.33      | 108.27   |
| 8   | Z     | 45  | GLU  | N-CA-C | -5.14 | 106.51      | 112.89   |
| 5   | N     | 94  | VAL  | N-CA-C | 5.14  | 112.64      | 107.55   |
| 1   | J     | 5   | ILE  | N-CA-C | 5.13  | 116.11      | 108.46   |
| 3   | 3     | 669 | VAL  | CA-C-N | 5.11  | 126.22      | 119.84   |
| 3   | 3     | 669 | VAL  | C-N-CA | 5.11  | 126.22      | 119.84   |
| 3   | C     | 566 | ALA  | N-CA-C | 5.11  | 117.15      | 109.23   |
| 2   | K     | 172 | CYS  | N-CA-C | 5.10  | 116.72      | 108.26   |
| 3   | L     | 684 | ARG  | CA-C-N | 5.10  | 125.10      | 120.21   |
| 3   | L     | 684 | ARG  | C-N-CA | 5.10  | 125.10      | 120.21   |
| 4   | 4     | 257 | TYR  | N-CA-C | -5.09 | 106.17      | 112.38   |
| 4   | 4     | 256 | GLY  | N-CA-C | -5.09 | 108.21      | 115.64   |
| 8   | Q     | 108 | ILE  | N-CA-C | 5.09  | 113.01      | 108.63   |
| 2   | B     | 73  | VAL  | CA-C-N | 5.09  | 126.20      | 119.84   |
| 2   | B     | 73  | VAL  | C-N-CA | 5.09  | 126.20      | 119.84   |
| 3   | U     | 11  | VAL  | N-CA-C | 5.08  | 115.97      | 108.45   |
| 3   | C     | 282 | VAL  | CA-C-N | 5.08  | 125.36      | 119.47   |
| 3   | C     | 282 | VAL  | C-N-CA | 5.08  | 125.36      | 119.47   |
| 8   | H     | 86  | LEU  | CA-C-N | 5.06  | 125.00      | 119.78   |
| 8   | H     | 86  | LEU  | C-N-CA | 5.06  | 125.00      | 119.78   |
| 3   | U     | 230 | CYS  | CA-C-N | 5.06  | 125.34      | 119.47   |
| 3   | U     | 230 | CYS  | C-N-CA | 5.06  | 125.34      | 119.47   |
| 3   | L     | 230 | CYS  | CA-C-N | 5.06  | 125.34      | 119.47   |
| 3   | L     | 230 | CYS  | C-N-CA | 5.06  | 125.34      | 119.47   |
| 3   | 3     | 764 | GLY  | CA-C-N | 5.05  | 126.16      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | 3     | 764 | GLY  | C-N-CA | 5.05  | 126.16      | 119.84   |
| 8   | 7     | 30  | ARG  | N-CA-C | 5.05  | 117.53      | 109.96   |
| 5   | N     | 172 | ALA  | N-CA-C | -5.04 | 107.30      | 113.50   |
| 8   | Z     | 108 | ILE  | N-CA-C | 5.04  | 112.96      | 108.63   |
| 8   | H     | 45  | GLU  | N-CA-C | -5.03 | 106.66      | 112.89   |
| 7   | P     | 101 | CYS  | N-CA-C | -5.03 | 107.28      | 113.41   |
| 5   | W     | 144 | HIS  | CA-C-N | 5.03  | 126.12      | 119.84   |
| 5   | W     | 144 | HIS  | C-N-CA | 5.03  | 126.12      | 119.84   |
| 8   | Q     | 30  | ARG  | N-CA-C | 5.02  | 117.48      | 109.96   |
| 3   | C     | 406 | ALA  | CA-C-N | 5.01  | 126.11      | 119.84   |
| 3   | C     | 406 | ALA  | C-N-CA | 5.01  | 126.11      | 119.84   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 3417  | 0        | 3388     | 211     | 0            |
| 1   | A     | 3417  | 0        | 3388     | 217     | 0            |
| 1   | J     | 3417  | 0        | 3388     | 218     | 0            |
| 1   | S     | 3417  | 0        | 3388     | 205     | 0            |
| 2   | 2     | 1406  | 0        | 1373     | 75      | 0            |
| 2   | B     | 1406  | 0        | 1373     | 79      | 0            |
| 2   | K     | 1406  | 0        | 1373     | 77      | 0            |
| 2   | T     | 1406  | 0        | 1373     | 79      | 0            |
| 3   | 3     | 5880  | 0        | 5911     | 370     | 0            |
| 3   | C     | 5880  | 0        | 5911     | 370     | 0            |
| 3   | L     | 5880  | 0        | 5911     | 373     | 0            |
| 3   | U     | 5880  | 0        | 5911     | 386     | 0            |
| 4   | 4     | 3011  | 0        | 3000     | 271     | 0            |
| 4   | D     | 3011  | 0        | 3000     | 288     | 0            |
| 4   | M     | 3011  | 0        | 3000     | 263     | 0            |
| 4   | V     | 3011  | 0        | 3000     | 290     | 0            |
| 5   | 5     | 1607  | 0        | 1574     | 112     | 0            |
| 5   | E     | 1607  | 0        | 1574     | 122     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | N     | 1607  | 0        | 1574     | 110     | 0            |
| 5   | W     | 1607  | 0        | 1574     | 131     | 0            |
| 6   | 6     | 1113  | 0        | 1121     | 111     | 0            |
| 6   | F     | 1113  | 0        | 1121     | 111     | 0            |
| 6   | O     | 1113  | 0        | 1121     | 110     | 0            |
| 6   | X     | 1113  | 0        | 1121     | 116     | 0            |
| 7   | 9     | 1193  | 0        | 1160     | 77      | 0            |
| 7   | G     | 1193  | 0        | 1160     | 77      | 0            |
| 7   | P     | 1193  | 0        | 1160     | 77      | 0            |
| 7   | Y     | 1193  | 0        | 1160     | 74      | 0            |
| 8   | 7     | 1031  | 0        | 1029     | 50      | 0            |
| 8   | H     | 1031  | 0        | 1029     | 58      | 0            |
| 8   | Q     | 1031  | 0        | 1029     | 55      | 0            |
| 8   | Z     | 1031  | 0        | 1029     | 50      | 0            |
| 9   | 1     | 8     | 0        | 0        | 0       | 0            |
| 9   | 3     | 24    | 0        | 0        | 3       | 0            |
| 9   | 6     | 8     | 0        | 0        | 2       | 0            |
| 9   | 9     | 16    | 0        | 0        | 2       | 0            |
| 9   | A     | 8     | 0        | 0        | 1       | 0            |
| 9   | C     | 24    | 0        | 0        | 1       | 0            |
| 9   | F     | 8     | 0        | 0        | 3       | 0            |
| 9   | G     | 16    | 0        | 0        | 2       | 0            |
| 9   | J     | 8     | 0        | 0        | 0       | 0            |
| 9   | L     | 24    | 0        | 0        | 3       | 0            |
| 9   | O     | 8     | 0        | 0        | 2       | 0            |
| 9   | P     | 16    | 0        | 0        | 2       | 0            |
| 9   | S     | 8     | 0        | 0        | 0       | 0            |
| 9   | U     | 24    | 0        | 0        | 2       | 0            |
| 9   | X     | 8     | 0        | 0        | 3       | 0            |
| 9   | Y     | 16    | 0        | 0        | 0       | 0            |
| 10  | 1     | 31    | 0        | 19       | 7       | 0            |
| 10  | A     | 31    | 0        | 19       | 6       | 0            |
| 10  | J     | 31    | 0        | 19       | 8       | 0            |
| 10  | S     | 31    | 0        | 19       | 6       | 0            |
| 11  | 2     | 4     | 0        | 0        | 1       | 0            |
| 11  | 3     | 4     | 0        | 0        | 0       | 0            |
| 11  | B     | 4     | 0        | 0        | 1       | 0            |
| 11  | C     | 4     | 0        | 0        | 1       | 0            |
| 11  | K     | 4     | 0        | 0        | 1       | 0            |
| 11  | L     | 4     | 0        | 0        | 0       | 0            |
| 11  | T     | 4     | 0        | 0        | 1       | 0            |
| 11  | U     | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12  | 2     | 1     | 0        | 0        | 0       | 0            |
| 12  | 3     | 2     | 0        | 0        | 0       | 0            |
| 12  | 9     | 1     | 0        | 0        | 0       | 0            |
| 12  | B     | 1     | 0        | 0        | 0       | 0            |
| 12  | C     | 1     | 0        | 0        | 0       | 0            |
| 12  | G     | 1     | 0        | 0        | 0       | 0            |
| 12  | H     | 1     | 0        | 0        | 0       | 0            |
| 12  | K     | 1     | 0        | 0        | 0       | 0            |
| 12  | L     | 2     | 0        | 0        | 0       | 0            |
| 12  | P     | 1     | 0        | 0        | 0       | 0            |
| 12  | T     | 1     | 0        | 0        | 0       | 0            |
| 12  | U     | 1     | 0        | 0        | 0       | 0            |
| 12  | Y     | 1     | 0        | 0        | 0       | 0            |
| 12  | Z     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 75028 | 0        | 74300    | 4758    | 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 32.

All (4758) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 4:D:188:PRO:HB3 | 3:U:724:ARG:CD   | 1.63                     | 1.27              |
| 3:C:46:ARG:HG2  | 3:C:46:ARG:HH11  | 1.05                     | 1.19              |
| 3:C:474:ARG:NH2 | 3:C:516:VAL:HG21 | 1.62                     | 1.13              |
| 6:X:145:GLU:HG2 | 7:Y:31:VAL:HG21  | 1.31                     | 1.11              |
| 4:D:188:PRO:CB  | 3:U:724:ARG:HD2  | 1.81                     | 1.11              |
| 3:3:46:ARG:HG2  | 3:3:46:ARG:HH11  | 0.98                     | 1.10              |
| 3:U:474:ARG:NH2 | 3:U:516:VAL:HG21 | 1.67                     | 1.09              |
| 3:L:474:ARG:NH2 | 3:L:516:VAL:HG21 | 1.67                     | 1.09              |
| 5:5:5:ARG:HH11  | 5:5:5:ARG:HG3    | 1.17                     | 1.07              |
| 5:W:121:LEU:HB3 | 5:W:146:LEU:HB2  | 1.36                     | 1.06              |
| 3:L:46:ARG:HG2  | 3:L:46:ARG:HH11  | 0.94                     | 1.05              |
| 3:3:474:ARG:NH2 | 3:3:516:VAL:HG21 | 1.71                     | 1.04              |
| 5:N:5:ARG:HG3   | 5:N:5:ARG:HH11   | 1.19                     | 1.03              |
| 5:5:121:LEU:HB3 | 5:5:146:LEU:HB2  | 1.39                     | 1.02              |
| 5:E:5:ARG:HH11  | 5:E:5:ARG:HG3    | 1.22                     | 1.02              |
| 7:Y:41:HIS:HB3  | 7:Y:113:ILE:HD11 | 1.42                     | 1.02              |
| 5:N:121:LEU:HB3 | 5:N:146:LEU:HB2  | 1.38                     | 1.02              |
| 7:P:41:HIS:HB3  | 7:P:113:ILE:HD11 | 1.42                     | 1.02              |
| 3:U:46:ARG:HG2  | 3:U:46:ARG:HH11  | 0.93                     | 1.02              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 5:W:5:ARG:HH11  | 5:W:5:ARG:HG3    | 1.19                     | 1.02              |
| 5:E:121:LEU:HB3 | 5:E:146:LEU:HB2  | 1.42                     | 1.01              |
| 4:D:72:HIS:O    | 4:D:73:ARG:HD2   | 1.60                     | 1.01              |
| 4:V:72:HIS:O    | 4:V:73:ARG:HD2   | 1.60                     | 1.01              |
| 1:1:185:GLU:HB2 | 1:1:218:ILE:HD12 | 1.38                     | 1.01              |
| 4:M:350:ARG:HE  | 4:M:403:VAL:HG23 | 1.22                     | 1.00              |
| 1:S:293:GLY:HA3 | 1:S:324:GLY:H    | 1.24                     | 1.00              |
| 1:1:293:GLY:HA3 | 1:1:324:GLY:H    | 1.26                     | 1.00              |
| 4:M:72:HIS:O    | 4:M:73:ARG:HD2   | 1.60                     | 1.00              |
| 3:C:117:LEU:N   | 4:D:321:MET:HE1  | 1.76                     | 1.00              |
| 3:U:501:LYS:H   | 3:U:501:LYS:HD2  | 1.24                     | 1.00              |
| 4:D:350:ARG:HE  | 4:D:403:VAL:HG23 | 1.27                     | 1.00              |
| 1:J:293:GLY:HA3 | 1:J:324:GLY:H    | 1.26                     | 0.99              |
| 4:M:129:HIS:CE1 | 4:M:349:ALA:HB1  | 1.97                     | 0.99              |
| 7:9:41:HIS:HB3  | 7:9:113:ILE:HD11 | 1.44                     | 0.99              |
| 4:4:72:HIS:O    | 4:4:73:ARG:HD2   | 1.61                     | 0.99              |
| 3:U:117:LEU:N   | 4:V:321:MET:HE1  | 1.77                     | 0.98              |
| 3:3:117:LEU:N   | 4:4:321:MET:HE1  | 1.77                     | 0.98              |
| 1:A:293:GLY:HA3 | 1:A:324:GLY:H    | 1.27                     | 0.98              |
| 3:3:87:VAL:HA   | 3:3:91:MET:HE1   | 1.45                     | 0.98              |
| 3:L:501:LYS:H   | 3:L:501:LYS:HD2  | 1.26                     | 0.98              |
| 6:6:145:GLU:HG2 | 7:9:31:VAL:HG21  | 1.45                     | 0.98              |
| 5:E:193:ARG:HG2 | 5:E:193:ARG:HH11 | 1.27                     | 0.98              |
| 5:W:145:PRO:HA  | 5:W:150:TYR:CD2  | 1.99                     | 0.98              |
| 3:3:501:LYS:H   | 3:3:501:LYS:HD2  | 1.27                     | 0.97              |
| 3:U:46:ARG:HG2  | 3:U:46:ARG:NH1   | 1.72                     | 0.97              |
| 3:C:501:LYS:H   | 3:C:501:LYS:HD2  | 1.28                     | 0.97              |
| 4:V:350:ARG:HE  | 4:V:403:VAL:HG23 | 1.28                     | 0.97              |
| 1:S:437:TRP:HB3 | 2:T:92:GLY:HA3   | 1.46                     | 0.97              |
| 4:V:254:TYR:HD1 | 4:V:255:SER:H    | 1.12                     | 0.96              |
| 6:F:145:GLU:HG2 | 7:G:31:VAL:HG21  | 1.47                     | 0.95              |
| 1:1:437:TRP:HB3 | 2:2:92:GLY:HA3   | 1.47                     | 0.95              |
| 3:L:715:GLU:H   | 3:L:761:SER:HB2  | 1.31                     | 0.95              |
| 6:O:145:GLU:HG2 | 7:P:31:VAL:HG21  | 1.48                     | 0.95              |
| 3:3:715:GLU:H   | 3:3:761:SER:HB2  | 1.31                     | 0.95              |
| 7:G:41:HIS:HB3  | 7:G:113:ILE:HD11 | 1.45                     | 0.95              |
| 1:S:185:GLU:HB2 | 1:S:218:ILE:HD12 | 1.49                     | 0.95              |
| 2:B:31:LEU:HD12 | 2:B:41:ILE:HD13  | 1.48                     | 0.94              |
| 4:4:350:ARG:HE  | 4:4:403:VAL:HG23 | 1.28                     | 0.94              |
| 3:L:136:GLU:HG2 | 5:N:189:ARG:HG2  | 1.48                     | 0.94              |
| 2:T:31:LEU:HD12 | 2:T:41:ILE:HD13  | 1.49                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:212:PRO:HG2  | 4:V:213:ILE:HD12 | 1.50                     | 0.94              |
| 5:N:42:LYS:HB3   | 5:N:107:LEU:HD13 | 1.46                     | 0.94              |
| 4:D:188:PRO:HB3  | 3:U:724:ARG:HD2  | 0.95                     | 0.93              |
| 4:D:212:PRO:HG2  | 4:D:213:ILE:HD12 | 1.50                     | 0.93              |
| 5:W:42:LYS:HB3   | 5:W:107:LEU:HD13 | 1.50                     | 0.93              |
| 4:D:129:HIS:CE1  | 4:D:349:ALA:HB1  | 2.02                     | 0.93              |
| 5:N:145:PRO:HA   | 5:N:150:TYR:CD2  | 2.03                     | 0.93              |
| 2:2:31:LEU:HD12  | 2:2:41:ILE:HD13  | 1.51                     | 0.93              |
| 5:5:145:PRO:HA   | 5:5:150:TYR:CD2  | 2.02                     | 0.93              |
| 3:L:87:VAL:HA    | 3:L:91:MET:HE1   | 1.47                     | 0.93              |
| 5:5:42:LYS:HB3   | 5:5:107:LEU:HD13 | 1.48                     | 0.93              |
| 5:W:193:ARG:HH11 | 5:W:193:ARG:HG2  | 1.28                     | 0.93              |
| 5:E:42:LYS:HB3   | 5:E:107:LEU:HD13 | 1.50                     | 0.93              |
| 3:3:509:ALA:HB1  | 3:3:768:GLY:HA3  | 1.52                     | 0.93              |
| 6:6:19:ILE:HD11  | 1:J:271:THR:HG21 | 1.51                     | 0.93              |
| 4:D:225:PRO:HG2  | 4:D:228:VAL:HB   | 1.51                     | 0.92              |
| 2:K:31:LEU:HD12  | 2:K:41:ILE:HD13  | 1.50                     | 0.92              |
| 3:L:117:LEU:N    | 4:M:321:MET:HE1  | 1.83                     | 0.92              |
| 4:4:254:TYR:HD1  | 4:4:255:SER:H    | 1.14                     | 0.92              |
| 3:C:87:VAL:HA    | 3:C:91:MET:HE1   | 1.48                     | 0.92              |
| 5:N:193:ARG:HG2  | 5:N:193:ARG:HH11 | 1.31                     | 0.92              |
| 5:5:193:ARG:HG2  | 5:5:193:ARG:HH11 | 1.33                     | 0.92              |
| 3:3:655:ARG:HB2  | 3:3:655:ARG:HH11 | 1.35                     | 0.92              |
| 3:L:561:PRO:HB3  | 3:L:576:ALA:HA   | 1.48                     | 0.92              |
| 5:E:175:THR:HG23 | 5:E:178:ASP:HB2  | 1.51                     | 0.92              |
| 4:M:254:TYR:HD1  | 4:M:255:SER:H    | 1.15                     | 0.92              |
| 4:4:367:ARG:NH1  | 4:4:369:LYS:HB2  | 1.85                     | 0.92              |
| 4:4:129:HIS:CE1  | 4:4:349:ALA:HB1  | 2.03                     | 0.92              |
| 3:3:561:PRO:HB3  | 3:3:576:ALA:HA   | 1.49                     | 0.92              |
| 3:C:715:GLU:H    | 3:C:761:SER:HB2  | 1.34                     | 0.92              |
| 1:A:185:GLU:HB2  | 1:A:218:ILE:HD12 | 1.49                     | 0.92              |
| 3:C:509:ALA:HB1  | 3:C:768:GLY:HA3  | 1.52                     | 0.91              |
| 5:E:145:PRO:HA   | 5:E:150:TYR:CD2  | 2.04                     | 0.91              |
| 3:U:715:GLU:H    | 3:U:761:SER:HB2  | 1.32                     | 0.91              |
| 3:U:561:PRO:HB3  | 3:U:576:ALA:HA   | 1.52                     | 0.91              |
| 4:4:212:PRO:HG2  | 4:4:213:ILE:HD12 | 1.50                     | 0.91              |
| 7:P:40:ARG:HB2   | 7:P:121:MET:HE1  | 1.52                     | 0.91              |
| 4:V:367:ARG:NH1  | 4:V:369:LYS:HB2  | 1.86                     | 0.91              |
| 3:3:46:ARG:HG2   | 3:3:46:ARG:NH1   | 1.77                     | 0.91              |
| 3:3:413:LEU:HD13 | 3:3:448:MET:HE1  | 1.50                     | 0.91              |
| 3:L:46:ARG:HG2   | 3:L:46:ARG:NH1   | 1.73                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:185:GLU:HB2  | 1:J:218:ILE:HD12 | 1.50                     | 0.90              |
| 6:X:163:TYR:HE1  | 7:Y:152:ARG:HD2  | 1.35                     | 0.90              |
| 4:D:254:TYR:HD1  | 4:D:255:SER:H    | 1.14                     | 0.90              |
| 3:L:509:ALA:HB1  | 3:L:768:GLY:HA3  | 1.53                     | 0.90              |
| 4:V:318:GLU:HB2  | 8:Z:39:ASP:HA    | 1.52                     | 0.90              |
| 6:6:108:MET:HE1  | 6:6:147:LEU:HG   | 1.54                     | 0.90              |
| 3:C:117:LEU:H    | 4:D:321:MET:HE1  | 1.35                     | 0.90              |
| 5:W:175:THR:HG23 | 5:W:178:ASP:HB2  | 1.54                     | 0.90              |
| 3:U:738:THR:HG22 | 3:U:739:PRO:HD2  | 1.54                     | 0.89              |
| 4:V:254:TYR:CE2  | 4:V:346:THR:HA   | 2.06                     | 0.89              |
| 1:S:90:ILE:HD11  | 1:S:211:LEU:HD22 | 1.53                     | 0.89              |
| 3:U:655:ARG:HH11 | 3:U:655:ARG:HB2  | 1.37                     | 0.89              |
| 6:X:108:MET:HE1  | 6:X:147:LEU:HG   | 1.52                     | 0.89              |
| 3:U:87:VAL:HA    | 3:U:91:MET:HE1   | 1.54                     | 0.89              |
| 3:C:136:GLU:HG2  | 5:E:189:ARG:HG2  | 1.54                     | 0.89              |
| 4:V:225:PRO:HG2  | 4:V:228:VAL:HB   | 1.54                     | 0.89              |
| 1:A:437:TRP:HB3  | 2:B:92:GLY:HA3   | 1.54                     | 0.89              |
| 3:C:561:PRO:HB3  | 3:C:576:ALA:HA   | 1.54                     | 0.88              |
| 5:5:175:THR:HG23 | 5:5:178:ASP:HB2  | 1.54                     | 0.88              |
| 6:F:108:MET:HE1  | 6:F:147:LEU:HG   | 1.56                     | 0.88              |
| 3:L:655:ARG:HB2  | 3:L:655:ARG:HH11 | 1.38                     | 0.88              |
| 7:9:40:ARG:HB2   | 7:9:121:MET:HE1  | 1.54                     | 0.88              |
| 4:M:225:PRO:HG2  | 4:M:228:VAL:HB   | 1.51                     | 0.88              |
| 4:V:129:HIS:CE1  | 4:V:349:ALA:HB1  | 2.09                     | 0.88              |
| 4:4:225:PRO:HG2  | 4:4:228:VAL:HB   | 1.52                     | 0.88              |
| 7:Y:33:LEU:HD11  | 7:Y:161:TYR:HB2  | 1.55                     | 0.88              |
| 1:J:437:TRP:HB3  | 2:K:92:GLY:HA3   | 1.56                     | 0.88              |
| 4:M:367:ARG:NH1  | 4:M:369:LYS:HB2  | 1.88                     | 0.88              |
| 5:W:26:TRP:NE1   | 5:W:91:ARG:HH21  | 1.71                     | 0.88              |
| 3:L:413:LEU:HD13 | 3:L:448:MET:HE1  | 1.53                     | 0.88              |
| 3:L:738:THR:HG22 | 3:L:739:PRO:HD2  | 1.56                     | 0.88              |
| 4:M:212:PRO:HG2  | 4:M:213:ILE:HD12 | 1.53                     | 0.88              |
| 7:G:40:ARG:HB2   | 7:G:121:MET:HE1  | 1.56                     | 0.87              |
| 3:3:117:LEU:H    | 4:4:321:MET:HE1  | 1.36                     | 0.87              |
| 5:N:42:LYS:HD3   | 5:N:107:LEU:HD22 | 1.55                     | 0.87              |
| 3:C:55:PRO:HG3   | 3:C:74:GLN:N     | 1.90                     | 0.87              |
| 3:C:738:THR:HG22 | 3:C:739:PRO:HD2  | 1.56                     | 0.87              |
| 3:U:509:ALA:HB1  | 3:U:768:GLY:HA3  | 1.54                     | 0.87              |
| 3:C:655:ARG:HB2  | 3:C:655:ARG:HH11 | 1.40                     | 0.87              |
| 6:X:81:ALA:HA    | 6:X:108:MET:HB3  | 1.57                     | 0.87              |
| 6:O:108:MET:HE1  | 6:O:147:LEU:HG   | 1.57                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:413:LEU:HD13 | 3:C:448:MET:HE1  | 1.56                     | 0.87              |
| 7:Y:40:ARG:HB2   | 7:Y:121:MET:HE1  | 1.53                     | 0.87              |
| 3:3:738:THR:HG22 | 3:3:739:PRO:HD2  | 1.57                     | 0.86              |
| 5:W:103:THR:HG22 | 5:W:126:PHE:HB3  | 1.57                     | 0.86              |
| 3:C:46:ARG:HG2   | 3:C:46:ARG:NH1   | 1.84                     | 0.86              |
| 4:D:318:GLU:HB2  | 8:H:39:ASP:HA    | 1.57                     | 0.86              |
| 2:B:139:GLU:HB2  | 2:B:140:PRO:HD2  | 1.56                     | 0.86              |
| 1:J:90:ILE:HD11  | 1:J:211:LEU:HD22 | 1.55                     | 0.86              |
| 4:4:314:ARG:HG2  | 4:4:314:ARG:HH11 | 1.40                     | 0.86              |
| 3:U:55:PRO:HG3   | 3:U:74:GLN:N     | 1.90                     | 0.86              |
| 2:2:139:GLU:HB2  | 2:2:140:PRO:HD2  | 1.56                     | 0.86              |
| 1:S:16:THR:HG21  | 1:S:229:PRO:HB3  | 1.57                     | 0.86              |
| 6:6:19:ILE:HD11  | 1:J:271:THR:CG2  | 2.06                     | 0.85              |
| 6:X:163:TYR:CE1  | 7:Y:152:ARG:HD2  | 2.10                     | 0.85              |
| 3:U:413:LEU:HD13 | 3:U:448:MET:HE1  | 1.56                     | 0.85              |
| 5:5:103:THR:HG22 | 5:5:126:PHE:HB3  | 1.56                     | 0.85              |
| 1:A:90:ILE:HD11  | 1:A:211:LEU:HD22 | 1.57                     | 0.85              |
| 5:E:103:THR:HG22 | 5:E:126:PHE:HB3  | 1.56                     | 0.85              |
| 3:L:55:PRO:HG3   | 3:L:74:GLN:N     | 1.90                     | 0.85              |
| 6:X:145:GLU:HG2  | 7:Y:31:VAL:CG2   | 2.05                     | 0.85              |
| 5:W:5:ARG:HG3    | 5:W:5:ARG:NH1    | 1.88                     | 0.85              |
| 3:3:136:GLU:HG2  | 5:5:189:ARG:HG2  | 1.57                     | 0.85              |
| 3:L:538:ALA:HB3  | 3:L:541:ALA:HB2  | 1.56                     | 0.85              |
| 3:U:136:GLU:HG2  | 5:W:189:ARG:HG2  | 1.58                     | 0.85              |
| 3:L:694:LEU:HB3  | 3:L:762:ALA:HB2  | 1.57                     | 0.85              |
| 4:M:254:TYR:CE2  | 4:M:346:THR:HA   | 2.12                     | 0.85              |
| 5:N:103:THR:HG22 | 5:N:126:PHE:HB3  | 1.57                     | 0.85              |
| 3:U:117:LEU:H    | 4:V:321:MET:HE1  | 1.37                     | 0.85              |
| 3:3:55:PRO:HG3   | 3:3:74:GLN:N     | 1.92                     | 0.85              |
| 4:D:61:TYR:HB3   | 6:F:88:MET:HE2   | 1.58                     | 0.85              |
| 5:E:193:ARG:HH11 | 5:E:193:ARG:CG   | 1.90                     | 0.84              |
| 7:G:33:LEU:HD11  | 7:G:161:TYR:HB2  | 1.58                     | 0.84              |
| 3:3:244:ALA:HB3  | 3:3:249:MET:HE2  | 1.59                     | 0.84              |
| 5:N:5:ARG:HG3    | 5:N:5:ARG:NH1    | 1.88                     | 0.84              |
| 2:K:139:GLU:HB2  | 2:K:140:PRO:HD2  | 1.58                     | 0.84              |
| 3:L:360:LEU:O    | 3:L:364:LEU:HB3  | 1.77                     | 0.84              |
| 1:S:397:ARG:HE   | 3:U:79:LEU:HD12  | 1.42                     | 0.84              |
| 5:W:193:ARG:HH11 | 5:W:193:ARG:CG   | 1.91                     | 0.84              |
| 5:N:175:THR:HG23 | 5:N:178:ASP:HB2  | 1.59                     | 0.84              |
| 4:D:314:ARG:HH11 | 4:D:314:ARG:HG2  | 1.41                     | 0.84              |
| 6:F:163:TYR:CE1  | 7:G:152:ARG:HD2  | 2.13                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:P:33:LEU:HD11  | 7:P:161:TYR:HB2  | 1.59                     | 0.84              |
| 2:T:139:GLU:HB2  | 2:T:140:PRO:HD2  | 1.58                     | 0.84              |
| 3:U:694:LEU:HB3  | 3:U:762:ALA:HB2  | 1.60                     | 0.84              |
| 1:1:16:THR:HG21  | 1:1:229:PRO:HB3  | 1.59                     | 0.83              |
| 4:D:88:LEU:HD21  | 6:F:48:ILE:HD13  | 1.60                     | 0.83              |
| 7:9:33:LEU:HD11  | 7:9:161:TYR:HB2  | 1.59                     | 0.83              |
| 1:J:16:THR:HG21  | 1:J:229:PRO:HB3  | 1.58                     | 0.83              |
| 3:U:360:LEU:O    | 3:U:364:LEU:HB3  | 1.78                     | 0.83              |
| 3:3:567:TYR:HA   | 3:3:584:VAL:HG23 | 1.60                     | 0.83              |
| 5:5:42:LYS:HD3   | 5:5:107:LEU:HD22 | 1.58                     | 0.83              |
| 1:A:16:THR:HG21  | 1:A:229:PRO:HB3  | 1.57                     | 0.83              |
| 3:C:567:TYR:HA   | 3:C:584:VAL:HG23 | 1.61                     | 0.83              |
| 3:C:694:LEU:HB3  | 3:C:762:ALA:HB2  | 1.58                     | 0.83              |
| 5:W:16:PRO:HD2   | 5:W:28:VAL:HG13  | 1.61                     | 0.83              |
| 3:L:216:PHE:HZ   | 8:Q:128:PHE:CD2  | 1.96                     | 0.83              |
| 3:3:216:PHE:HZ   | 8:7:128:PHE:CD2  | 1.96                     | 0.83              |
| 3:3:285:VAL:HG13 | 3:3:286:ASN:H    | 1.43                     | 0.83              |
| 3:C:614:LEU:HD11 | 3:C:624:LEU:HD12 | 1.60                     | 0.83              |
| 4:D:94:ASP:HB3   | 4:D:173:ILE:HG21 | 1.60                     | 0.83              |
| 5:N:193:ARG:HH11 | 5:N:193:ARG:CG   | 1.92                     | 0.83              |
| 3:L:567:TYR:HA   | 3:L:584:VAL:HG23 | 1.60                     | 0.83              |
| 1:1:184:GLU:OE1  | 1:1:186:THR:HG22 | 1.79                     | 0.82              |
| 3:3:374:ARG:NH2  | 3:3:684:ARG:HG3  | 1.94                     | 0.82              |
| 4:4:254:TYR:CE2  | 4:4:346:THR:HA   | 2.14                     | 0.82              |
| 4:D:367:ARG:NH1  | 4:D:369:LYS:HB2  | 1.94                     | 0.82              |
| 4:M:94:ASP:HB3   | 4:M:173:ILE:HG21 | 1.60                     | 0.82              |
| 5:5:5:ARG:HG3    | 5:5:5:ARG:NH1    | 1.85                     | 0.82              |
| 4:V:314:ARG:HG2  | 4:V:314:ARG:HH11 | 1.42                     | 0.82              |
| 4:D:254:TYR:CE2  | 4:D:346:THR:HA   | 2.14                     | 0.82              |
| 3:3:694:LEU:HB3  | 3:3:762:ALA:HB2  | 1.61                     | 0.82              |
| 3:3:360:LEU:O    | 3:3:364:LEU:HB3  | 1.80                     | 0.82              |
| 1:1:90:ILE:HD11  | 1:1:211:LEU:HD22 | 1.61                     | 0.82              |
| 5:E:5:ARG:HG3    | 5:E:5:ARG:NH1    | 1.90                     | 0.82              |
| 5:E:26:TRP:NE1   | 5:E:91:ARG:HH21  | 1.76                     | 0.82              |
| 3:U:386:SER:HB2  | 3:U:675:ARG:NH1  | 1.95                     | 0.82              |
| 4:4:367:ARG:HH12 | 4:4:369:LYS:HB2  | 1.45                     | 0.82              |
| 1:A:33:LEU:HD23  | 1:A:37:GLY:HA3   | 1.61                     | 0.82              |
| 5:E:42:LYS:HD3   | 5:E:107:LEU:HD22 | 1.61                     | 0.82              |
| 3:3:614:LEU:HD11 | 3:3:624:LEU:HD12 | 1.62                     | 0.81              |
| 6:6:163:TYR:HD2  | 6:6:169:ARG:HA   | 1.45                     | 0.81              |
| 2:B:7:LYS:H      | 2:B:7:LYS:HD2    | 1.44                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:W:193:ARG:HG2  | 5:W:193:ARG:NH1  | 1.90                     | 0.81              |
| 3:C:244:ALA:HB3  | 3:C:249:MET:HE2  | 1.63                     | 0.81              |
| 5:W:52:ILE:HG23  | 5:W:114:LEU:HB3  | 1.62                     | 0.81              |
| 3:3:538:ALA:HB3  | 3:3:541:ALA:HB2  | 1.60                     | 0.81              |
| 4:M:314:ARG:HG2  | 4:M:314:ARG:HH11 | 1.45                     | 0.81              |
| 4:V:94:ASP:HB3   | 4:V:173:ILE:HG21 | 1.61                     | 0.81              |
| 6:6:81:ALA:HA    | 6:6:108:MET:HB3  | 1.63                     | 0.81              |
| 3:U:567:TYR:HA   | 3:U:584:VAL:HG23 | 1.62                     | 0.81              |
| 5:E:193:ARG:HG2  | 5:E:193:ARG:NH1  | 1.90                     | 0.81              |
| 2:K:79:HIS:ND1   | 2:K:118:SER:HB2  | 1.96                     | 0.81              |
| 3:L:115:HIS:CG   | 3:L:116:PRO:HD2  | 2.16                     | 0.81              |
| 3:C:206:GLY:O    | 3:C:209:THR:HG23 | 1.81                     | 0.80              |
| 5:5:16:PRO:HD2   | 5:5:28:VAL:HG13  | 1.63                     | 0.80              |
| 3:3:115:HIS:CG   | 3:3:116:PRO:HD2  | 2.16                     | 0.80              |
| 1:A:310:PRO:HG2  | 1:A:315:HIS:CD2  | 2.16                     | 0.80              |
| 4:M:235:THR:HA   | 4:M:239:LEU:HD12 | 1.64                     | 0.80              |
| 3:U:538:ALA:HB3  | 3:U:541:ALA:HB2  | 1.64                     | 0.80              |
| 5:W:42:LYS:HD3   | 5:W:107:LEU:HD22 | 1.63                     | 0.80              |
| 4:4:235:THR:HA   | 4:4:239:LEU:HD12 | 1.64                     | 0.80              |
| 3:C:538:ALA:HB3  | 3:C:541:ALA:HB2  | 1.61                     | 0.80              |
| 6:F:163:TYR:HD2  | 6:F:169:ARG:HA   | 1.47                     | 0.80              |
| 3:3:46:ARG:HH11  | 3:3:46:ARG:CG    | 1.89                     | 0.80              |
| 5:5:193:ARG:HH11 | 5:5:193:ARG:CG   | 1.94                     | 0.80              |
| 2:K:7:LYS:H      | 2:K:7:LYS:HD2    | 1.46                     | 0.80              |
| 3:L:11:VAL:HG11  | 3:L:25:HIS:CD2   | 2.16                     | 0.80              |
| 3:L:374:ARG:NH2  | 3:L:684:ARG:HG3  | 1.97                     | 0.80              |
| 1:S:33:LEU:HD23  | 1:S:37:GLY:HA3   | 1.63                     | 0.80              |
| 5:5:193:ARG:HG2  | 5:5:193:ARG:NH1  | 1.94                     | 0.80              |
| 6:F:81:ALA:HA    | 6:F:108:MET:HB3  | 1.61                     | 0.80              |
| 6:O:99:MET:HG2   | 6:O:100:PRO:HD2  | 1.61                     | 0.80              |
| 4:4:94:ASP:HB3   | 4:4:173:ILE:HG21 | 1.62                     | 0.80              |
| 5:5:52:ILE:HG23  | 5:5:114:LEU:HB3  | 1.64                     | 0.80              |
| 5:E:52:ILE:HG23  | 5:E:114:LEU:HB3  | 1.64                     | 0.80              |
| 5:N:52:ILE:HG23  | 5:N:114:LEU:HB3  | 1.63                     | 0.80              |
| 3:U:115:HIS:HB3  | 4:V:321:MET:HE3  | 1.64                     | 0.80              |
| 6:X:163:TYR:HD2  | 6:X:169:ARG:HA   | 1.45                     | 0.80              |
| 3:3:545:GLU:HA   | 3:3:550:LEU:HD11 | 1.63                     | 0.80              |
| 3:C:515:THR:HG23 | 3:C:683:LEU:HD12 | 1.62                     | 0.80              |
| 5:N:193:ARG:HG2  | 5:N:193:ARG:NH1  | 1.93                     | 0.80              |
| 3:U:374:ARG:NH2  | 3:U:684:ARG:HG3  | 1.95                     | 0.80              |
| 6:O:163:TYR:HD2  | 6:O:169:ARG:HA   | 1.47                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:115:HIS:CG   | 3:U:116:PRO:HD2  | 2.18                     | 0.79              |
| 1:1:33:LEU:HD23  | 1:1:37:GLY:HA3   | 1.64                     | 0.79              |
| 3:C:474:ARG:HH21 | 3:C:516:VAL:HG21 | 1.43                     | 0.79              |
| 3:C:545:GLU:HA   | 3:C:550:LEU:HD11 | 1.65                     | 0.79              |
| 3:L:11:VAL:HG11  | 3:L:25:HIS:HD2   | 1.46                     | 0.79              |
| 3:L:614:LEU:HD11 | 3:L:624:LEU:HD12 | 1.64                     | 0.79              |
| 5:N:26:TRP:NE1   | 5:N:91:ARG:HH21  | 1.81                     | 0.79              |
| 2:T:110:GLU:HA   | 8:Z:121:ARG:HH12 | 1.47                     | 0.79              |
| 6:F:96:TRP:HA    | 6:F:99:MET:HE3   | 1.65                     | 0.79              |
| 5:E:80:TRP:HA    | 5:E:80:TRP:CE3   | 2.16                     | 0.79              |
| 4:M:350:ARG:NE   | 4:M:403:VAL:HG23 | 1.96                     | 0.79              |
| 6:O:81:ALA:HA    | 6:O:108:MET:HB3  | 1.65                     | 0.79              |
| 3:U:205:ARG:HA   | 3:U:209:THR:HG22 | 1.64                     | 0.79              |
| 2:B:79:HIS:ND1   | 2:B:118:SER:HB2  | 1.97                     | 0.79              |
| 3:C:285:VAL:HG13 | 3:C:286:ASN:H    | 1.45                     | 0.79              |
| 3:U:285:VAL:HG13 | 3:U:286:ASN:H    | 1.48                     | 0.79              |
| 2:K:146:THR:HG23 | 2:K:149:ARG:HB2  | 1.63                     | 0.79              |
| 7:Y:26:TYR:N     | 7:Y:27:PRO:HD3   | 1.97                     | 0.79              |
| 2:2:7:LYS:H      | 2:2:7:LYS:HD2    | 1.48                     | 0.79              |
| 7:9:26:TYR:N     | 7:9:27:PRO:HD3   | 1.97                     | 0.78              |
| 3:C:20:MET:HE3   | 3:C:432:PHE:HB3  | 1.65                     | 0.78              |
| 3:C:360:LEU:O    | 3:C:364:LEU:HB3  | 1.82                     | 0.78              |
| 3:C:386:SER:HB2  | 3:C:675:ARG:NH1  | 1.97                     | 0.78              |
| 4:D:64:THR:HG23  | 6:F:123:ILE:HD11 | 1.65                     | 0.78              |
| 3:L:205:ARG:HA   | 3:L:209:THR:HG22 | 1.65                     | 0.78              |
| 6:X:143:ARG:HG2  | 6:X:145:GLU:OE1  | 1.83                     | 0.78              |
| 5:5:80:TRP:HA    | 5:5:80:TRP:CE3   | 2.18                     | 0.78              |
| 3:3:11:VAL:HG11  | 3:3:25:HIS:HD2   | 1.48                     | 0.78              |
| 1:A:184:GLU:OE1  | 1:A:186:THR:HG22 | 1.83                     | 0.78              |
| 2:B:146:THR:HG23 | 2:B:149:ARG:HB2  | 1.65                     | 0.78              |
| 5:N:80:TRP:CE3   | 5:N:80:TRP:HA    | 2.19                     | 0.78              |
| 3:L:515:THR:HG23 | 3:L:683:LEU:HD12 | 1.64                     | 0.78              |
| 2:T:79:HIS:ND1   | 2:T:118:SER:HB2  | 1.99                     | 0.78              |
| 3:3:11:VAL:HG11  | 3:3:25:HIS:CD2   | 2.19                     | 0.78              |
| 6:6:99:MET:HG2   | 6:6:100:PRO:HD2  | 1.63                     | 0.78              |
| 4:M:61:TYR:HB3   | 6:O:88:MET:HE2   | 1.63                     | 0.78              |
| 4:V:105:LEU:HB3  | 4:V:337:PRO:HB3  | 1.65                     | 0.78              |
| 3:L:386:SER:HB2  | 3:L:675:ARG:NH1  | 1.98                     | 0.78              |
| 5:W:39:ALA:HA    | 5:W:107:LEU:HD12 | 1.64                     | 0.78              |
| 6:X:99:MET:HG2   | 6:X:100:PRO:HD2  | 1.65                     | 0.78              |
| 4:4:88:LEU:HD21  | 6:6:48:ILE:HD13  | 1.64                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:163:TYR:HE1  | 7:G:152:ARG:HD2  | 1.47                     | 0.78              |
| 1:S:184:GLU:OE1  | 1:S:186:THR:HG22 | 1.84                     | 0.78              |
| 5:E:16:PRO:HD2   | 5:E:28:VAL:HG13  | 1.64                     | 0.78              |
| 3:L:206:GLY:O    | 3:L:209:THR:HG23 | 1.84                     | 0.78              |
| 1:1:243:THR:HG22 | 1:1:244:GLU:H    | 1.49                     | 0.78              |
| 4:4:371:ARG:HG3  | 5:5:51:ASP:OD1   | 1.83                     | 0.77              |
| 3:U:11:VAL:HG11  | 3:U:25:HIS:CD2   | 2.19                     | 0.77              |
| 4:V:350:ARG:NE   | 4:V:403:VAL:HG23 | 1.99                     | 0.77              |
| 6:X:148:ILE:HG21 | 7:Y:27:PRO:HG3   | 1.64                     | 0.77              |
| 3:3:205:ARG:HA   | 3:3:209:THR:HG22 | 1.66                     | 0.77              |
| 5:5:39:ALA:HA    | 5:5:107:LEU:HD12 | 1.65                     | 0.77              |
| 3:U:409:LEU:HD12 | 3:U:535:MET:HE2  | 1.66                     | 0.77              |
| 4:4:74:THR:HG22  | 4:4:76:LEU:H     | 1.49                     | 0.77              |
| 3:L:545:GLU:HA   | 3:L:550:LEU:HD11 | 1.65                     | 0.77              |
| 4:V:235:THR:HA   | 4:V:239:LEU:HD12 | 1.67                     | 0.77              |
| 1:J:33:LEU:HD23  | 1:J:37:GLY:HA3   | 1.64                     | 0.77              |
| 5:5:26:TRP:NE1   | 5:5:91:ARG:HH21  | 1.83                     | 0.77              |
| 3:L:409:LEU:HD12 | 3:L:535:MET:HE2  | 1.67                     | 0.77              |
| 4:4:234:LEU:O    | 4:4:239:LEU:HG   | 1.84                     | 0.77              |
| 3:C:205:ARG:HA   | 3:C:209:THR:HG22 | 1.67                     | 0.77              |
| 3:C:614:LEU:HD11 | 3:C:624:LEU:CD1  | 2.14                     | 0.77              |
| 4:M:367:ARG:HH12 | 4:M:369:LYS:HB2  | 1.48                     | 0.77              |
| 6:X:96:TRP:HA    | 6:X:99:MET:HE3   | 1.65                     | 0.77              |
| 3:L:117:LEU:H    | 4:M:321:MET:HE1  | 1.48                     | 0.77              |
| 4:V:222:GLY:HA3  | 4:V:396:ILE:HD11 | 1.67                     | 0.77              |
| 3:3:440:ARG:HG2  | 3:3:440:ARG:HH11 | 1.48                     | 0.77              |
| 4:D:167:ARG:HD3  | 6:F:143:ARG:HH12 | 1.50                     | 0.77              |
| 3:U:545:GLU:HA   | 3:U:550:LEU:HD11 | 1.64                     | 0.77              |
| 3:U:614:LEU:HD11 | 3:U:624:LEU:HD12 | 1.67                     | 0.77              |
| 5:W:80:TRP:HA    | 5:W:80:TRP:CE3   | 2.17                     | 0.77              |
| 4:D:350:ARG:NE   | 4:D:403:VAL:HG23 | 1.99                     | 0.77              |
| 2:T:7:LYS:H      | 2:T:7:LYS:HD2    | 1.50                     | 0.77              |
| 4:V:367:ARG:HH12 | 4:V:369:LYS:HB2  | 1.47                     | 0.77              |
| 3:U:244:ALA:HB3  | 3:U:249:MET:HE2  | 1.66                     | 0.77              |
| 3:3:614:LEU:HD11 | 3:3:624:LEU:CD1  | 2.15                     | 0.76              |
| 5:5:175:THR:O    | 5:5:177:LYS:N    | 2.18                     | 0.76              |
| 5:E:39:ALA:HA    | 5:E:107:LEU:HD12 | 1.66                     | 0.76              |
| 1:A:139:ARG:HG2  | 2:B:140:PRO:HD3  | 1.67                     | 0.76              |
| 3:3:206:GLY:O    | 3:3:209:THR:HG23 | 1.84                     | 0.76              |
| 1:A:16:THR:HG21  | 1:A:229:PRO:CB   | 2.15                     | 0.76              |
| 1:J:184:GLU:OE1  | 1:J:186:THR:HG22 | 1.86                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:11:VAL:HG11  | 3:U:25:HIS:HD2   | 1.50                     | 0.76              |
| 2:T:146:THR:HG23 | 2:T:149:ARG:HB2  | 1.67                     | 0.76              |
| 3:U:474:ARG:HH21 | 3:U:516:VAL:HG21 | 1.50                     | 0.76              |
| 4:4:389:GLN:HG3  | 4:4:391:PRO:HD2  | 1.68                     | 0.76              |
| 3:C:115:HIS:CG   | 3:C:116:PRO:HD2  | 2.20                     | 0.76              |
| 7:G:26:TYR:N     | 7:G:27:PRO:HD3   | 2.00                     | 0.76              |
| 4:M:222:GLY:HA3  | 4:M:396:ILE:HD11 | 1.67                     | 0.76              |
| 4:4:89:HIS:CE1   | 4:4:92:ALA:HB2   | 2.20                     | 0.76              |
| 3:C:11:VAL:HG11  | 3:C:25:HIS:HD2   | 1.51                     | 0.76              |
| 1:J:192:LEU:HD22 | 1:J:211:LEU:HD11 | 1.67                     | 0.76              |
| 1:S:192:LEU:HD22 | 1:S:211:LEU:HD11 | 1.68                     | 0.76              |
| 1:S:243:THR:HG22 | 1:S:244:GLU:H    | 1.50                     | 0.76              |
| 3:C:11:VAL:HG11  | 3:C:25:HIS:CD2   | 2.20                     | 0.76              |
| 6:O:143:ARG:HG2  | 6:O:145:GLU:OE1  | 1.84                     | 0.75              |
| 4:V:59:ILE:HD11  | 5:W:135:ILE:HG23 | 1.66                     | 0.75              |
| 1:1:253:GLN:HG2  | 1:1:327:GLY:HA2  | 1.69                     | 0.75              |
| 2:K:139:GLU:CB   | 2:K:140:PRO:HD2  | 2.16                     | 0.75              |
| 3:L:244:ALA:HB3  | 3:L:249:MET:HE2  | 1.68                     | 0.75              |
| 8:Z:121:ARG:HH11 | 8:Z:121:ARG:HG3  | 1.50                     | 0.75              |
| 3:U:614:LEU:HD11 | 3:U:624:LEU:CD1  | 2.17                     | 0.75              |
| 6:X:164:ASN:HB2  | 7:Y:128:ASP:OD2  | 1.85                     | 0.75              |
| 3:C:157:PHE:CE1  | 3:C:159:PHE:HB2  | 2.20                     | 0.75              |
| 5:E:80:TRP:HA    | 5:E:80:TRP:HE3   | 1.50                     | 0.75              |
| 3:3:386:SER:HB2  | 3:3:675:ARG:NH1  | 2.01                     | 0.75              |
| 3:L:474:ARG:HH21 | 3:L:516:VAL:HG21 | 1.47                     | 0.75              |
| 2:2:139:GLU:CB   | 2:2:140:PRO:HD2  | 2.16                     | 0.75              |
| 6:6:96:TRP:HA    | 6:6:99:MET:HE3   | 1.68                     | 0.75              |
| 2:B:139:GLU:CB   | 2:B:140:PRO:HD2  | 2.15                     | 0.75              |
| 7:G:175:ALA:O    | 7:G:177:THR:HG23 | 1.86                     | 0.75              |
| 1:J:243:THR:HG22 | 1:J:244:GLU:H    | 1.51                     | 0.75              |
| 3:L:614:LEU:HD11 | 3:L:624:LEU:CD1  | 2.17                     | 0.75              |
| 4:D:105:LEU:HB3  | 4:D:337:PRO:HB3  | 1.69                     | 0.75              |
| 2:T:139:GLU:CB   | 2:T:140:PRO:HD2  | 2.16                     | 0.75              |
| 3:3:515:THR:HG23 | 3:3:683:LEU:HD12 | 1.67                     | 0.75              |
| 6:F:148:ILE:HG21 | 7:G:27:PRO:HG3   | 1.69                     | 0.75              |
| 4:M:341:GLU:HG2  | 4:M:358:VAL:HG22 | 1.69                     | 0.75              |
| 4:V:252:TYR:HE2  | 5:W:87:ARG:HH21  | 1.35                     | 0.75              |
| 8:7:121:ARG:HH11 | 8:7:121:ARG:HG3  | 1.49                     | 0.75              |
| 7:P:26:TYR:N     | 7:P:27:PRO:HD3   | 2.01                     | 0.75              |
| 6:X:114:SER:HB2  | 7:Y:97:ARG:HD2   | 1.69                     | 0.75              |
| 4:M:105:LEU:HB3  | 4:M:337:PRO:HB3  | 1.68                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:243:THR:HG22 | 1:A:244:GLU:H    | 1.51                     | 0.74              |
| 3:C:115:HIS:HB3  | 4:D:321:MET:HE3  | 1.69                     | 0.74              |
| 1:J:370:LEU:O    | 1:J:374:ILE:HG22 | 1.88                     | 0.74              |
| 5:W:175:THR:O    | 5:W:177:LYS:N    | 2.20                     | 0.74              |
| 4:4:371:ARG:HH22 | 4:4:376:VAL:HG21 | 1.52                     | 0.74              |
| 4:V:241:ALA:HA   | 4:V:278:VAL:HG21 | 1.69                     | 0.74              |
| 1:1:107:LEU:O    | 1:1:111:PRO:HG3  | 1.86                     | 0.74              |
| 4:D:371:ARG:HH22 | 4:D:376:VAL:HG21 | 1.53                     | 0.74              |
| 4:D:389:GLN:HG3  | 4:D:391:PRO:HD2  | 1.70                     | 0.74              |
| 6:F:99:MET:HG2   | 6:F:100:PRO:HD2  | 1.69                     | 0.74              |
| 1:1:397:ARG:HE   | 3:3:79:LEU:HD12  | 1.53                     | 0.74              |
| 6:6:163:TYR:CE1  | 7:9:152:ARG:HD2  | 2.22                     | 0.74              |
| 4:4:222:GLY:HA3  | 4:4:396:ILE:HD11 | 1.69                     | 0.74              |
| 4:M:389:GLN:HG3  | 4:M:391:PRO:HD2  | 1.70                     | 0.74              |
| 3:3:409:LEU:HD12 | 3:3:535:MET:HE2  | 1.70                     | 0.74              |
| 5:5:5:ARG:HH11   | 5:5:5:ARG:CG     | 1.99                     | 0.74              |
| 5:N:66:GLU:CG    | 5:N:95:PRO:HA    | 2.17                     | 0.74              |
| 4:V:234:LEU:O    | 4:V:239:LEU:HG   | 1.88                     | 0.74              |
| 4:M:234:LEU:O    | 4:M:239:LEU:HG   | 1.87                     | 0.74              |
| 3:U:157:PHE:CE1  | 3:U:159:PHE:HB2  | 2.23                     | 0.74              |
| 4:4:120:LEU:HD13 | 4:4:160:PHE:HE1  | 1.53                     | 0.74              |
| 8:H:121:ARG:HH11 | 8:H:121:ARG:HG3  | 1.52                     | 0.74              |
| 4:M:371:ARG:HG3  | 5:N:51:ASP:OD1   | 1.87                     | 0.73              |
| 5:N:13:LYS:HZ3   | 5:N:33:ARG:HH21  | 1.36                     | 0.73              |
| 2:2:146:THR:HG23 | 2:2:149:ARG:HB2  | 1.69                     | 0.73              |
| 5:5:80:TRP:HA    | 5:5:80:TRP:HE3   | 1.52                     | 0.73              |
| 4:D:235:THR:HA   | 4:D:239:LEU:HD12 | 1.69                     | 0.73              |
| 3:L:556:ALA:HB2  | 3:L:562:GLY:HA3  | 1.69                     | 0.73              |
| 3:U:20:MET:HE3   | 3:U:432:PHE:HB3  | 1.69                     | 0.73              |
| 3:3:115:HIS:HB3  | 4:4:321:MET:HE3  | 1.70                     | 0.73              |
| 5:W:80:TRP:HA    | 5:W:80:TRP:HE3   | 1.52                     | 0.73              |
| 3:3:474:ARG:HH21 | 3:3:516:VAL:HG21 | 1.51                     | 0.73              |
| 4:4:350:ARG:NE   | 4:4:403:VAL:HG23 | 2.01                     | 0.73              |
| 6:6:148:ILE:HG21 | 7:9:27:PRO:HG3   | 1.69                     | 0.73              |
| 3:U:46:ARG:HH11  | 3:U:46:ARG:CG    | 1.85                     | 0.73              |
| 1:1:16:THR:HG21  | 1:1:229:PRO:CB   | 2.18                     | 0.73              |
| 4:D:89:HIS:CE1   | 4:D:92:ALA:HB2   | 2.24                     | 0.73              |
| 6:X:112:ALA:O    | 6:X:127:VAL:HG23 | 1.89                     | 0.73              |
| 6:6:145:GLU:HG2  | 7:9:31:VAL:CG2   | 2.19                     | 0.73              |
| 3:L:157:PHE:CE1  | 3:L:159:PHE:HB2  | 2.23                     | 0.73              |
| 4:4:236:GLY:HA2  | 4:4:351:GLY:HA3  | 1.71                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:556:ALA:HB2  | 3:C:562:GLY:HA3  | 1.70                     | 0.73              |
| 3:L:229:ILE:HD11 | 3:L:289:TRP:CZ3  | 2.24                     | 0.73              |
| 6:O:163:TYR:CE1  | 7:P:152:ARG:HD2  | 2.23                     | 0.73              |
| 1:S:246:SER:HB3  | 1:S:268:MET:HG2  | 1.71                     | 0.73              |
| 1:1:246:SER:HB3  | 1:1:268:MET:HG2  | 1.70                     | 0.73              |
| 3:3:157:PHE:CE1  | 3:3:159:PHE:HB2  | 2.23                     | 0.73              |
| 3:C:374:ARG:NH2  | 3:C:684:ARG:HG3  | 2.02                     | 0.73              |
| 4:D:367:ARG:HH12 | 4:D:369:LYS:HB2  | 1.53                     | 0.72              |
| 3:L:55:PRO:HG2   | 3:L:73:ILE:N     | 2.05                     | 0.72              |
| 1:J:253:GLN:HG2  | 1:J:327:GLY:HA2  | 1.71                     | 0.72              |
| 6:O:96:TRP:HA    | 6:O:99:MET:HE3   | 1.69                     | 0.72              |
| 1:1:192:LEU:HD22 | 1:1:211:LEU:HD11 | 1.71                     | 0.72              |
| 5:E:1:MET:SD     | 8:Z:113:GLU:CD   | 2.71                     | 0.72              |
| 5:E:13:LYS:HZ3   | 5:E:33:ARG:HH21  | 1.37                     | 0.72              |
| 1:S:16:THR:HG21  | 1:S:229:PRO:CB   | 2.19                     | 0.72              |
| 3:C:684:ARG:HG2  | 3:C:684:ARG:HH11 | 1.54                     | 0.72              |
| 3:L:440:ARG:HG2  | 3:L:440:ARG:HH11 | 1.53                     | 0.72              |
| 1:A:192:LEU:HD22 | 1:A:211:LEU:HD11 | 1.70                     | 0.72              |
| 5:N:80:TRP:HA    | 5:N:80:TRP:HE3   | 1.53                     | 0.72              |
| 1:S:6:LEU:HD21   | 1:S:12:ARG:HG3   | 1.72                     | 0.72              |
| 3:3:629:ILE:HG22 | 3:3:630:GLU:H    | 1.54                     | 0.72              |
| 6:6:143:ARG:HG2  | 6:6:145:GLU:OE1  | 1.88                     | 0.72              |
| 4:M:250:LYS:HE2  | 4:M:262:PHE:HB3  | 1.70                     | 0.72              |
| 3:U:497:TRP:NE1  | 3:U:524:LEU:HD11 | 2.04                     | 0.72              |
| 2:2:110:GLU:HA   | 8:7:121:ARG:HH12 | 1.54                     | 0.72              |
| 4:4:61:TYR:HB3   | 6:6:88:MET:HE2   | 1.70                     | 0.72              |
| 4:M:47:LEU:HD13  | 4:M:52:VAL:HA    | 1.70                     | 0.72              |
| 5:N:16:PRO:HD2   | 5:N:28:VAL:HG13  | 1.72                     | 0.72              |
| 5:N:175:THR:O    | 5:N:177:LYS:N    | 2.23                     | 0.72              |
| 4:V:74:THR:HG22  | 4:V:76:LEU:H     | 1.54                     | 0.72              |
| 4:V:371:ARG:HH22 | 4:V:376:VAL:HG21 | 1.54                     | 0.72              |
| 5:W:13:LYS:HZ3   | 5:W:33:ARG:HH21  | 1.36                     | 0.72              |
| 4:4:224:ILE:HD11 | 4:4:275:ARG:NH1  | 2.05                     | 0.72              |
| 5:5:66:GLU:CG    | 5:5:95:PRO:HA    | 2.19                     | 0.72              |
| 5:E:175:THR:O    | 5:E:177:LYS:N    | 2.22                     | 0.72              |
| 1:J:310:PRO:HG2  | 1:J:315:HIS:CD2  | 2.25                     | 0.72              |
| 3:L:629:ILE:HG22 | 3:L:630:GLU:H    | 1.55                     | 0.72              |
| 3:U:515:THR:HG23 | 3:U:683:LEU:HD12 | 1.72                     | 0.72              |
| 4:D:234:LEU:O    | 4:D:239:LEU:HG   | 1.88                     | 0.72              |
| 6:F:41:PHE:CE2   | 6:F:92:MET:HB2   | 2.24                     | 0.72              |
| 1:J:139:ARG:HG2  | 2:K:140:PRO:HD3  | 1.70                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:190:LEU:O    | 4:M:194:LEU:HB2  | 1.90                     | 0.72              |
| 4:V:389:GLN:HG3  | 4:V:391:PRO:HD2  | 1.70                     | 0.72              |
| 4:4:105:LEU:HB3  | 4:4:337:PRO:HB3  | 1.71                     | 0.71              |
| 4:4:314:ARG:HG2  | 4:4:314:ARG:NH1  | 2.05                     | 0.71              |
| 3:C:629:ILE:HG22 | 3:C:630:GLU:H    | 1.53                     | 0.71              |
| 4:D:74:THR:HG22  | 4:D:76:LEU:H     | 1.54                     | 0.71              |
| 4:M:74:THR:HG22  | 4:M:76:LEU:H     | 1.54                     | 0.71              |
| 5:N:39:ALA:HA    | 5:N:107:LEU:HD12 | 1.70                     | 0.71              |
| 3:U:55:PRO:HG2   | 3:U:73:ILE:N     | 2.04                     | 0.71              |
| 3:3:398:VAL:HB   | 3:3:450:LEU:HD22 | 1.71                     | 0.71              |
| 6:6:163:TYR:HE1  | 7:9:152:ARG:HD2  | 1.54                     | 0.71              |
| 3:C:229:ILE:HD11 | 3:C:289:TRP:CZ3  | 2.26                     | 0.71              |
| 2:K:122:VAL:HG12 | 2:K:123:GLU:H    | 1.54                     | 0.71              |
| 4:M:88:LEU:HD21  | 6:O:48:ILE:HD13  | 1.71                     | 0.71              |
| 4:V:236:GLY:HA2  | 4:V:351:GLY:HA3  | 1.72                     | 0.71              |
| 3:3:31:PRO:HB2   | 3:3:47:MET:HB3   | 1.72                     | 0.71              |
| 1:S:310:PRO:HG2  | 1:S:315:HIS:CD2  | 2.24                     | 0.71              |
| 3:U:31:PRO:HB2   | 3:U:47:MET:HB3   | 1.72                     | 0.71              |
| 4:V:88:LEU:HD21  | 6:X:48:ILE:HD13  | 1.72                     | 0.71              |
| 3:3:55:PRO:HG2   | 3:3:73:ILE:N     | 2.06                     | 0.71              |
| 3:C:31:PRO:HB2   | 3:C:47:MET:HB3   | 1.71                     | 0.71              |
| 3:C:55:PRO:HG2   | 3:C:73:ILE:N     | 2.04                     | 0.71              |
| 3:U:206:GLY:O    | 3:U:209:THR:HG23 | 1.90                     | 0.71              |
| 3:L:203:ILE:HG22 | 3:L:204:GLU:N    | 2.05                     | 0.71              |
| 2:T:134:ILE:HG13 | 2:T:145:VAL:HG21 | 1.72                     | 0.71              |
| 2:2:79:HIS:ND1   | 2:2:118:SER:HB2  | 2.05                     | 0.71              |
| 4:D:254:TYR:O    | 4:D:256:GLY:N    | 2.23                     | 0.71              |
| 4:M:241:ALA:HA   | 4:M:278:VAL:HG21 | 1.71                     | 0.71              |
| 1:J:107:LEU:O    | 1:J:111:PRO:HG3  | 1.90                     | 0.71              |
| 1:J:246:SER:HB3  | 1:J:268:MET:HG2  | 1.71                     | 0.71              |
| 2:K:110:GLU:HA   | 8:Q:121:ARG:HH12 | 1.55                     | 0.71              |
| 3:U:556:ALA:HB2  | 3:U:562:GLY:HA3  | 1.73                     | 0.71              |
| 3:3:655:ARG:HB2  | 3:3:655:ARG:NH1  | 2.05                     | 0.71              |
| 4:4:252:TYR:HE2  | 5:5:87:ARG:HH21  | 1.37                     | 0.71              |
| 2:B:122:VAL:HG12 | 2:B:123:GLU:H    | 1.54                     | 0.71              |
| 4:M:64:THR:HG23  | 6:O:123:ILE:HD11 | 1.72                     | 0.71              |
| 4:M:89:HIS:CE1   | 4:M:92:ALA:HB2   | 2.26                     | 0.71              |
| 3:3:556:ALA:HB2  | 3:3:562:GLY:HA3  | 1.71                     | 0.71              |
| 3:L:285:VAL:HG13 | 3:L:286:ASN:H    | 1.55                     | 0.71              |
| 4:M:120:LEU:HD13 | 4:M:160:PHE:HE1  | 1.56                     | 0.71              |
| 4:M:224:ILE:HD11 | 4:M:275:ARG:NH1  | 2.06                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:P:40:ARG:HB2   | 7:P:121:MET:CE   | 2.19                     | 0.71              |
| 5:W:66:GLU:CG    | 5:W:95:PRO:HA    | 2.21                     | 0.71              |
| 6:X:41:PHE:CE2   | 6:X:92:MET:HB2   | 2.26                     | 0.71              |
| 2:T:122:VAL:HG12 | 2:T:123:GLU:H    | 1.55                     | 0.70              |
| 1:A:253:GLN:HG2  | 1:A:327:GLY:HA2  | 1.73                     | 0.70              |
| 4:D:222:GLY:HA3  | 4:D:396:ILE:HD11 | 1.72                     | 0.70              |
| 6:O:148:ILE:HG21 | 7:P:27:PRO:HG3   | 1.73                     | 0.70              |
| 1:A:219:ASN:HD22 | 1:A:223:THR:HG21 | 1.56                     | 0.70              |
| 4:M:236:GLY:HA2  | 4:M:351:GLY:HA3  | 1.73                     | 0.70              |
| 3:C:112:LEU:HD12 | 4:D:322:GLU:HG3  | 1.71                     | 0.70              |
| 5:E:66:GLU:CG    | 5:E:95:PRO:HA    | 2.22                     | 0.70              |
| 6:F:143:ARG:HG2  | 6:F:145:GLU:OE1  | 1.91                     | 0.70              |
| 6:F:145:GLU:HG2  | 7:G:31:VAL:CG2   | 2.20                     | 0.70              |
| 8:Q:121:ARG:HG3  | 8:Q:121:ARG:HH11 | 1.54                     | 0.70              |
| 7:Y:175:ALA:O    | 7:Y:177:THR:HG23 | 1.92                     | 0.70              |
| 3:3:216:PHE:HZ   | 8:7:128:PHE:HD2  | 1.37                     | 0.70              |
| 4:4:341:GLU:HG2  | 4:4:358:VAL:HG22 | 1.74                     | 0.70              |
| 3:L:46:ARG:HH11  | 3:L:46:ARG:CG    | 1.85                     | 0.70              |
| 4:V:85:MET:HE3   | 4:V:409:ARG:HG3  | 1.71                     | 0.70              |
| 3:3:285:VAL:HG13 | 3:3:286:ASN:N    | 2.05                     | 0.70              |
| 4:4:236:GLY:HA2  | 4:4:351:GLY:CA   | 2.22                     | 0.70              |
| 6:6:163:TYR:HB3  | 6:6:168:GLU:O    | 1.91                     | 0.70              |
| 4:V:84:ARG:NE    | 6:X:117:MET:HE1  | 2.06                     | 0.70              |
| 7:9:40:ARG:HB2   | 7:9:121:MET:CE   | 2.21                     | 0.70              |
| 4:D:85:MET:HE3   | 4:D:409:ARG:HG3  | 1.72                     | 0.70              |
| 3:L:20:MET:HE3   | 3:L:432:PHE:HB3  | 1.73                     | 0.70              |
| 4:4:59:ILE:HD11  | 5:5:135:ILE:HG23 | 1.72                     | 0.70              |
| 3:C:337:ARG:H    | 3:C:337:ARG:HD2  | 1.56                     | 0.70              |
| 4:D:64:THR:HG23  | 6:F:123:ILE:CD1  | 2.21                     | 0.70              |
| 4:M:254:TYR:O    | 4:M:256:GLY:N    | 2.22                     | 0.70              |
| 1:S:289:ALA:HB3  | 1:S:337:MET:HE3  | 1.74                     | 0.70              |
| 4:V:238:SER:HB3  | 4:V:279:ARG:NH2  | 2.07                     | 0.70              |
| 3:3:229:ILE:HD11 | 3:3:289:TRP:CZ3  | 2.27                     | 0.70              |
| 3:C:508:GLY:O    | 3:C:512:LEU:HB2  | 1.92                     | 0.70              |
| 3:C:550:LEU:HB3  | 3:C:684:ARG:HH21 | 1.57                     | 0.70              |
| 3:L:402:PRO:HG3  | 3:L:535:MET:HE1  | 1.74                     | 0.70              |
| 3:U:337:ARG:H    | 3:U:337:ARG:HD2  | 1.55                     | 0.70              |
| 1:A:397:ARG:H    | 1:A:397:ARG:HD2  | 1.56                     | 0.69              |
| 3:L:186:ARG:HD3  | 3:L:229:ILE:HG22 | 1.73                     | 0.69              |
| 4:4:367:ARG:HH12 | 4:4:369:LYS:CB   | 2.05                     | 0.69              |
| 7:P:34:LYS:HB3   | 7:P:35:PRO:HD2   | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:216:PHE:HZ   | 8:Z:128:PHE:CD2  | 2.09                     | 0.69              |
| 7:Y:40:ARG:HB2   | 7:Y:121:MET:CE   | 2.21                     | 0.69              |
| 1:J:397:ARG:HE   | 3:L:79:LEU:HD12  | 1.58                     | 0.69              |
| 3:L:216:PHE:HZ   | 8:Q:128:PHE:HD2  | 1.38                     | 0.69              |
| 4:V:47:LEU:HD13  | 4:V:52:VAL:HA    | 1.74                     | 0.69              |
| 3:3:20:MET:HE3   | 3:3:432:PHE:HB3  | 1.73                     | 0.69              |
| 1:A:370:LEU:O    | 1:A:374:ILE:HG22 | 1.93                     | 0.69              |
| 3:L:603:PRO:HB2  | 3:L:634:ALA:HB2  | 1.73                     | 0.69              |
| 3:L:684:ARG:HG2  | 3:L:684:ARG:HH11 | 1.55                     | 0.69              |
| 6:O:145:GLU:HG2  | 7:P:31:VAL:CG2   | 2.22                     | 0.69              |
| 1:S:139:ARG:HG2  | 2:T:140:PRO:HD3  | 1.75                     | 0.69              |
| 4:4:241:ALA:HA   | 4:4:278:VAL:HG21 | 1.73                     | 0.69              |
| 2:B:110:GLU:HA   | 8:H:121:ARG:HH12 | 1.58                     | 0.69              |
| 4:D:120:LEU:HD13 | 4:D:160:PHE:HE1  | 1.57                     | 0.69              |
| 3:L:229:ILE:HD11 | 3:L:289:TRP:HZ3  | 1.57                     | 0.69              |
| 3:L:534:ALA:HB3  | 3:L:542:ARG:HH12 | 1.56                     | 0.69              |
| 4:M:239:LEU:HD22 | 4:M:244:VAL:HB   | 1.74                     | 0.69              |
| 6:O:163:TYR:HB3  | 6:O:168:GLU:O    | 1.93                     | 0.69              |
| 3:U:229:ILE:HD11 | 3:U:289:TRP:CZ3  | 2.27                     | 0.69              |
| 3:3:684:ARG:HG2  | 3:3:684:ARG:HH11 | 1.56                     | 0.69              |
| 4:4:85:MET:HE3   | 4:4:409:ARG:HG3  | 1.74                     | 0.69              |
| 1:J:65:ARG:CZ    | 1:J:268:MET:HE1  | 2.21                     | 0.69              |
| 4:M:129:HIS:HE1  | 4:M:349:ALA:HB1  | 1.57                     | 0.69              |
| 1:S:393:LEU:HD22 | 3:U:106:GLY:HA3  | 1.75                     | 0.69              |
| 4:V:213:ILE:HG21 | 4:V:217:ARG:HH11 | 1.58                     | 0.69              |
| 1:1:397:ARG:H    | 1:1:397:ARG:HD2  | 1.57                     | 0.69              |
| 3:3:171:SER:HB2  | 3:3:172:PRO:HD2  | 1.75                     | 0.69              |
| 3:3:337:ARG:H    | 3:3:337:ARG:HD2  | 1.55                     | 0.69              |
| 7:9:34:LYS:HB3   | 7:9:35:PRO:HD2   | 1.74                     | 0.69              |
| 3:C:440:ARG:HG2  | 3:C:440:ARG:HH11 | 1.58                     | 0.69              |
| 1:J:16:THR:HG21  | 1:J:229:PRO:CB   | 2.22                     | 0.69              |
| 4:M:85:MET:HE3   | 4:M:409:ARG:HG3  | 1.72                     | 0.69              |
| 1:1:289:ALA:HB3  | 1:1:337:MET:HE3  | 1.75                     | 0.69              |
| 4:4:190:LEU:O    | 4:4:194:LEU:HB2  | 1.92                     | 0.69              |
| 6:6:112:ALA:O    | 6:6:127:VAL:HG23 | 1.92                     | 0.69              |
| 1:A:246:SER:HB3  | 1:A:268:MET:HG2  | 1.74                     | 0.69              |
| 3:C:203:ILE:HG22 | 3:C:204:GLU:N    | 2.06                     | 0.69              |
| 4:D:236:GLY:HA2  | 4:D:351:GLY:HA3  | 1.73                     | 0.69              |
| 7:G:45:ARG:NH2   | 7:G:137:LEU:HD23 | 2.07                     | 0.69              |
| 3:L:31:PRO:HB2   | 3:L:47:MET:HB3   | 1.75                     | 0.69              |
| 4:M:314:ARG:HG2  | 4:M:314:ARG:NH1  | 2.07                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:N:66:GLU:HG3   | 5:N:95:PRO:HA    | 1.73                     | 0.69              |
| 3:U:655:ARG:HB2  | 3:U:655:ARG:NH1  | 2.07                     | 0.69              |
| 4:4:105:LEU:HD23 | 4:4:337:PRO:HG3  | 1.74                     | 0.69              |
| 3:L:31:PRO:HG3   | 3:L:137:TYR:CD1  | 2.28                     | 0.69              |
| 1:S:438:ARG:H    | 1:S:438:ARG:HD2  | 1.57                     | 0.69              |
| 3:C:285:VAL:HG13 | 3:C:286:ASN:N    | 2.08                     | 0.69              |
| 3:C:716:LEU:HD21 | 3:C:758:LEU:HB3  | 1.74                     | 0.69              |
| 1:S:55:GLU:O     | 1:S:59:ARG:HB2   | 1.93                     | 0.69              |
| 3:U:440:ARG:HH11 | 3:U:440:ARG:HG2  | 1.58                     | 0.69              |
| 3:C:438:LYS:O    | 3:C:441:MET:HG3  | 1.93                     | 0.68              |
| 7:G:40:ARG:HB2   | 7:G:121:MET:CE   | 2.23                     | 0.68              |
| 1:S:370:LEU:O    | 1:S:374:ILE:HG22 | 1.92                     | 0.68              |
| 3:U:438:LYS:O    | 3:U:441:MET:HG3  | 1.92                     | 0.68              |
| 6:X:153:GLN:HG3  | 7:Y:124:TYR:CZ   | 2.28                     | 0.68              |
| 4:D:167:ARG:HD3  | 6:F:143:ARG:NH1  | 2.08                     | 0.68              |
| 1:J:65:ARG:NH2   | 1:J:268:MET:HE1  | 2.08                     | 0.68              |
| 1:S:397:ARG:H    | 1:S:397:ARG:HD2  | 1.57                     | 0.68              |
| 4:4:250:LYS:HE2  | 4:4:262:PHE:HB3  | 1.74                     | 0.68              |
| 1:A:351:GLU:HA   | 3:C:205:ARG:HH12 | 1.58                     | 0.68              |
| 4:V:254:TYR:HD1  | 4:V:255:SER:N    | 1.87                     | 0.68              |
| 4:D:47:LEU:HD13  | 4:D:52:VAL:HA    | 1.75                     | 0.68              |
| 4:D:190:LEU:O    | 4:D:194:LEU:HB2  | 1.94                     | 0.68              |
| 7:G:34:LYS:HB3   | 7:G:35:PRO:HD2   | 1.74                     | 0.68              |
| 3:U:31:PRO:HG3   | 3:U:137:TYR:CD1  | 2.29                     | 0.68              |
| 3:U:550:LEU:HB3  | 3:U:684:ARG:HH21 | 1.58                     | 0.68              |
| 1:1:310:PRO:HG2  | 1:1:315:HIS:CD2  | 2.29                     | 0.68              |
| 2:2:122:VAL:HG12 | 2:2:123:GLU:H    | 1.57                     | 0.68              |
| 4:4:318:GLU:HB2  | 8:7:39:ASP:HA    | 1.74                     | 0.68              |
| 7:9:175:ALA:O    | 7:9:177:THR:HG23 | 1.92                     | 0.68              |
| 3:L:508:GLY:O    | 3:L:512:LEU:HB2  | 1.94                     | 0.68              |
| 3:U:629:ILE:HG22 | 3:U:630:GLU:H    | 1.58                     | 0.68              |
| 4:V:254:TYR:O    | 4:V:256:GLY:N    | 2.25                     | 0.68              |
| 4:D:252:TYR:HE2  | 5:E:87:ARG:HH21  | 1.39                     | 0.68              |
| 1:J:289:ALA:HB3  | 1:J:337:MET:HE3  | 1.76                     | 0.68              |
| 3:L:337:ARG:H    | 3:L:337:ARG:HD2  | 1.57                     | 0.68              |
| 7:P:175:ALA:O    | 7:P:177:THR:HG23 | 1.92                     | 0.68              |
| 1:1:55:GLU:O     | 1:1:59:ARG:HB2   | 1.93                     | 0.68              |
| 4:4:254:TYR:O    | 4:4:256:GLY:N    | 2.23                     | 0.68              |
| 4:M:371:ARG:HH22 | 4:M:376:VAL:HG21 | 1.58                     | 0.68              |
| 5:N:18:GLU:HB2   | 5:N:26:TRP:HB2   | 1.76                     | 0.68              |
| 6:O:165:GLU:HG2  | 7:P:148:ARG:HH11 | 1.58                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:47:LEU:HD13  | 4:4:52:VAL:HA    | 1.74                     | 0.68              |
| 4:D:237:GLY:HA2  | 4:D:240:ARG:CZ   | 2.23                     | 0.68              |
| 8:H:108:ILE:HG22 | 8:H:114:ARG:NH1  | 2.09                     | 0.68              |
| 3:U:186:ARG:HD3  | 3:U:229:ILE:HG22 | 1.75                     | 0.68              |
| 4:V:367:ARG:HH12 | 4:V:369:LYS:CB   | 2.06                     | 0.68              |
| 5:5:13:LYS:NZ    | 5:5:33:ARG:HH21  | 1.90                     | 0.68              |
| 4:V:250:LYS:HE2  | 4:V:262:PHE:HB3  | 1.76                     | 0.68              |
| 3:3:203:ILE:HG22 | 3:3:204:GLU:N    | 2.08                     | 0.68              |
| 3:3:550:LEU:HB3  | 3:3:684:ARG:HH21 | 1.59                     | 0.68              |
| 4:D:236:GLY:HA2  | 4:D:351:GLY:CA   | 2.24                     | 0.68              |
| 5:E:13:LYS:NZ    | 5:E:33:ARG:HH21  | 1.92                     | 0.68              |
| 3:L:507:LEU:HD22 | 3:L:511:VAL:HG11 | 1.76                     | 0.68              |
| 4:M:133:LEU:HD21 | 4:M:204:TYR:CD2  | 2.29                     | 0.68              |
| 4:M:252:TYR:HE2  | 5:N:87:ARG:HH21  | 1.42                     | 0.68              |
| 5:N:168:ALA:HA   | 5:N:171:ARG:NH1  | 2.09                     | 0.68              |
| 1:S:253:GLN:HG2  | 1:S:327:GLY:HA2  | 1.75                     | 0.68              |
| 4:V:371:ARG:HG3  | 5:W:51:ASP:OD1   | 1.93                     | 0.68              |
| 3:3:6:VAL:HG12   | 3:3:7:ASN:N      | 2.08                     | 0.67              |
| 3:3:507:LEU:HD22 | 3:3:511:VAL:HG11 | 1.76                     | 0.67              |
| 4:4:254:TYR:HD1  | 4:4:255:SER:N    | 1.89                     | 0.67              |
| 3:C:6:VAL:HG12   | 3:C:7:ASN:N      | 2.09                     | 0.67              |
| 4:V:190:LEU:O    | 4:V:194:LEU:HB2  | 1.94                     | 0.67              |
| 4:V:237:GLY:HA2  | 4:V:240:ARG:CZ   | 2.24                     | 0.67              |
| 5:W:18:GLU:HB2   | 5:W:26:TRP:HB2   | 1.76                     | 0.67              |
| 1:1:219:ASN:HD22 | 1:1:223:THR:HG21 | 1.59                     | 0.67              |
| 5:5:66:GLU:HG3   | 5:5:95:PRO:HA    | 1.75                     | 0.67              |
| 4:V:236:GLY:HA2  | 4:V:351:GLY:CA   | 2.24                     | 0.67              |
| 3:C:171:SER:HB2  | 3:C:172:PRO:HD2  | 1.74                     | 0.67              |
| 4:D:142:ALA:HB1  | 4:D:145:PRO:HG2  | 1.77                     | 0.67              |
| 4:M:236:GLY:HA2  | 4:M:351:GLY:CA   | 2.24                     | 0.67              |
| 4:V:350:ARG:O    | 4:V:373:PRO:HB2  | 1.95                     | 0.67              |
| 5:W:66:GLU:HG3   | 5:W:95:PRO:HA    | 1.77                     | 0.67              |
| 6:X:163:TYR:HB3  | 6:X:168:GLU:O    | 1.94                     | 0.67              |
| 2:B:87:SER:HB3   | 11:B:182:FES:S2  | 2.35                     | 0.67              |
| 2:B:134:ILE:HG13 | 2:B:145:VAL:HG21 | 1.76                     | 0.67              |
| 3:C:655:ARG:HB2  | 3:C:655:ARG:NH1  | 2.10                     | 0.67              |
| 3:C:229:ILE:HD11 | 3:C:289:TRP:HZ3  | 1.60                     | 0.67              |
| 1:J:55:GLU:O     | 1:J:59:ARG:HB2   | 1.94                     | 0.67              |
| 4:V:311:PRO:HD3  | 4:V:330:HIS:NE2  | 2.09                     | 0.67              |
| 3:3:31:PRO:HG3   | 3:3:137:TYR:CD1  | 2.29                     | 0.67              |
| 3:C:337:ARG:H    | 3:C:337:ARG:CD   | 2.08                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:371:ARG:HG3  | 5:E:51:ASP:OD1   | 1.94                     | 0.67              |
| 1:S:397:ARG:HE   | 3:U:79:LEU:CD1   | 2.07                     | 0.67              |
| 3:L:550:LEU:HB3  | 3:L:684:ARG:HH21 | 1.58                     | 0.67              |
| 2:T:87:SER:HB3   | 11:T:182:FES:S2  | 2.34                     | 0.67              |
| 4:V:213:ILE:HG21 | 4:V:217:ARG:NH1  | 2.10                     | 0.67              |
| 1:1:139:ARG:HG2  | 2:2:140:PRO:HD3  | 1.75                     | 0.67              |
| 3:3:716:LEU:HD21 | 3:3:758:LEU:HB3  | 1.76                     | 0.67              |
| 3:C:216:PHE:HZ   | 8:H:128:PHE:CD2  | 2.12                     | 0.67              |
| 1:J:267:PRO:HG2  | 1:J:270:THR:HG22 | 1.77                     | 0.67              |
| 4:M:254:TYR:HD1  | 4:M:255:SER:N    | 1.90                     | 0.67              |
| 3:U:337:ARG:H    | 3:U:337:ARG:CD   | 2.07                     | 0.67              |
| 4:V:44:MET:HA    | 4:V:44:MET:CE    | 2.25                     | 0.67              |
| 1:A:393:LEU:HD22 | 3:C:106:GLY:HA3  | 1.77                     | 0.67              |
| 1:J:397:ARG:H    | 1:J:397:ARG:HD2  | 1.59                     | 0.67              |
| 5:N:13:LYS:NZ    | 5:N:33:ARG:HH21  | 1.92                     | 0.67              |
| 6:O:163:TYR:HE1  | 7:P:152:ARG:HD2  | 1.57                     | 0.67              |
| 3:U:20:MET:HE3   | 3:U:432:PHE:CB   | 2.25                     | 0.67              |
| 3:U:125:GLY:HA3  | 3:U:246:ASN:HD22 | 1.60                     | 0.67              |
| 3:C:507:LEU:HD22 | 3:C:511:VAL:HG11 | 1.77                     | 0.67              |
| 5:E:66:GLU:HG3   | 5:E:95:PRO:HA    | 1.77                     | 0.67              |
| 1:J:6:LEU:HD21   | 1:J:12:ARG:HG3   | 1.77                     | 0.67              |
| 4:V:89:HIS:CE1   | 4:V:92:ALA:HB2   | 2.29                     | 0.67              |
| 1:1:370:LEU:O    | 1:1:374:ILE:HG22 | 1.95                     | 0.66              |
| 4:D:224:ILE:HD11 | 4:D:275:ARG:NH1  | 2.11                     | 0.66              |
| 1:J:438:ARG:H    | 1:J:438:ARG:HD2  | 1.60                     | 0.66              |
| 3:U:285:VAL:HG13 | 3:U:286:ASN:N    | 2.09                     | 0.66              |
| 1:1:6:LEU:HD21   | 1:1:12:ARG:HG3   | 1.77                     | 0.66              |
| 6:F:114:SER:HB2  | 7:G:97:ARG:HD2   | 1.77                     | 0.66              |
| 3:L:655:ARG:HB2  | 3:L:655:ARG:NH1  | 2.09                     | 0.66              |
| 4:M:237:GLY:HA2  | 4:M:240:ARG:CZ   | 2.25                     | 0.66              |
| 3:C:534:ALA:HB3  | 3:C:542:ARG:HH12 | 1.59                     | 0.66              |
| 4:V:105:LEU:HD23 | 4:V:337:PRO:HG3  | 1.77                     | 0.66              |
| 1:1:438:ARG:H    | 1:1:438:ARG:HD2  | 1.60                     | 0.66              |
| 6:6:114:SER:HB2  | 7:9:97:ARG:HD2   | 1.77                     | 0.66              |
| 1:J:393:LEU:HD22 | 3:L:106:GLY:HA3  | 1.77                     | 0.66              |
| 1:S:219:ASN:HD22 | 1:S:223:THR:HG21 | 1.61                     | 0.66              |
| 3:U:684:ARG:HG2  | 3:U:684:ARG:HH11 | 1.60                     | 0.66              |
| 4:V:120:LEU:HD13 | 4:V:160:PHE:HE1  | 1.59                     | 0.66              |
| 4:V:133:LEU:HD21 | 4:V:204:TYR:CD2  | 2.31                     | 0.66              |
| 4:V:341:GLU:HG2  | 4:V:358:VAL:HG22 | 1.78                     | 0.66              |
| 7:Y:48:ASN:HB2   | 7:Y:50:LEU:HD23  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:184:GLU:CD   | 1:1:186:THR:HG22 | 2.21                     | 0.66              |
| 3:3:337:ARG:H    | 3:3:337:ARG:CD   | 2.08                     | 0.66              |
| 1:A:6:LEU:HD21   | 1:A:12:ARG:HG3   | 1.78                     | 0.66              |
| 1:A:107:LEU:O    | 1:A:111:PRO:HG3  | 1.96                     | 0.66              |
| 3:C:497:TRP:NE1  | 3:C:524:LEU:HD11 | 2.11                     | 0.66              |
| 4:D:44:MET:CE    | 4:D:44:MET:HA    | 2.26                     | 0.66              |
| 7:G:153:THR:HG22 | 7:G:155:LYS:H    | 1.60                     | 0.66              |
| 5:W:13:LYS:NZ    | 5:W:33:ARG:HH21  | 1.94                     | 0.66              |
| 7:Y:153:THR:HG22 | 7:Y:155:LYS:H    | 1.61                     | 0.66              |
| 3:3:534:ALA:HB3  | 3:3:542:ARG:HH12 | 1.59                     | 0.66              |
| 4:4:225:PRO:CG   | 4:4:228:VAL:HB   | 2.26                     | 0.66              |
| 1:A:184:GLU:CD   | 1:A:186:THR:HG22 | 2.21                     | 0.66              |
| 4:D:59:ILE:HD11  | 5:E:135:ILE:HG23 | 1.78                     | 0.66              |
| 1:S:65:ARG:CZ    | 1:S:268:MET:HE1  | 2.26                     | 0.66              |
| 1:A:50:PRO:O     | 1:A:53:VAL:HG12  | 1.95                     | 0.66              |
| 4:D:133:LEU:HD21 | 4:D:204:TYR:CD2  | 2.31                     | 0.66              |
| 4:D:241:ALA:HA   | 4:D:278:VAL:HG21 | 1.77                     | 0.66              |
| 1:J:110:VAL:N    | 1:J:111:PRO:HD3  | 2.11                     | 0.66              |
| 4:M:40:VAL:HG22  | 4:M:40:VAL:O     | 1.96                     | 0.66              |
| 4:V:239:LEU:HD22 | 4:V:244:VAL:HB   | 1.77                     | 0.66              |
| 6:6:41:PHE:CE2   | 6:6:92:MET:HB2   | 2.30                     | 0.66              |
| 3:C:398:VAL:HB   | 3:C:450:LEU:HD22 | 1.78                     | 0.66              |
| 3:C:409:LEU:HD12 | 3:C:535:MET:HE2  | 1.77                     | 0.66              |
| 4:D:213:ILE:HG21 | 4:D:217:ARG:HH11 | 1.61                     | 0.66              |
| 4:D:225:PRO:CG   | 4:D:228:VAL:HB   | 2.25                     | 0.66              |
| 5:E:135:ILE:HG22 | 5:E:136:LEU:HG   | 1.78                     | 0.66              |
| 3:L:716:LEU:HD21 | 3:L:758:LEU:HB3  | 1.77                     | 0.66              |
| 4:M:367:ARG:HH12 | 4:M:369:LYS:CB   | 2.08                     | 0.66              |
| 1:S:184:GLU:CD   | 1:S:186:THR:HG22 | 2.21                     | 0.66              |
| 1:S:214:LYS:O    | 1:S:216:THR:HG23 | 1.96                     | 0.66              |
| 1:1:267:PRO:HG2  | 1:1:270:THR:HG22 | 1.78                     | 0.66              |
| 3:3:87:VAL:HA    | 3:3:91:MET:CE    | 2.24                     | 0.66              |
| 3:3:205:ARG:CA   | 3:3:209:THR:HG22 | 2.26                     | 0.66              |
| 4:4:64:THR:HG23  | 6:6:123:ILE:HD11 | 1.77                     | 0.66              |
| 4:D:250:LYS:HE2  | 4:D:262:PHE:HB3  | 1.77                     | 0.66              |
| 4:M:44:MET:HA    | 4:M:44:MET:CE    | 2.26                     | 0.66              |
| 3:U:398:VAL:HB   | 3:U:450:LEU:HD22 | 1.77                     | 0.66              |
| 1:1:50:PRO:O     | 1:1:53:VAL:HG12  | 1.94                     | 0.65              |
| 4:4:44:MET:HA    | 4:4:44:MET:CE    | 2.26                     | 0.65              |
| 1:A:10:ASP:OD1   | 1:A:11:PRO:HD2   | 1.96                     | 0.65              |
| 4:M:105:LEU:HD23 | 4:M:337:PRO:HG3  | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:253:GLN:N    | 1:S:253:GLN:HE21 | 1.95                     | 0.65              |
| 7:P:48:ASN:HB2   | 7:P:50:LEU:HD23  | 1.78                     | 0.65              |
| 3:U:507:LEU:HD22 | 3:U:511:VAL:HG11 | 1.77                     | 0.65              |
| 4:V:249:ARG:HB3  | 4:V:257:TYR:HD1  | 1.60                     | 0.65              |
| 3:3:186:ARG:HD3  | 3:3:229:ILE:HG22 | 1.78                     | 0.65              |
| 3:3:402:PRO:HG3  | 3:3:535:MET:HE1  | 1.78                     | 0.65              |
| 4:D:238:SER:HB3  | 4:D:279:ARG:NH2  | 2.11                     | 0.65              |
| 6:O:41:PHE:CE2   | 6:O:92:MET:HB2   | 2.31                     | 0.65              |
| 6:O:117:MET:HB3  | 7:P:99:ILE:HD13  | 1.79                     | 0.65              |
| 4:V:142:ALA:HB1  | 4:V:145:PRO:HG2  | 1.79                     | 0.65              |
| 7:Y:34:LYS:HB3   | 7:Y:35:PRO:HD2   | 1.78                     | 0.65              |
| 3:3:497:TRP:NE1  | 3:3:524:LEU:HD11 | 2.12                     | 0.65              |
| 6:F:112:ALA:O    | 6:F:127:VAL:HG23 | 1.96                     | 0.65              |
| 3:L:6:VAL:HG12   | 3:L:7:ASN:N      | 2.11                     | 0.65              |
| 4:V:213:ILE:HG22 | 4:V:217:ARG:CG   | 2.27                     | 0.65              |
| 4:4:84:ARG:NE    | 6:6:117:MET:HE1  | 2.11                     | 0.65              |
| 4:4:237:GLY:HA2  | 4:4:240:ARG:CZ   | 2.27                     | 0.65              |
| 4:4:311:PRO:HD3  | 4:4:330:HIS:NE2  | 2.11                     | 0.65              |
| 4:D:239:LEU:HD22 | 4:D:244:VAL:HB   | 1.78                     | 0.65              |
| 4:M:213:ILE:HG21 | 4:M:217:ARG:HH11 | 1.61                     | 0.65              |
| 3:3:384:PRO:HG3  | 3:3:542:ARG:HE   | 1.62                     | 0.65              |
| 3:3:440:ARG:HH11 | 3:3:440:ARG:CG   | 2.09                     | 0.65              |
| 4:D:105:LEU:HD23 | 4:D:337:PRO:HG3  | 1.77                     | 0.65              |
| 4:D:254:TYR:HD1  | 4:D:255:SER:N    | 1.89                     | 0.65              |
| 7:P:45:ARG:NH2   | 7:P:137:LEU:HD23 | 2.12                     | 0.65              |
| 8:Q:108:ILE:HG22 | 8:Q:114:ARG:NH1  | 2.12                     | 0.65              |
| 1:S:50:PRO:O     | 1:S:53:VAL:HG12  | 1.95                     | 0.65              |
| 5:5:18:GLU:HB2   | 5:5:26:TRP:HB2   | 1.78                     | 0.65              |
| 1:A:214:LYS:O    | 1:A:216:THR:HG23 | 1.96                     | 0.65              |
| 1:A:267:PRO:HG2  | 1:A:270:THR:HG22 | 1.77                     | 0.65              |
| 3:C:31:PRO:HG3   | 3:C:137:TYR:CD1  | 2.32                     | 0.65              |
| 5:E:5:ARG:HH11   | 5:E:5:ARG:CG     | 2.04                     | 0.65              |
| 6:F:163:TYR:HB3  | 6:F:168:GLU:O    | 1.97                     | 0.65              |
| 1:S:397:ARG:NE   | 3:U:79:LEU:HD12  | 2.12                     | 0.65              |
| 6:X:83:ARG:HA    | 6:X:111:CYS:HB3  | 1.78                     | 0.65              |
| 4:4:133:LEU:HD21 | 4:4:204:TYR:CD2  | 2.32                     | 0.65              |
| 1:A:366:PHE:CD1  | 1:A:370:LEU:HD21 | 2.31                     | 0.65              |
| 3:U:229:ILE:HD11 | 3:U:289:TRP:HZ3  | 1.61                     | 0.65              |
| 3:U:603:PRO:HB2  | 3:U:634:ALA:HB2  | 1.78                     | 0.65              |
| 1:1:214:LYS:O    | 1:1:216:THR:HG23 | 1.96                     | 0.65              |
| 1:A:438:ARG:HD2  | 1:A:438:ARG:H    | 1.61                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:219:ASN:HD22 | 1:J:223:THR:HG21 | 1.61                     | 0.65              |
| 1:1:360:ARG:O    | 3:3:207:VAL:HG13 | 1.97                     | 0.65              |
| 3:3:508:GLY:O    | 3:3:512:LEU:HB2  | 1.97                     | 0.65              |
| 5:5:135:ILE:HG22 | 5:5:136:LEU:HG   | 1.77                     | 0.65              |
| 3:U:534:ALA:HB3  | 3:U:542:ARG:HH12 | 1.62                     | 0.65              |
| 1:1:110:VAL:N    | 1:1:111:PRO:HD3  | 2.13                     | 0.64              |
| 3:C:20:MET:HE3   | 3:C:432:PHE:CB   | 2.26                     | 0.64              |
| 7:G:48:ASN:HB2   | 7:G:50:LEU:HD23  | 1.79                     | 0.64              |
| 7:P:153:THR:HG22 | 7:P:155:LYS:H    | 1.62                     | 0.64              |
| 7:9:153:THR:HG22 | 7:9:155:LYS:H    | 1.62                     | 0.64              |
| 4:D:314:ARG:HG2  | 4:D:314:ARG:NH1  | 2.05                     | 0.64              |
| 3:L:115:HIS:HB3  | 4:M:321:MET:HE3  | 1.80                     | 0.64              |
| 3:U:173:PHE:HB3  | 3:U:296:PHE:CE1  | 2.32                     | 0.64              |
| 4:V:84:ARG:CD    | 6:X:117:MET:HE1  | 2.27                     | 0.64              |
| 4:V:122:GLU:HB2  | 4:V:290:ILE:HD11 | 1.79                     | 0.64              |
| 4:V:225:PRO:CG   | 4:V:228:VAL:HB   | 2.27                     | 0.64              |
| 3:U:112:LEU:HD12 | 4:V:322:GLU:HG3  | 1.79                     | 0.64              |
| 3:U:508:GLY:O    | 3:U:512:LEU:HB2  | 1.97                     | 0.64              |
| 5:W:5:ARG:HH11   | 5:W:5:ARG:CG     | 2.01                     | 0.64              |
| 1:1:186:THR:CG2  | 1:1:200:ARG:H    | 2.10                     | 0.64              |
| 1:1:341:MET:HE1  | 1:1:409:PRO:HB2  | 1.78                     | 0.64              |
| 3:L:87:VAL:HA    | 3:L:91:MET:CE    | 2.24                     | 0.64              |
| 1:A:344:LEU:O    | 1:A:347:PHE:HB3  | 1.98                     | 0.64              |
| 3:C:120:PRO:HG2  | 8:H:42:TYR:OH    | 1.97                     | 0.64              |
| 4:D:371:ARG:NH2  | 4:D:376:VAL:HG21 | 2.12                     | 0.64              |
| 1:J:50:PRO:O     | 1:J:53:VAL:HG12  | 1.96                     | 0.64              |
| 3:L:205:ARG:CA   | 3:L:209:THR:HG22 | 2.28                     | 0.64              |
| 3:L:337:ARG:H    | 3:L:337:ARG:CD   | 2.09                     | 0.64              |
| 3:U:6:VAL:HG12   | 3:U:7:ASN:N      | 2.12                     | 0.64              |
| 4:V:254:TYR:HE2  | 4:V:346:THR:HA   | 1.58                     | 0.64              |
| 4:4:213:ILE:HG21 | 4:4:217:ARG:HH11 | 1.62                     | 0.64              |
| 4:4:381:LEU:HD11 | 4:4:397:ILE:HG12 | 1.80                     | 0.64              |
| 4:M:122:GLU:HB2  | 4:M:290:ILE:HD11 | 1.79                     | 0.64              |
| 3:U:205:ARG:CA   | 3:U:209:THR:HG22 | 2.28                     | 0.64              |
| 3:3:438:LYS:O    | 3:3:441:MET:HG3  | 1.98                     | 0.64              |
| 1:A:364:ALA:HB1  | 3:C:207:VAL:HG22 | 1.79                     | 0.64              |
| 3:C:603:PRO:HB2  | 3:C:634:ALA:HB2  | 1.80                     | 0.64              |
| 4:D:40:VAL:O     | 4:D:40:VAL:HG22  | 1.98                     | 0.64              |
| 3:L:715:GLU:HB3  | 3:L:746:ARG:CZ   | 2.27                     | 0.64              |
| 4:M:102:GLU:HG2  | 4:M:175:ILE:O    | 1.98                     | 0.64              |
| 4:M:142:ALA:HB1  | 4:M:145:PRO:HG2  | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:N:104:VAL:HG12 | 5:N:108:TRP:HE3  | 1.63                     | 0.64              |
| 1:S:316:LEU:HD12 | 1:S:323:LEU:HB2  | 1.80                     | 0.64              |
| 1:1:393:LEU:HD22 | 3:3:106:GLY:HA3  | 1.80                     | 0.64              |
| 3:3:300:TRP:CD1  | 3:3:300:TRP:H    | 2.16                     | 0.64              |
| 4:4:239:LEU:HD22 | 4:4:244:VAL:HB   | 1.80                     | 0.64              |
| 1:A:55:GLU:O     | 1:A:59:ARG:HB2   | 1.97                     | 0.64              |
| 1:A:65:ARG:CZ    | 1:A:268:MET:HE1  | 2.27                     | 0.64              |
| 1:A:253:GLN:N    | 1:A:253:GLN:HE21 | 1.96                     | 0.64              |
| 4:D:213:ILE:HG21 | 4:D:217:ARG:NH1  | 2.13                     | 0.64              |
| 4:D:249:ARG:HB3  | 4:D:257:TYR:HD1  | 1.63                     | 0.64              |
| 6:6:77:VAL:HG22  | 6:6:104:TRP:HB2  | 1.79                     | 0.64              |
| 1:A:110:VAL:N    | 1:A:111:PRO:HD3  | 2.13                     | 0.64              |
| 3:C:30:VAL:HG22  | 3:C:48:CYS:HA    | 1.80                     | 0.64              |
| 5:E:18:GLU:HB2   | 5:E:26:TRP:HB2   | 1.80                     | 0.64              |
| 7:G:153:THR:HG22 | 7:G:155:LYS:N    | 2.11                     | 0.64              |
| 4:V:371:ARG:NH2  | 4:V:376:VAL:HG21 | 2.12                     | 0.64              |
| 4:D:84:ARG:HG2   | 9:F:182:SF4:S2   | 2.39                     | 0.64              |
| 5:W:26:TRP:HE1   | 5:W:91:ARG:HH21  | 1.45                     | 0.64              |
| 4:4:238:SER:HB3  | 4:4:279:ARG:NH2  | 2.12                     | 0.63              |
| 3:C:402:PRO:HG3  | 3:C:535:MET:HE1  | 1.80                     | 0.63              |
| 1:S:65:ARG:NH2   | 1:S:268:MET:HE1  | 2.13                     | 0.63              |
| 1:S:115:ILE:O    | 1:S:119:ILE:HG13 | 1.98                     | 0.63              |
| 3:U:171:SER:HB2  | 3:U:172:PRO:HD2  | 1.79                     | 0.63              |
| 3:3:285:VAL:HG22 | 3:3:286:ASN:N    | 2.14                     | 0.63              |
| 4:4:371:ARG:NH2  | 4:4:376:VAL:HG21 | 2.12                     | 0.63              |
| 4:D:102:GLU:HG2  | 4:D:175:ILE:O    | 1.99                     | 0.63              |
| 3:L:584:VAL:HG12 | 3:L:600:VAL:HB   | 1.80                     | 0.63              |
| 7:Y:71:GLU:HB2   | 7:Y:90:VAL:HB    | 1.80                     | 0.63              |
| 4:4:213:ILE:HD12 | 4:4:213:ILE:H    | 1.64                     | 0.63              |
| 6:6:153:GLN:HG3  | 7:9:124:TYR:CZ   | 2.34                     | 0.63              |
| 6:6:165:GLU:HG2  | 7:9:148:ARG:HH11 | 1.62                     | 0.63              |
| 4:4:40:VAL:O     | 4:4:40:VAL:HG22  | 1.98                     | 0.63              |
| 4:4:142:ALA:HB1  | 4:4:145:PRO:HG2  | 1.80                     | 0.63              |
| 8:7:108:ILE:HG22 | 8:7:114:ARG:NH1  | 2.14                     | 0.63              |
| 4:M:64:THR:HG23  | 6:O:123:ILE:CD1  | 2.28                     | 0.63              |
| 1:S:344:LEU:O    | 1:S:347:PHE:HB3  | 1.99                     | 0.63              |
| 4:V:64:THR:HG23  | 6:X:123:ILE:HD11 | 1.81                     | 0.63              |
| 7:Y:153:THR:HG22 | 7:Y:155:LYS:N    | 2.13                     | 0.63              |
| 1:A:186:THR:CG2  | 1:A:200:ARG:H    | 2.12                     | 0.63              |
| 3:C:469:ARG:HB2  | 3:C:470:PRO:HD2  | 1.81                     | 0.63              |
| 3:L:300:TRP:CD1  | 3:L:300:TRP:H    | 2.16                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:393:MET:O    | 4:M:396:ILE:HG22 | 1.99                     | 0.63              |
| 5:N:71:VAL:HG11  | 5:N:89:PHE:HD2   | 1.64                     | 0.63              |
| 3:U:30:VAL:HG22  | 3:U:48:CYS:HA    | 1.79                     | 0.63              |
| 4:V:164:THR:OG1  | 4:V:170:HIS:HB3  | 1.99                     | 0.63              |
| 1:1:65:ARG:CZ    | 1:1:268:MET:HE1  | 2.28                     | 0.63              |
| 3:3:603:PRO:HB2  | 3:3:634:ALA:HB2  | 1.79                     | 0.63              |
| 3:C:125:GLY:HA3  | 3:C:246:ASN:HD22 | 1.63                     | 0.63              |
| 1:J:366:PHE:CD1  | 1:J:370:LEU:HD21 | 2.33                     | 0.63              |
| 2:K:134:ILE:HG13 | 2:K:145:VAL:HG21 | 1.79                     | 0.63              |
| 4:V:84:ARG:HD3   | 6:X:117:MET:HE1  | 1.80                     | 0.63              |
| 8:Z:108:ILE:HG22 | 8:Z:114:ARG:NH1  | 2.14                     | 0.63              |
| 1:1:332:PRO:HD2  | 2:2:90:LEU:HD23  | 1.80                     | 0.63              |
| 3:3:317:LEU:HD22 | 3:3:317:LEU:N    | 2.13                     | 0.63              |
| 3:C:509:ALA:HB1  | 3:C:768:GLY:CA   | 2.27                     | 0.63              |
| 3:L:285:VAL:HG22 | 3:L:286:ASN:N    | 2.14                     | 0.63              |
| 4:M:64:THR:HB    | 4:M:66:PHE:CE1   | 2.34                     | 0.63              |
| 3:U:716:LEU:HD21 | 3:U:758:LEU:HB3  | 1.81                     | 0.63              |
| 5:W:104:VAL:HG12 | 5:W:108:TRP:HE3  | 1.63                     | 0.63              |
| 4:M:222:GLY:CA   | 4:M:396:ILE:HD11 | 2.28                     | 0.63              |
| 3:U:509:ALA:HB1  | 3:U:768:GLY:CA   | 2.29                     | 0.63              |
| 4:V:155:THR:HB   | 4:V:193:LEU:HD12 | 1.80                     | 0.63              |
| 1:1:65:ARG:NH2   | 1:1:268:MET:HE1  | 2.13                     | 0.63              |
| 1:1:364:ALA:HB1  | 3:3:207:VAL:HG22 | 1.81                     | 0.63              |
| 3:3:30:VAL:HG22  | 3:3:48:CYS:HA    | 1.79                     | 0.63              |
| 3:3:509:ALA:HB1  | 3:3:768:GLY:CA   | 2.27                     | 0.63              |
| 5:5:13:LYS:HZ3   | 5:5:33:ARG:HH21  | 1.44                     | 0.63              |
| 7:9:48:ASN:HB2   | 7:9:50:LEU:HD23  | 1.80                     | 0.63              |
| 1:A:115:ILE:O    | 1:A:119:ILE:HG13 | 1.98                     | 0.63              |
| 4:D:140:LEU:O    | 4:D:140:LEU:HD23 | 1.98                     | 0.63              |
| 5:E:168:ALA:HA   | 5:E:171:ARG:NH1  | 2.14                     | 0.63              |
| 4:M:64:THR:OG1   | 6:O:83:ARG:NH1   | 2.30                     | 0.63              |
| 1:S:107:LEU:O    | 1:S:111:PRO:HG3  | 1.99                     | 0.63              |
| 3:U:216:PHE:HZ   | 8:Z:128:PHE:HD2  | 1.46                     | 0.63              |
| 3:U:317:LEU:HD22 | 3:U:317:LEU:N    | 2.14                     | 0.63              |
| 3:U:398:VAL:HG21 | 3:U:448:MET:HE2  | 1.81                     | 0.63              |
| 4:V:230:ILE:HD11 | 4:V:244:VAL:HG21 | 1.80                     | 0.63              |
| 5:W:42:LYS:HB2   | 5:W:108:TRP:CZ2  | 2.34                     | 0.63              |
| 5:5:104:VAL:HG12 | 5:5:108:TRP:HE3  | 1.63                     | 0.62              |
| 1:A:53:VAL:HG23  | 1:A:231:MET:HE2  | 1.81                     | 0.62              |
| 4:D:64:THR:OG1   | 6:F:83:ARG:NH1   | 2.32                     | 0.62              |
| 1:J:115:ILE:O    | 1:J:119:ILE:HG13 | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:357:ALA:HB2  | 3:L:641:LEU:HD11 | 1.81                     | 0.62              |
| 3:L:509:ALA:HB1  | 3:L:768:GLY:CA   | 2.26                     | 0.62              |
| 2:2:61:MET:HE2   | 3:3:214:MET:HG2  | 1.81                     | 0.62              |
| 3:3:229:ILE:HD11 | 3:3:289:TRP:HZ3  | 1.63                     | 0.62              |
| 4:4:64:THR:HB    | 4:4:66:PHE:CE1   | 2.35                     | 0.62              |
| 4:M:230:ILE:HD11 | 4:M:244:VAL:HG21 | 1.81                     | 0.62              |
| 4:M:311:PRO:HD3  | 4:M:330:HIS:NE2  | 2.14                     | 0.62              |
| 1:1:436:LEU:HD23 | 2:2:90:LEU:HA    | 1.81                     | 0.62              |
| 4:D:236:GLY:C    | 4:D:238:SER:H    | 2.07                     | 0.62              |
| 4:M:238:SER:HB3  | 4:M:279:ARG:NH2  | 2.14                     | 0.62              |
| 6:O:112:ALA:O    | 6:O:127:VAL:HG23 | 1.99                     | 0.62              |
| 3:U:373:GLY:HA3  | 3:U:538:ALA:HB2  | 1.81                     | 0.62              |
| 3:U:571:VAL:HG21 | 3:U:591:HIS:CD2  | 2.34                     | 0.62              |
| 4:V:236:GLY:C    | 4:V:238:SER:H    | 2.08                     | 0.62              |
| 2:T:110:GLU:HA   | 8:Z:121:ARG:NH1  | 2.14                     | 0.62              |
| 1:1:366:PHE:CD1  | 1:1:370:LEU:HD21 | 2.34                     | 0.62              |
| 4:4:213:ILE:HG22 | 4:4:217:ARG:CG   | 2.29                     | 0.62              |
| 4:D:212:PRO:CG   | 4:D:213:ILE:HD12 | 2.27                     | 0.62              |
| 4:D:341:GLU:HG2  | 4:D:358:VAL:HG22 | 1.81                     | 0.62              |
| 5:E:104:VAL:HG12 | 5:E:108:TRP:HE3  | 1.64                     | 0.62              |
| 1:J:186:THR:CG2  | 1:J:200:ARG:H    | 2.12                     | 0.62              |
| 3:L:13:VAL:HG21  | 3:L:17:THR:HG21  | 1.82                     | 0.62              |
| 3:L:438:LYS:O    | 3:L:441:MET:HG3  | 2.00                     | 0.62              |
| 3:L:440:ARG:HH11 | 3:L:440:ARG:CG   | 2.12                     | 0.62              |
| 3:L:469:ARG:HB2  | 3:L:470:PRO:HD2  | 1.80                     | 0.62              |
| 3:L:546:ALA:HA   | 3:L:678:PHE:CE2  | 2.34                     | 0.62              |
| 4:M:84:ARG:HG2   | 9:O:182:SF4:S2   | 2.39                     | 0.62              |
| 4:V:167:ARG:HD3  | 6:X:143:ARG:HH12 | 1.64                     | 0.62              |
| 4:V:265:PRO:HG2  | 4:V:282:GLU:HG2  | 1.80                     | 0.62              |
| 4:4:252:TYR:HE2  | 5:5:87:ARG:NH2   | 1.98                     | 0.62              |
| 2:B:42:ARG:H     | 2:B:45:ARG:HG3   | 1.64                     | 0.62              |
| 3:C:165:ASP:HB3  | 3:C:178:ARG:HD2  | 1.80                     | 0.62              |
| 4:D:70:MET:HG2   | 4:D:78:ASN:OD1   | 2.00                     | 0.62              |
| 4:V:222:GLY:CA   | 4:V:396:ILE:HD11 | 2.28                     | 0.62              |
| 7:Y:45:ARG:NH2   | 7:Y:137:LEU:HD23 | 2.14                     | 0.62              |
| 4:4:262:PHE:HD1  | 4:4:289:ILE:HD11 | 1.65                     | 0.62              |
| 7:9:153:THR:HG22 | 7:9:155:LYS:N    | 2.15                     | 0.62              |
| 3:C:205:ARG:CA   | 3:C:209:THR:HG22 | 2.28                     | 0.62              |
| 1:J:184:GLU:CD   | 1:J:186:THR:HG22 | 2.24                     | 0.62              |
| 6:O:114:SER:HB2  | 7:P:97:ARG:HD2   | 1.81                     | 0.62              |
| 6:O:153:GLN:HG3  | 7:P:124:TYR:CZ   | 2.35                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:242:GLY:HA2  | 1:S:268:MET:O    | 1.99                     | 0.62              |
| 3:U:203:ILE:HG22 | 3:U:204:GLU:N    | 2.13                     | 0.62              |
| 4:V:43:LEU:HD11  | 4:V:397:ILE:HD11 | 1.82                     | 0.62              |
| 4:V:64:THR:HB    | 4:V:66:PHE:CE1   | 2.35                     | 0.62              |
| 3:3:469:ARG:HB2  | 3:3:470:PRO:HD2  | 1.81                     | 0.62              |
| 1:A:16:THR:CG2   | 1:A:229:PRO:HB3  | 2.29                     | 0.62              |
| 4:D:238:SER:HB3  | 4:D:279:ARG:HH22 | 1.65                     | 0.62              |
| 4:M:213:ILE:HG21 | 4:M:217:ARG:NH1  | 2.13                     | 0.62              |
| 3:U:715:GLU:HB3  | 3:U:746:ARG:CZ   | 2.30                     | 0.62              |
| 5:W:135:ILE:HG22 | 5:W:136:LEU:HG   | 1.79                     | 0.62              |
| 6:X:138:PRO:CG   | 7:Y:121:MET:HG3  | 2.29                     | 0.62              |
| 3:3:20:MET:HE3   | 3:3:432:PHE:CB   | 2.30                     | 0.62              |
| 1:A:65:ARG:NH2   | 1:A:268:MET:HE1  | 2.15                     | 0.62              |
| 5:E:42:LYS:HB2   | 5:E:108:TRP:CZ2  | 2.34                     | 0.62              |
| 1:J:364:ALA:HB1  | 3:L:207:VAL:HG22 | 1.81                     | 0.62              |
| 7:P:153:THR:HG22 | 7:P:155:LYS:N    | 2.15                     | 0.62              |
| 1:S:436:LEU:HD23 | 2:T:90:LEU:HA    | 1.80                     | 0.62              |
| 4:V:314:ARG:HG2  | 4:V:314:ARG:NH1  | 2.08                     | 0.62              |
| 1:A:289:ALA:HB3  | 1:A:337:MET:HE3  | 1.81                     | 0.62              |
| 1:A:397:ARG:HE   | 3:C:79:LEU:HD12  | 1.63                     | 0.62              |
| 1:S:332:PRO:CD   | 2:T:90:LEU:HD23  | 2.30                     | 0.62              |
| 3:U:591:HIS:ND1  | 3:U:592:PRO:HD2  | 2.15                     | 0.62              |
| 4:V:381:LEU:HD11 | 4:V:397:ILE:HG12 | 1.80                     | 0.62              |
| 1:1:332:PRO:CD   | 2:2:90:LEU:HD23  | 2.29                     | 0.61              |
| 4:4:213:ILE:HG21 | 4:4:217:ARG:NH1  | 2.13                     | 0.61              |
| 4:4:249:ARG:HB3  | 4:4:257:TYR:HD1  | 1.65                     | 0.61              |
| 3:C:186:ARG:HD3  | 3:C:229:ILE:HG22 | 1.82                     | 0.61              |
| 3:C:300:TRP:CD1  | 3:C:300:TRP:H    | 2.16                     | 0.61              |
| 4:D:213:ILE:HD12 | 4:D:213:ILE:H    | 1.64                     | 0.61              |
| 3:L:398:VAL:HB   | 3:L:450:LEU:HD22 | 1.81                     | 0.61              |
| 4:M:140:LEU:O    | 4:M:140:LEU:HD23 | 1.99                     | 0.61              |
| 1:S:10:ASP:OD1   | 1:S:11:PRO:HD2   | 1.99                     | 0.61              |
| 2:2:134:ILE:HG13 | 2:2:145:VAL:HG21 | 1.82                     | 0.61              |
| 1:J:341:MET:HE1  | 1:J:409:PRO:HB2  | 1.81                     | 0.61              |
| 3:L:282:VAL:HG22 | 3:L:285:VAL:HG12 | 1.82                     | 0.61              |
| 6:X:43:LEU:HD13  | 6:X:83:ARG:O     | 1.99                     | 0.61              |
| 4:4:230:ILE:HG22 | 4:4:230:ILE:O    | 2.00                     | 0.61              |
| 5:5:42:LYS:HB2   | 5:5:108:TRP:CZ2  | 2.35                     | 0.61              |
| 4:D:213:ILE:HG22 | 4:D:217:ARG:CG   | 2.30                     | 0.61              |
| 3:L:384:PRO:HG3  | 3:L:542:ARG:HE   | 1.66                     | 0.61              |
| 4:M:236:GLY:C    | 4:M:238:SER:H    | 2.09                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:249:ARG:HB3  | 4:M:257:TYR:HD1  | 1.65                     | 0.61              |
| 4:M:254:TYR:HE2  | 4:M:346:THR:HA   | 1.64                     | 0.61              |
| 1:S:259:LYS:HA   | 1:S:284:LEU:HD21 | 1.83                     | 0.61              |
| 1:S:366:PHE:CD1  | 1:S:370:LEU:HD21 | 2.35                     | 0.61              |
| 3:U:300:TRP:CD1  | 3:U:300:TRP:H    | 2.17                     | 0.61              |
| 7:Y:33:LEU:CD1   | 7:Y:161:TYR:HB2  | 2.28                     | 0.61              |
| 3:3:586:HIS:CD2  | 3:3:604:ALA:HB2  | 2.36                     | 0.61              |
| 3:L:591:HIS:ND1  | 3:L:592:PRO:HD2  | 2.16                     | 0.61              |
| 4:M:213:ILE:HD12 | 4:M:213:ILE:H    | 1.66                     | 0.61              |
| 5:N:92:VAL:O     | 5:N:92:VAL:HG23  | 2.00                     | 0.61              |
| 4:V:215:TYR:O    | 4:V:219:ARG:HB2  | 1.99                     | 0.61              |
| 3:3:169:PRO:HA   | 3:3:175:ILE:HA   | 1.83                     | 0.61              |
| 3:3:205:ARG:C    | 3:3:209:THR:HG22 | 2.25                     | 0.61              |
| 4:4:122:GLU:HB2  | 4:4:290:ILE:HD11 | 1.82                     | 0.61              |
| 4:4:222:GLY:CA   | 4:4:396:ILE:HD11 | 2.29                     | 0.61              |
| 3:C:317:LEU:HD22 | 3:C:317:LEU:N    | 2.15                     | 0.61              |
| 3:C:722:THR:HG21 | 3:C:756:GLY:N    | 2.16                     | 0.61              |
| 7:G:71:GLU:HB2   | 7:G:90:VAL:HB    | 1.82                     | 0.61              |
| 5:N:42:LYS:HB2   | 5:N:108:TRP:CZ2  | 2.35                     | 0.61              |
| 5:W:71:VAL:HG11  | 5:W:89:PHE:HD2   | 1.66                     | 0.61              |
| 1:1:88:TYR:HB2   | 1:1:216:THR:HG22 | 1.82                     | 0.61              |
| 3:3:690:GLY:HA3  | 3:3:770:ARG:NH2  | 2.16                     | 0.61              |
| 3:C:586:HIS:CD2  | 3:C:604:ALA:HB2  | 2.35                     | 0.61              |
| 5:E:35:LYS:HD3   | 5:E:102:PRO:HB2  | 1.83                     | 0.61              |
| 3:U:87:VAL:HA    | 3:U:91:MET:CE    | 2.28                     | 0.61              |
| 5:W:168:ALA:HA   | 5:W:171:ARG:NH1  | 2.16                     | 0.61              |
| 3:3:120:PRO:HG2  | 8:7:42:TYR:OH    | 2.00                     | 0.61              |
| 1:A:278:GLU:OE2  | 6:X:19:ILE:N     | 2.31                     | 0.61              |
| 4:D:96:ALA:HB2   | 4:D:346:THR:HG21 | 1.82                     | 0.61              |
| 4:D:188:PRO:HB3  | 3:U:724:ARG:HD3  | 1.71                     | 0.61              |
| 4:D:252:TYR:HE2  | 5:E:87:ARG:NH2   | 1.99                     | 0.61              |
| 3:U:285:VAL:HG22 | 3:U:286:ASN:N    | 2.15                     | 0.61              |
| 7:9:46:HIS:CE1   | 7:9:52:LYS:HG2   | 2.35                     | 0.61              |
| 4:D:262:PHE:HD1  | 4:D:289:ILE:HD11 | 1.65                     | 0.61              |
| 5:N:34:PHE:HE1   | 5:N:38:MET:SD    | 2.23                     | 0.61              |
| 6:O:16:ARG:O     | 6:O:21:PHE:HD2   | 1.83                     | 0.61              |
| 1:S:186:THR:CG2  | 1:S:200:ARG:H    | 2.13                     | 0.61              |
| 3:U:169:PRO:HA   | 3:U:175:ILE:HA   | 1.82                     | 0.61              |
| 3:U:584:VAL:HG12 | 3:U:600:VAL:HB   | 1.82                     | 0.61              |
| 4:V:44:MET:HA    | 4:V:44:MET:HE2   | 1.83                     | 0.61              |
| 5:W:167:PRO:HB3  | 7:Y:66:TYR:CE2   | 2.36                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:X:77:VAL:HG22  | 6:X:104:TRP:HB2  | 1.83                     | 0.61              |
| 1:1:242:GLY:HA2  | 1:1:268:MET:O    | 2.01                     | 0.61              |
| 3:3:398:VAL:HG21 | 3:3:448:MET:HE2  | 1.83                     | 0.61              |
| 6:6:153:GLN:HG3  | 7:9:124:TYR:OH   | 2.01                     | 0.61              |
| 1:A:197:ALA:HB3  | 2:B:66:PHE:CZ    | 2.35                     | 0.61              |
| 3:C:586:HIS:NE2  | 3:C:604:ALA:HB2  | 2.14                     | 0.61              |
| 4:D:230:ILE:HD11 | 4:D:244:VAL:HG21 | 1.82                     | 0.61              |
| 4:D:367:ARG:HH12 | 4:D:369:LYS:CB   | 2.14                     | 0.61              |
| 2:K:87:SER:HB3   | 11:K:182:FES:S2  | 2.41                     | 0.61              |
| 4:M:213:ILE:HG22 | 4:M:217:ARG:CG   | 2.31                     | 0.61              |
| 3:U:398:VAL:C    | 3:U:399:LEU:HD12 | 2.26                     | 0.61              |
| 3:U:546:ALA:HA   | 3:U:678:PHE:CE2  | 2.36                     | 0.61              |
| 6:X:153:GLN:HG3  | 7:Y:124:TYR:OH   | 1.99                     | 0.61              |
| 4:4:393:MET:O    | 4:4:396:ILE:HG22 | 2.01                     | 0.61              |
| 5:5:168:ALA:HA   | 5:5:171:ARG:NH1  | 2.16                     | 0.61              |
| 1:A:360:ARG:O    | 3:C:207:VAL:HG13 | 2.01                     | 0.61              |
| 1:J:253:GLN:HE21 | 1:J:253:GLN:N    | 1.98                     | 0.61              |
| 2:K:136:VAL:HG12 | 2:K:137:ASN:N    | 2.16                     | 0.61              |
| 3:L:173:PHE:HB3  | 3:L:296:PHE:CE1  | 2.35                     | 0.61              |
| 4:M:161:GLU:OE1  | 7:P:34:LYS:HG2   | 2.00                     | 0.61              |
| 5:N:5:ARG:HH11   | 5:N:5:ARG:CG     | 2.01                     | 0.61              |
| 4:V:224:ILE:HD11 | 4:V:275:ARG:NH1  | 2.15                     | 0.61              |
| 1:1:162:LEU:O    | 1:1:165:THR:HG22 | 2.01                     | 0.60              |
| 3:3:13:VAL:HG21  | 3:3:17:THR:HG21  | 1.83                     | 0.60              |
| 3:3:254:THR:OG1  | 3:3:624:LEU:HD23 | 2.01                     | 0.60              |
| 3:3:571:VAL:HG21 | 3:3:591:HIS:CD2  | 2.35                     | 0.60              |
| 1:J:97:GLU:O     | 1:J:100:SER:HB3  | 2.00                     | 0.60              |
| 3:U:200:LEU:O    | 3:U:201:ASP:HB2  | 2.01                     | 0.60              |
| 1:1:92:ASN:ND2   | 10:1:440:FMN:C2  | 2.64                     | 0.60              |
| 2:2:87:SER:HB3   | 11:2:182:FES:S2  | 2.41                     | 0.60              |
| 3:3:546:ALA:HA   | 3:3:678:PHE:CE2  | 2.36                     | 0.60              |
| 4:4:155:THR:HB   | 4:4:193:LEU:HD12 | 1.83                     | 0.60              |
| 4:4:236:GLY:C    | 4:4:238:SER:H    | 2.09                     | 0.60              |
| 6:6:117:MET:HB3  | 7:9:99:ILE:HD13  | 1.84                     | 0.60              |
| 4:D:350:ARG:O    | 4:D:373:PRO:HB2  | 2.01                     | 0.60              |
| 7:G:33:LEU:CD1   | 7:G:161:TYR:HB2  | 2.29                     | 0.60              |
| 1:J:92:ASN:ND2   | 10:J:440:FMN:N1  | 2.49                     | 0.60              |
| 3:L:690:GLY:HA3  | 3:L:770:ARG:NH2  | 2.16                     | 0.60              |
| 4:V:238:SER:HB3  | 4:V:279:ARG:HH22 | 1.63                     | 0.60              |
| 3:3:584:VAL:HG12 | 3:3:600:VAL:HB   | 1.83                     | 0.60              |
| 4:4:153:ARG:HH11 | 4:4:153:ARG:HG3  | 1.66                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:212:PRO:CG   | 4:4:213:ILE:HD12 | 2.28                     | 0.60              |
| 4:4:350:ARG:O    | 4:4:373:PRO:HB2  | 2.01                     | 0.60              |
| 6:6:99:MET:CG    | 6:6:100:PRO:HD2  | 2.31                     | 0.60              |
| 3:C:216:PHE:HZ   | 8:H:128:PHE:HD2  | 1.49                     | 0.60              |
| 3:C:694:LEU:HB3  | 3:C:762:ALA:CB   | 2.31                     | 0.60              |
| 4:M:230:ILE:O    | 4:M:230:ILE:HG22 | 2.01                     | 0.60              |
| 4:M:381:LEU:HD11 | 4:M:397:ILE:HG12 | 1.82                     | 0.60              |
| 3:U:690:GLY:HA3  | 3:U:770:ARG:NH2  | 2.16                     | 0.60              |
| 6:X:99:MET:CG    | 6:X:100:PRO:HD2  | 2.32                     | 0.60              |
| 1:1:253:GLN:N    | 1:1:253:GLN:HE21 | 1.98                     | 0.60              |
| 1:1:259:LYS:HA   | 1:1:284:LEU:HD21 | 1.83                     | 0.60              |
| 1:A:242:GLY:HA2  | 1:A:268:MET:O    | 2.01                     | 0.60              |
| 3:C:584:VAL:HG12 | 3:C:600:VAL:HB   | 1.82                     | 0.60              |
| 3:L:171:SER:HB2  | 3:L:172:PRO:HD2  | 1.83                     | 0.60              |
| 4:M:363:SER:HB2  | 5:N:174:LEU:H    | 1.66                     | 0.60              |
| 5:N:135:ILE:HG22 | 5:N:136:LEU:HG   | 1.82                     | 0.60              |
| 5:N:174:LEU:HD22 | 5:N:180:GLY:HA2  | 1.84                     | 0.60              |
| 4:V:61:TYR:HB3   | 6:X:88:MET:HE2   | 1.83                     | 0.60              |
| 3:3:715:GLU:HB3  | 3:3:746:ARG:CZ   | 2.30                     | 0.60              |
| 8:7:89:ALA:O     | 8:7:91:ILE:HG13  | 2.01                     | 0.60              |
| 1:J:160:LYS:HG3  | 1:J:161:ASN:H    | 1.66                     | 0.60              |
| 4:M:263:ASP:HB2  | 4:M:285:GLU:CD   | 2.26                     | 0.60              |
| 3:U:185:LYS:HG2  | 3:U:188:VAL:HG22 | 1.84                     | 0.60              |
| 4:4:230:ILE:HD11 | 4:4:244:VAL:HG21 | 1.83                     | 0.60              |
| 6:F:16:ARG:O     | 6:F:21:PHE:HD2   | 1.85                     | 0.60              |
| 6:F:77:VAL:HG22  | 6:F:104:TRP:HB2  | 1.83                     | 0.60              |
| 6:F:138:PRO:CG   | 7:G:121:MET:HG3  | 2.31                     | 0.60              |
| 3:L:30:VAL:HG22  | 3:L:48:CYS:HA    | 1.83                     | 0.60              |
| 6:O:16:ARG:HG2   | 6:O:21:PHE:CE2   | 2.37                     | 0.60              |
| 6:O:153:GLN:HG3  | 7:P:124:TYR:OH   | 2.02                     | 0.60              |
| 1:S:88:TYR:HB2   | 1:S:216:THR:HG22 | 1.83                     | 0.60              |
| 2:T:42:ARG:H     | 2:T:45:ARG:HG3   | 1.67                     | 0.60              |
| 1:S:160:LYS:HG3  | 1:S:161:ASN:H    | 1.67                     | 0.60              |
| 4:V:110:PRO:HB3  | 4:V:301:PRO:HG2  | 1.83                     | 0.60              |
| 4:4:148:TYR:HB3  | 4:4:200:ARG:NH1  | 2.17                     | 0.60              |
| 4:4:238:SER:HB3  | 4:4:279:ARG:HH22 | 1.65                     | 0.60              |
| 1:A:341:MET:HE1  | 1:A:409:PRO:HB2  | 1.83                     | 0.60              |
| 4:D:222:GLY:CA   | 4:D:396:ILE:HD11 | 2.32                     | 0.60              |
| 5:E:116:ARG:HG3  | 5:E:129:HIS:CE1  | 2.36                     | 0.60              |
| 5:E:175:THR:CG2  | 5:E:178:ASP:HB2  | 2.29                     | 0.60              |
| 3:3:112:LEU:HD12 | 4:4:322:GLU:HG3  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:141:GLU:OE2  | 3:3:143:TYR:HE1  | 1.85                     | 0.60              |
| 4:4:116:ILE:HD11 | 4:4:182:LEU:HG   | 1.84                     | 0.60              |
| 4:D:64:THR:HB    | 4:D:66:PHE:CE1   | 2.36                     | 0.60              |
| 3:L:20:MET:HE3   | 3:L:432:PHE:CB   | 2.32                     | 0.60              |
| 4:V:148:TYR:HB3  | 4:V:200:ARG:NH1  | 2.17                     | 0.60              |
| 1:1:97:GLU:O     | 1:1:100:SER:HB3  | 2.01                     | 0.60              |
| 3:C:87:VAL:HA    | 3:C:91:MET:CE    | 2.29                     | 0.60              |
| 3:C:546:ALA:HA   | 3:C:678:PHE:CE2  | 2.36                     | 0.60              |
| 3:C:715:GLU:HB3  | 3:C:746:ARG:CZ   | 2.31                     | 0.60              |
| 4:D:263:ASP:HB2  | 4:D:285:GLU:CD   | 2.27                     | 0.60              |
| 3:U:240:ALA:CB   | 3:U:276:ARG:HB2  | 2.32                     | 0.60              |
| 4:V:367:ARG:HE   | 5:W:122:PHE:HZ   | 1.50                     | 0.60              |
| 1:1:41:ALA:HB2   | 1:1:116:GLU:HG3  | 1.84                     | 0.59              |
| 1:1:53:VAL:HG23  | 1:1:231:MET:HE2  | 1.84                     | 0.59              |
| 5:5:174:LEU:HD22 | 5:5:180:GLY:HA2  | 1.84                     | 0.59              |
| 8:7:33:LYS:HD2   | 8:7:36:ASP:OD1   | 2.02                     | 0.59              |
| 3:C:169:PRO:HA   | 3:C:175:ILE:HA   | 1.84                     | 0.59              |
| 4:D:122:GLU:HB2  | 4:D:290:ILE:HD11 | 1.83                     | 0.59              |
| 1:J:88:TYR:HB2   | 1:J:216:THR:HG22 | 1.84                     | 0.59              |
| 2:K:40:TRP:CD1   | 2:K:74:PRO:HA    | 2.37                     | 0.59              |
| 4:M:110:PRO:HB3  | 4:M:301:PRO:HG2  | 1.82                     | 0.59              |
| 4:M:155:THR:HB   | 4:M:193:LEU:HD12 | 1.84                     | 0.59              |
| 5:N:42:LYS:CB    | 5:N:107:LEU:HD13 | 2.26                     | 0.59              |
| 6:O:99:MET:CG    | 6:O:100:PRO:HD2  | 2.31                     | 0.59              |
| 4:V:252:TYR:HE2  | 5:W:87:ARG:NH2   | 1.97                     | 0.59              |
| 7:Y:33:LEU:HD11  | 7:Y:161:TYR:CB   | 2.29                     | 0.59              |
| 2:2:86:LEU:O     | 2:2:90:LEU:HD12  | 2.02                     | 0.59              |
| 3:3:216:PHE:CZ   | 8:7:128:PHE:CD2  | 2.86                     | 0.59              |
| 4:4:43:LEU:HD11  | 4:4:397:ILE:HD11 | 1.84                     | 0.59              |
| 7:9:71:GLU:HB2   | 7:9:90:VAL:HB    | 1.84                     | 0.59              |
| 3:C:240:ALA:CB   | 3:C:276:ARG:HB2  | 2.31                     | 0.59              |
| 3:C:384:PRO:HG3  | 3:C:542:ARG:HE   | 1.67                     | 0.59              |
| 3:C:571:VAL:HG21 | 3:C:591:HIS:CD2  | 2.37                     | 0.59              |
| 4:D:84:ARG:O     | 6:F:83:ARG:NH2   | 2.35                     | 0.59              |
| 4:D:393:MET:O    | 4:D:396:ILE:HG22 | 2.02                     | 0.59              |
| 3:L:317:LEU:HD22 | 3:L:317:LEU:N    | 2.16                     | 0.59              |
| 3:L:497:TRP:NE1  | 3:L:524:LEU:HD11 | 2.17                     | 0.59              |
| 3:L:571:VAL:CG2  | 3:L:587:LEU:HD11 | 2.31                     | 0.59              |
| 4:M:59:ILE:HD11  | 5:N:135:ILE:HG23 | 1.83                     | 0.59              |
| 3:U:254:THR:OG1  | 3:U:624:LEU:HD23 | 2.02                     | 0.59              |
| 5:W:116:ARG:HG3  | 5:W:129:HIS:CE1  | 2.37                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:X:148:ILE:HG22 | 6:X:149:TYR:N    | 2.16                     | 0.59              |
| 1:1:115:ILE:O    | 1:1:119:ILE:HG13 | 2.02                     | 0.59              |
| 1:1:437:TRP:CZ3  | 2:2:96:LEU:HB2   | 2.37                     | 0.59              |
| 1:A:363:VAL:HA   | 1:A:367:MET:HB2  | 1.83                     | 0.59              |
| 3:C:205:ARG:C    | 3:C:209:THR:HG22 | 2.27                     | 0.59              |
| 4:D:153:ARG:HH11 | 4:D:153:ARG:HG3  | 1.67                     | 0.59              |
| 1:J:332:PRO:HD2  | 2:K:90:LEU:HD23  | 1.84                     | 0.59              |
| 1:J:344:LEU:O    | 1:J:347:PHE:HB3  | 2.01                     | 0.59              |
| 3:L:240:ALA:CB   | 3:L:276:ARG:HB2  | 2.32                     | 0.59              |
| 4:M:350:ARG:O    | 4:M:373:PRO:HB2  | 2.02                     | 0.59              |
| 4:M:371:ARG:NH2  | 4:M:376:VAL:HG21 | 2.16                     | 0.59              |
| 3:U:330:LYS:HA   | 3:U:647:ALA:HB1  | 1.85                     | 0.59              |
| 6:X:16:ARG:O     | 6:X:21:PHE:HD2   | 1.85                     | 0.59              |
| 4:4:96:ALA:HB2   | 4:4:346:THR:HG21 | 1.85                     | 0.59              |
| 8:7:37:PHE:CD1   | 8:7:55:MET:HB2   | 2.37                     | 0.59              |
| 2:B:139:GLU:HB2  | 2:B:140:PRO:CD   | 2.31                     | 0.59              |
| 3:C:173:PHE:HB3  | 3:C:296:PHE:CE1  | 2.37                     | 0.59              |
| 3:C:477:LEU:HD22 | 3:C:517:ALA:HB1  | 1.84                     | 0.59              |
| 6:F:83:ARG:HA    | 6:F:111:CYS:HB3  | 1.84                     | 0.59              |
| 1:J:10:ASP:OD1   | 1:J:11:PRO:HD2   | 2.02                     | 0.59              |
| 3:L:216:PHE:CZ   | 8:Q:128:PHE:CD2  | 2.86                     | 0.59              |
| 3:L:285:VAL:HG13 | 3:L:286:ASN:N    | 2.16                     | 0.59              |
| 3:L:722:THR:HG21 | 3:L:756:GLY:N    | 2.18                     | 0.59              |
| 4:M:247:ASP:OD1  | 4:M:249:ARG:HG3  | 2.02                     | 0.59              |
| 6:O:77:VAL:HG22  | 6:O:104:TRP:HB2  | 1.83                     | 0.59              |
| 6:O:148:ILE:HG22 | 6:O:149:TYR:N    | 2.17                     | 0.59              |
| 3:U:55:PRO:HG3   | 3:U:74:GLN:H     | 1.67                     | 0.59              |
| 4:V:213:ILE:CG2  | 4:V:217:ARG:HH11 | 2.16                     | 0.59              |
| 2:2:81:GLN:HB3   | 2:2:122:VAL:HG21 | 1.84                     | 0.59              |
| 3:3:165:ASP:HB3  | 3:3:178:ARG:HD2  | 1.83                     | 0.59              |
| 4:4:254:TYR:HE2  | 4:4:346:THR:HA   | 1.66                     | 0.59              |
| 4:4:363:SER:HB2  | 5:5:174:LEU:H    | 1.67                     | 0.59              |
| 4:M:367:ARG:HE   | 5:N:122:PHE:HZ   | 1.49                     | 0.59              |
| 1:S:16:THR:CG2   | 1:S:229:PRO:HB3  | 2.31                     | 0.59              |
| 3:U:202:PHE:C    | 3:U:203:ILE:HD13 | 2.28                     | 0.59              |
| 3:3:586:HIS:NE2  | 3:3:604:ALA:HB2  | 2.18                     | 0.59              |
| 2:B:106:ILE:HG22 | 2:B:110:GLU:HB2  | 1.85                     | 0.59              |
| 3:C:192:GLU:OE2  | 3:C:440:ARG:HA   | 2.03                     | 0.59              |
| 4:D:116:ILE:HD11 | 4:D:182:LEU:HG   | 1.85                     | 0.59              |
| 5:E:134:LYS:HD3  | 5:E:137:THR:OG1  | 2.02                     | 0.59              |
| 6:F:77:VAL:O     | 6:F:77:VAL:HG12  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:53:VAL:HG23  | 1:J:231:MET:HE2  | 1.85                     | 0.59              |
| 2:K:114:ASP:OD2  | 2:K:116:LEU:HD21 | 2.03                     | 0.59              |
| 4:V:161:GLU:OE1  | 7:Y:34:LYS:HG2   | 2.02                     | 0.59              |
| 2:2:77:LYS:H     | 2:2:116:LEU:HA   | 1.67                     | 0.59              |
| 3:C:689:LYS:HE3  | 3:C:771:VAL:HG13 | 1.85                     | 0.59              |
| 3:L:202:PHE:C    | 3:L:203:ILE:HD13 | 2.28                     | 0.59              |
| 3:L:689:LYS:HE3  | 3:L:771:VAL:HG13 | 1.83                     | 0.59              |
| 8:Q:37:PHE:CD1   | 8:Q:55:MET:HB2   | 2.38                     | 0.59              |
| 2:T:136:VAL:HG12 | 2:T:137:ASN:N    | 2.18                     | 0.59              |
| 4:V:140:LEU:HD23 | 4:V:140:LEU:O    | 2.02                     | 0.59              |
| 4:V:240:ARG:HG3  | 4:V:265:PRO:O    | 2.02                     | 0.59              |
| 6:X:77:VAL:O     | 6:X:77:VAL:HG12  | 2.02                     | 0.59              |
| 1:1:351:GLU:HA   | 3:3:205:ARG:HH12 | 1.67                     | 0.59              |
| 4:D:148:TYR:HB3  | 4:D:200:ARG:NH1  | 2.17                     | 0.59              |
| 4:D:211:SER:HB2  | 4:D:214:PHE:HB3  | 1.85                     | 0.59              |
| 6:F:16:ARG:HG2   | 6:F:21:PHE:CE2   | 2.37                     | 0.59              |
| 1:J:332:PRO:CD   | 2:K:90:LEU:HD23  | 2.32                     | 0.59              |
| 1:J:351:GLU:HA   | 3:L:205:ARG:HH12 | 1.67                     | 0.59              |
| 5:W:167:PRO:HB3  | 7:Y:66:TYR:CD2   | 2.37                     | 0.59              |
| 7:Y:128:ASP:O    | 7:Y:144:LYS:HD3  | 2.03                     | 0.59              |
| 3:L:254:THR:OG1  | 3:L:624:LEU:HD23 | 2.03                     | 0.59              |
| 7:P:71:GLU:HB2   | 7:P:90:VAL:HB    | 1.84                     | 0.59              |
| 8:Q:13:TRP:CE2   | 8:Q:17:LEU:HD11  | 2.38                     | 0.59              |
| 4:V:64:THR:HG23  | 6:X:123:ILE:CD1  | 2.33                     | 0.59              |
| 4:V:213:ILE:HD12 | 4:V:213:ILE:H    | 1.68                     | 0.59              |
| 6:6:16:ARG:HG2   | 6:6:21:PHE:CE2   | 2.38                     | 0.59              |
| 4:D:44:MET:HA    | 4:D:44:MET:HE2   | 1.84                     | 0.59              |
| 4:D:155:THR:HB   | 4:D:193:LEU:HD12 | 1.85                     | 0.59              |
| 4:D:164:THR:OG1  | 4:D:170:HIS:HB3  | 2.02                     | 0.59              |
| 3:L:169:PRO:HA   | 3:L:175:ILE:HA   | 1.85                     | 0.59              |
| 4:M:225:PRO:CG   | 4:M:228:VAL:HB   | 2.27                     | 0.59              |
| 4:M:265:PRO:HG2  | 4:M:282:GLU:HG2  | 1.84                     | 0.59              |
| 1:S:110:VAL:N    | 1:S:111:PRO:HD3  | 2.18                     | 0.59              |
| 3:U:458:LEU:H    | 3:U:458:LEU:HD12 | 1.67                     | 0.59              |
| 4:V:102:GLU:HG2  | 4:V:175:ILE:O    | 2.03                     | 0.59              |
| 3:3:173:PHE:HB3  | 3:3:296:PHE:CE1  | 2.37                     | 0.58              |
| 3:3:693:TYR:HB3  | 3:3:759:TYR:CD2  | 2.39                     | 0.58              |
| 1:A:92:ASN:ND2   | 10:A:440:FMN:C2  | 2.66                     | 0.58              |
| 6:F:115:GLY:HA2  | 6:F:125:GLN:HA   | 1.85                     | 0.58              |
| 6:F:148:ILE:HG22 | 6:F:149:TYR:N    | 2.18                     | 0.58              |
| 7:G:33:LEU:HD11  | 7:G:161:TYR:CB   | 2.30                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:259:LYS:HA   | 1:J:284:LEU:HD21 | 1.85                     | 0.58              |
| 1:S:332:PRO:HD2  | 2:T:90:LEU:HD23  | 1.85                     | 0.58              |
| 3:U:227:THR:HG21 | 3:U:237:ASP:HB2  | 1.85                     | 0.58              |
| 7:Y:123:ASP:HB2  | 7:Y:129:LEU:HD21 | 1.85                     | 0.58              |
| 3:C:494:LYS:O    | 3:C:498:GLU:HG2  | 2.02                     | 0.58              |
| 3:U:469:ARG:HB2  | 3:U:470:PRO:HD2  | 1.85                     | 0.58              |
| 3:U:670:PRO:HD2  | 3:U:676:LEU:HD23 | 1.83                     | 0.58              |
| 4:V:230:ILE:HG22 | 4:V:230:ILE:O    | 2.03                     | 0.58              |
| 5:W:35:LYS:HD3   | 5:W:102:PRO:HB2  | 1.84                     | 0.58              |
| 8:Z:33:LYS:HD2   | 8:Z:36:ASP:OD1   | 2.03                     | 0.58              |
| 2:B:86:LEU:O     | 2:B:90:LEU:HD12  | 2.03                     | 0.58              |
| 1:J:342:TRP:HE3  | 1:J:342:TRP:O    | 1.86                     | 0.58              |
| 3:L:136:GLU:CG   | 5:N:189:ARG:HG2  | 2.30                     | 0.58              |
| 4:M:238:SER:HB3  | 4:M:279:ARG:HH22 | 1.66                     | 0.58              |
| 5:W:59:THR:HG22  | 5:W:59:THR:O     | 2.03                     | 0.58              |
| 1:1:53:VAL:O     | 1:1:57:VAL:HG23  | 2.03                     | 0.58              |
| 3:3:344:TYR:CD1  | 3:3:568:TYR:CE1  | 2.92                     | 0.58              |
| 4:4:110:PRO:HB3  | 4:4:301:PRO:HG2  | 1.85                     | 0.58              |
| 5:5:42:LYS:CB    | 5:5:107:LEU:HD13 | 2.28                     | 0.58              |
| 4:D:265:PRO:HG2  | 4:D:282:GLU:HG2  | 1.83                     | 0.58              |
| 6:F:43:LEU:HD13  | 6:F:83:ARG:O     | 2.03                     | 0.58              |
| 2:K:42:ARG:H     | 2:K:45:ARG:HG3   | 1.68                     | 0.58              |
| 3:L:165:ASP:HB3  | 3:L:178:ARG:HD2  | 1.85                     | 0.58              |
| 4:M:148:TYR:HB3  | 4:M:200:ARG:NH1  | 2.19                     | 0.58              |
| 3:U:402:PRO:CB   | 3:U:535:MET:HE1  | 2.33                     | 0.58              |
| 4:4:115:THR:CG2  | 4:4:297:LEU:HD23 | 2.34                     | 0.58              |
| 5:5:71:VAL:HG11  | 5:5:89:PHE:HD2   | 1.67                     | 0.58              |
| 5:5:175:THR:CG2  | 5:5:178:ASP:HB2  | 2.32                     | 0.58              |
| 4:D:129:HIS:HE1  | 4:D:349:ALA:HB1  | 1.66                     | 0.58              |
| 5:E:71:VAL:HG11  | 5:E:89:PHE:HD2   | 1.68                     | 0.58              |
| 8:H:33:LYS:HD2   | 8:H:36:ASP:OD1   | 2.03                     | 0.58              |
| 1:J:92:ASN:ND2   | 10:J:440:FMN:C2  | 2.67                     | 0.58              |
| 3:U:13:VAL:HG21  | 3:U:17:THR:HG21  | 1.84                     | 0.58              |
| 3:U:112:LEU:HD21 | 3:U:130:LEU:HD11 | 1.84                     | 0.58              |
| 3:U:402:PRO:HG3  | 3:U:535:MET:HE1  | 1.85                     | 0.58              |
| 3:U:683:LEU:HD23 | 3:U:683:LEU:N    | 2.19                     | 0.58              |
| 4:V:263:ASP:HB2  | 4:V:285:GLU:CD   | 2.28                     | 0.58              |
| 6:X:16:ARG:HG2   | 6:X:21:PHE:CE2   | 2.37                     | 0.58              |
| 3:3:591:HIS:ND1  | 3:3:592:PRO:HD2  | 2.19                     | 0.58              |
| 4:4:409:ARG:O    | 4:4:409:ARG:HG2  | 2.03                     | 0.58              |
| 2:B:81:GLN:HB3   | 2:B:122:VAL:HG21 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:385:ALA:HB2  | 3:C:531:LYS:HB3  | 1.85                     | 0.58              |
| 4:D:367:ARG:HE   | 5:E:122:PHE:HZ   | 1.51                     | 0.58              |
| 6:F:115:GLY:HA3  | 6:F:125:GLN:OE1  | 2.04                     | 0.58              |
| 2:K:58:THR:HG21  | 3:L:200:LEU:N    | 2.18                     | 0.58              |
| 3:U:586:HIS:NE2  | 3:U:604:ALA:HB2  | 2.18                     | 0.58              |
| 4:V:287:VAL:O    | 4:V:291:LYS:HG3  | 2.03                     | 0.58              |
| 3:3:440:ARG:CG   | 3:3:440:ARG:NH1  | 2.67                     | 0.58              |
| 4:4:64:THR:HG23  | 6:6:123:ILE:CD1  | 2.33                     | 0.58              |
| 4:4:164:THR:OG1  | 4:4:170:HIS:HB3  | 2.02                     | 0.58              |
| 4:4:263:ASP:HB2  | 4:4:285:GLU:CD   | 2.28                     | 0.58              |
| 4:D:409:ARG:O    | 4:D:409:ARG:HG2  | 2.03                     | 0.58              |
| 1:J:360:ARG:O    | 3:L:207:VAL:HG13 | 2.04                     | 0.58              |
| 3:U:344:TYR:CD1  | 3:U:568:TYR:CE1  | 2.92                     | 0.58              |
| 4:V:212:PRO:CG   | 4:V:213:ILE:HD12 | 2.29                     | 0.58              |
| 2:2:40:TRP:CD1   | 2:2:74:PRO:HA    | 2.39                     | 0.58              |
| 3:3:202:PHE:C    | 3:3:203:ILE:HD13 | 2.29                     | 0.58              |
| 4:M:212:PRO:CG   | 4:M:213:ILE:HD12 | 2.31                     | 0.58              |
| 1:S:437:TRP:CZ3  | 2:T:96:LEU:HB2   | 2.39                     | 0.58              |
| 2:T:81:GLN:HB3   | 2:T:122:VAL:HG21 | 1.85                     | 0.58              |
| 3:U:694:LEU:HB3  | 3:U:762:ALA:CB   | 2.32                     | 0.58              |
| 1:1:303:THR:OG1  | 1:1:306:VAL:HG23 | 2.03                     | 0.58              |
| 2:2:42:ARG:H     | 2:2:45:ARG:HG3   | 1.68                     | 0.58              |
| 3:C:684:ARG:HG2  | 3:C:684:ARG:NH1  | 2.18                     | 0.58              |
| 4:D:43:LEU:HD11  | 4:D:397:ILE:HD11 | 1.84                     | 0.58              |
| 4:D:110:PRO:HB3  | 4:D:301:PRO:HG2  | 1.85                     | 0.58              |
| 5:E:42:LYS:CB    | 5:E:107:LEU:HD13 | 2.30                     | 0.58              |
| 1:J:197:ALA:HB3  | 2:K:66:PHE:CZ    | 2.38                     | 0.58              |
| 2:K:86:LEU:O     | 2:K:90:LEU:HD12  | 2.04                     | 0.58              |
| 3:L:494:LYS:O    | 3:L:498:GLU:HG2  | 2.03                     | 0.58              |
| 3:L:572:PRO:HD2  | 3:L:577:LEU:HD21 | 1.84                     | 0.58              |
| 3:L:586:HIS:CD2  | 3:L:604:ALA:HB2  | 2.39                     | 0.58              |
| 5:N:33:ARG:O     | 5:N:37:GLU:HB2   | 2.03                     | 0.58              |
| 3:U:282:VAL:HG22 | 3:U:285:VAL:HG12 | 1.84                     | 0.58              |
| 4:V:40:VAL:O     | 4:V:40:VAL:HG22  | 2.02                     | 0.58              |
| 4:V:363:SER:HB2  | 5:W:174:LEU:H    | 1.69                     | 0.58              |
| 1:1:92:ASN:ND2   | 10:1:440:FMN:N1  | 2.52                     | 0.58              |
| 3:3:373:GLY:HA3  | 3:3:538:ALA:HB2  | 1.84                     | 0.58              |
| 4:4:102:GLU:HG2  | 4:4:175:ILE:O    | 2.04                     | 0.58              |
| 5:5:92:VAL:HG23  | 5:5:92:VAL:O     | 2.04                     | 0.58              |
| 1:A:197:ALA:HB3  | 2:B:66:PHE:CE1   | 2.39                     | 0.58              |
| 4:D:311:PRO:HD3  | 4:D:330:HIS:NE2  | 2.19                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:153:GLN:HG3  | 7:G:124:TYR:CZ   | 2.39                     | 0.58              |
| 1:J:109:ASP:C    | 1:J:111:PRO:HD3  | 2.29                     | 0.58              |
| 3:L:205:ARG:C    | 3:L:209:THR:HG22 | 2.29                     | 0.58              |
| 3:U:477:LEU:HD22 | 3:U:517:ALA:HB1  | 1.86                     | 0.58              |
| 3:U:546:ALA:C    | 3:U:547:MET:HE2  | 2.29                     | 0.58              |
| 2:2:81:GLN:HB3   | 2:2:122:VAL:CG2  | 2.34                     | 0.57              |
| 4:4:262:PHE:CD1  | 4:4:289:ILE:HD11 | 2.38                     | 0.57              |
| 1:A:250:LYS:HB3  | 1:A:252:TYR:CE2  | 2.39                     | 0.57              |
| 2:B:130:THR:HB   | 2:B:144:CYS:SG   | 2.43                     | 0.57              |
| 3:C:254:THR:OG1  | 3:C:624:LEU:HD23 | 2.03                     | 0.57              |
| 4:D:215:TYR:O    | 4:D:219:ARG:HB2  | 2.04                     | 0.57              |
| 1:J:104:ARG:HH21 | 2:K:127:SER:CB   | 2.17                     | 0.57              |
| 1:J:301:PRO:O    | 1:J:306:VAL:HG21 | 2.04                     | 0.57              |
| 3:L:684:ARG:HG2  | 3:L:684:ARG:NH1  | 2.18                     | 0.57              |
| 5:N:35:LYS:HD3   | 5:N:102:PRO:HB2  | 1.85                     | 0.57              |
| 1:S:341:MET:HE1  | 1:S:409:PRO:HB2  | 1.86                     | 0.57              |
| 3:U:586:HIS:CD2  | 3:U:604:ALA:HB2  | 2.38                     | 0.57              |
| 3:U:689:LYS:HE3  | 3:U:771:VAL:HG13 | 1.85                     | 0.57              |
| 4:V:254:TYR:CD2  | 4:V:346:THR:HA   | 2.38                     | 0.57              |
| 6:6:43:LEU:HD13  | 6:6:83:ARG:O     | 2.04                     | 0.57              |
| 3:C:497:TRP:O    | 3:C:528:LYS:HE3  | 2.04                     | 0.57              |
| 4:D:230:ILE:HG22 | 4:D:230:ILE:O    | 2.03                     | 0.57              |
| 4:D:262:PHE:CD1  | 4:D:289:ILE:HD11 | 2.38                     | 0.57              |
| 3:L:671:GLU:HA   | 3:L:671:GLU:OE2  | 2.05                     | 0.57              |
| 4:M:215:TYR:CE2  | 4:M:219:ARG:HG3  | 2.39                     | 0.57              |
| 6:O:77:VAL:HA    | 6:O:104:TRP:O    | 2.05                     | 0.57              |
| 6:O:78:MET:HG3   | 6:O:78:MET:O     | 2.03                     | 0.57              |
| 1:S:274:GLU:HG2  | 1:S:279:TRP:HE1  | 1.69                     | 0.57              |
| 1:1:16:THR:CG2   | 1:1:229:PRO:HB3  | 2.30                     | 0.57              |
| 3:3:722:THR:HG21 | 3:3:756:GLY:N    | 2.19                     | 0.57              |
| 5:5:134:LYS:HD3  | 5:5:137:THR:OG1  | 2.03                     | 0.57              |
| 3:C:13:VAL:HG21  | 3:C:17:THR:HG21  | 1.87                     | 0.57              |
| 3:C:185:LYS:HG2  | 3:C:188:VAL:HG22 | 1.85                     | 0.57              |
| 4:D:73:ARG:HG3   | 4:D:77:GLN:OE1   | 2.04                     | 0.57              |
| 6:F:164:ASN:HB2  | 7:G:128:ASP:OD2  | 2.03                     | 0.57              |
| 3:L:693:TYR:HB3  | 3:L:759:TYR:CD2  | 2.40                     | 0.57              |
| 3:L:715:GLU:HB3  | 3:L:746:ARG:NH1  | 2.19                     | 0.57              |
| 4:M:44:MET:HA    | 4:M:44:MET:HE2   | 1.85                     | 0.57              |
| 4:V:211:SER:HB2  | 4:V:214:PHE:HB3  | 1.85                     | 0.57              |
| 1:1:250:LYS:HB3  | 1:1:252:TYR:CE2  | 2.39                     | 0.57              |
| 1:1:344:LEU:O    | 1:1:347:PHE:HB3  | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:140:LEU:O    | 4:4:140:LEU:HD23 | 2.03                     | 0.57              |
| 7:9:45:ARG:NH2   | 7:9:137:LEU:HD23 | 2.20                     | 0.57              |
| 8:7:121:ARG:HG3  | 8:7:121:ARG:NH1  | 2.19                     | 0.57              |
| 1:A:356:CYS:HB3  | 1:A:358:PRO:HG2  | 1.84                     | 0.57              |
| 3:L:694:LEU:HB3  | 3:L:762:ALA:CB   | 2.31                     | 0.57              |
| 4:M:262:PHE:HD1  | 4:M:289:ILE:HD11 | 1.70                     | 0.57              |
| 5:N:58:LEU:O     | 5:N:58:LEU:HD12  | 2.05                     | 0.57              |
| 3:U:385:ALA:HB2  | 3:U:531:LYS:HB3  | 1.86                     | 0.57              |
| 4:V:70:MET:HG2   | 4:V:78:ASN:OD1   | 2.03                     | 0.57              |
| 1:1:186:THR:HG23 | 1:1:200:ARG:H    | 1.69                     | 0.57              |
| 3:3:185:LYS:HG3  | 3:3:202:PHE:HE2  | 1.69                     | 0.57              |
| 3:3:671:GLU:HA   | 3:3:671:GLU:OE2  | 2.04                     | 0.57              |
| 3:3:684:ARG:HG2  | 3:3:684:ARG:NH1  | 2.19                     | 0.57              |
| 6:6:148:ILE:HG22 | 6:6:149:TYR:N    | 2.18                     | 0.57              |
| 1:A:238:PHE:HE1  | 1:A:249:MET:CE   | 2.16                     | 0.57              |
| 3:C:281:GLU:HG2  | 3:C:283:PRO:HD3  | 1.87                     | 0.57              |
| 1:J:242:GLY:HA2  | 1:J:268:MET:O    | 2.04                     | 0.57              |
| 5:N:66:GLU:HG2   | 5:N:95:PRO:HA    | 1.86                     | 0.57              |
| 6:O:138:PRO:CG   | 7:P:121:MET:HG3  | 2.35                     | 0.57              |
| 3:U:494:LYS:O    | 3:U:498:GLU:HG2  | 2.04                     | 0.57              |
| 1:1:10:ASP:OD1   | 1:1:11:PRO:HD2   | 2.04                     | 0.57              |
| 3:3:469:ARG:HA   | 3:3:754:PRO:HG3  | 1.86                     | 0.57              |
| 1:A:53:VAL:O     | 1:A:57:VAL:HG23  | 2.04                     | 0.57              |
| 6:F:153:GLN:HG3  | 7:G:124:TYR:OH   | 2.05                     | 0.57              |
| 7:G:45:ARG:HH21  | 7:G:137:LEU:HD23 | 1.70                     | 0.57              |
| 2:K:61:MET:HE2   | 3:L:214:MET:HG2  | 1.87                     | 0.57              |
| 3:L:309:PRO:HG2  | 3:L:320:ALA:O    | 2.05                     | 0.57              |
| 3:L:670:PRO:HD2  | 3:L:676:LEU:HD23 | 1.87                     | 0.57              |
| 3:U:194:VAL:HG12 | 3:U:411:LEU:HD22 | 1.87                     | 0.57              |
| 3:U:326:PHE:CE2  | 3:U:330:LYS:HE3  | 2.39                     | 0.57              |
| 2:2:106:ILE:HG22 | 2:2:110:GLU:HB2  | 1.87                     | 0.57              |
| 2:2:139:GLU:HB2  | 2:2:140:PRO:CD   | 2.32                     | 0.57              |
| 3:3:125:GLY:HA3  | 3:3:246:ASN:HD22 | 1.68                     | 0.57              |
| 3:3:240:ALA:CB   | 3:3:276:ARG:HB2  | 2.35                     | 0.57              |
| 3:3:497:TRP:O    | 3:3:528:LYS:HE3  | 2.04                     | 0.57              |
| 5:5:25:LEU:CD2   | 5:5:25:LEU:N     | 2.68                     | 0.57              |
| 1:A:41:ALA:HB2   | 1:A:116:GLU:HG3  | 1.86                     | 0.57              |
| 6:F:165:GLU:HG2  | 7:G:148:ARG:HH11 | 1.68                     | 0.57              |
| 1:J:356:CYS:HB3  | 1:J:358:PRO:HG2  | 1.85                     | 0.57              |
| 3:L:402:PRO:CG   | 3:L:535:MET:HE1  | 2.35                     | 0.57              |
| 4:M:43:LEU:HD11  | 4:M:397:ILE:HD11 | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:O:83:ARG:HA    | 6:O:111:CYS:HB3  | 1.86                     | 0.57              |
| 6:O:107:SER:O    | 6:O:137:VAL:HG12 | 2.04                     | 0.57              |
| 3:U:384:PRO:HG3  | 3:U:542:ARG:HE   | 1.68                     | 0.57              |
| 4:V:119:ILE:O    | 4:V:123:LEU:HB2  | 2.05                     | 0.57              |
| 4:4:64:THR:OG1   | 6:6:83:ARG:NH1   | 2.37                     | 0.57              |
| 2:B:129:HIS:CD2  | 2:B:130:THR:HG23 | 2.40                     | 0.57              |
| 3:C:546:ALA:C    | 3:C:547:MET:HE2  | 2.29                     | 0.57              |
| 3:C:591:HIS:ND1  | 3:C:592:PRO:HD2  | 2.19                     | 0.57              |
| 4:D:168:PHE:HE1  | 6:F:141:PRO:HG3  | 1.69                     | 0.57              |
| 2:K:81:GLN:HB3   | 2:K:122:VAL:HG21 | 1.85                     | 0.57              |
| 3:L:402:PRO:CB   | 3:L:535:MET:HE1  | 2.34                     | 0.57              |
| 4:M:153:ARG:HH11 | 4:M:153:ARG:HG3  | 1.69                     | 0.57              |
| 4:M:211:SER:HB2  | 4:M:214:PHE:HB3  | 1.87                     | 0.57              |
| 7:P:30:PRO:HB2   | 7:P:162:VAL:HG13 | 1.86                     | 0.57              |
| 4:V:63:HIS:O     | 6:X:122:ALA:HB1  | 2.05                     | 0.57              |
| 3:3:341:VAL:HG21 | 3:3:364:LEU:HD11 | 1.85                     | 0.57              |
| 4:4:44:MET:HA    | 4:4:44:MET:HE2   | 1.87                     | 0.57              |
| 6:6:83:ARG:HA    | 6:6:111:CYS:HB3  | 1.85                     | 0.57              |
| 2:B:114:ASP:OD2  | 2:B:116:LEU:HD21 | 2.05                     | 0.57              |
| 3:C:690:GLY:HA3  | 3:C:770:ARG:NH2  | 2.19                     | 0.57              |
| 6:F:82:GLY:HA2   | 9:F:182:SF4:S4   | 2.45                     | 0.57              |
| 4:M:164:THR:OG1  | 4:M:170:HIS:HB3  | 2.04                     | 0.57              |
| 6:O:164:ASN:HB2  | 7:P:128:ASP:OD2  | 2.04                     | 0.57              |
| 4:V:73:ARG:HG3   | 4:V:77:GLN:OE1   | 2.05                     | 0.57              |
| 6:X:138:PRO:HG3  | 7:Y:121:MET:HG3  | 1.87                     | 0.57              |
| 7:Y:48:ASN:CB    | 7:Y:50:LEU:HD23  | 2.35                     | 0.57              |
| 8:Z:82:ILE:HG23  | 8:Z:95:ALA:HB3   | 1.87                     | 0.57              |
| 1:A:266:LEU:HB3  | 1:A:270:THR:HG21 | 1.87                     | 0.57              |
| 1:J:214:LYS:O    | 1:J:216:THR:HG23 | 2.04                     | 0.57              |
| 1:J:287:ILE:HG22 | 1:J:302:PHE:CG   | 2.40                     | 0.57              |
| 4:M:215:TYR:O    | 4:M:219:ARG:HB2  | 2.03                     | 0.57              |
| 5:N:25:LEU:CD2   | 5:N:25:LEU:N     | 2.68                     | 0.57              |
| 1:S:53:VAL:O     | 1:S:57:VAL:HG23  | 2.04                     | 0.57              |
| 1:S:162:LEU:O    | 1:S:165:THR:HG22 | 2.04                     | 0.57              |
| 7:Y:46:HIS:CE1   | 7:Y:52:LYS:HG2   | 2.40                     | 0.57              |
| 8:Z:121:ARG:HG3  | 8:Z:121:ARG:NH1  | 2.20                     | 0.57              |
| 3:3:458:LEU:HD12 | 3:3:458:LEU:H    | 1.69                     | 0.56              |
| 3:3:497:TRP:O    | 3:3:500:ALA:HB3  | 2.05                     | 0.56              |
| 1:A:160:LYS:HG3  | 1:A:161:ASN:H    | 1.70                     | 0.56              |
| 3:C:671:GLU:HA   | 3:C:671:GLU:OE2  | 2.04                     | 0.56              |
| 2:T:101:THR:HG23 | 2:T:106:ILE:O    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:114:ASP:OD2  | 2:T:116:LEU:HD21 | 2.05                     | 0.56              |
| 3:U:688:ARG:HB3  | 3:U:770:ARG:HD3  | 1.87                     | 0.56              |
| 6:6:115:GLY:HA2  | 6:6:125:GLN:HA   | 1.87                     | 0.56              |
| 1:A:270:THR:O    | 1:A:311:MET:HG3  | 2.05                     | 0.56              |
| 3:C:497:TRP:O    | 3:C:500:ALA:HB3  | 2.05                     | 0.56              |
| 8:H:89:ALA:O     | 8:H:91:ILE:HG13  | 2.05                     | 0.56              |
| 3:L:398:VAL:C    | 3:L:399:LEU:HD12 | 2.30                     | 0.56              |
| 1:S:97:GLU:O     | 1:S:100:SER:HB3  | 2.05                     | 0.56              |
| 1:S:287:ILE:HG22 | 1:S:302:PHE:CG   | 2.40                     | 0.56              |
| 2:2:136:VAL:HG12 | 2:2:137:ASN:N    | 2.20                     | 0.56              |
| 3:3:494:LYS:O    | 3:3:498:GLU:HG2  | 2.05                     | 0.56              |
| 3:3:670:PRO:HD2  | 3:3:676:LEU:HD23 | 1.87                     | 0.56              |
| 4:4:153:ARG:HG3  | 4:4:153:ARG:NH1  | 2.20                     | 0.56              |
| 1:A:88:TYR:HB2   | 1:A:216:THR:HG22 | 1.88                     | 0.56              |
| 1:A:303:THR:OG1  | 1:A:306:VAL:HG23 | 2.05                     | 0.56              |
| 2:B:10:PHE:CZ    | 2:B:33:ARG:HG3   | 2.40                     | 0.56              |
| 2:B:40:TRP:CD1   | 2:B:74:PRO:HA    | 2.40                     | 0.56              |
| 2:B:139:GLU:CB   | 2:B:140:PRO:CD   | 2.82                     | 0.56              |
| 3:C:285:VAL:HG22 | 3:C:286:ASN:N    | 2.20                     | 0.56              |
| 3:C:398:VAL:C    | 3:C:399:LEU:HD12 | 2.30                     | 0.56              |
| 3:C:571:VAL:CG2  | 3:C:587:LEU:HD11 | 2.36                     | 0.56              |
| 4:D:254:TYR:CD1  | 4:D:255:SER:N    | 2.70                     | 0.56              |
| 5:E:92:VAL:HG23  | 5:E:92:VAL:O     | 2.05                     | 0.56              |
| 6:F:117:MET:HB3  | 7:G:99:ILE:HD13  | 1.86                     | 0.56              |
| 1:J:16:THR:CG2   | 1:J:229:PRO:HB3  | 2.33                     | 0.56              |
| 4:M:84:ARG:NE    | 6:O:117:MET:HE1  | 2.21                     | 0.56              |
| 5:N:175:THR:CG2  | 5:N:178:ASP:HB2  | 2.34                     | 0.56              |
| 7:P:134:GLU:H    | 7:P:134:GLU:CD   | 2.12                     | 0.56              |
| 1:S:53:VAL:HG23  | 1:S:231:MET:HE2  | 1.88                     | 0.56              |
| 1:S:186:THR:HG23 | 1:S:200:ARG:H    | 1.69                     | 0.56              |
| 1:S:438:ARG:HD2  | 1:S:438:ARG:N    | 2.20                     | 0.56              |
| 2:T:106:ILE:HG22 | 2:T:110:GLU:HB2  | 1.87                     | 0.56              |
| 3:U:701:ALA:HB2  | 3:U:763:LEU:HB2  | 1.86                     | 0.56              |
| 4:V:43:LEU:HD11  | 4:V:397:ILE:CD1  | 2.36                     | 0.56              |
| 5:W:25:LEU:N     | 5:W:25:LEU:CD2   | 2.68                     | 0.56              |
| 6:X:77:VAL:HA    | 6:X:104:TRP:O    | 2.06                     | 0.56              |
| 7:Y:30:PRO:HB2   | 7:Y:162:VAL:HG13 | 1.87                     | 0.56              |
| 3:3:402:PRO:CB   | 3:3:535:MET:HE1  | 2.35                     | 0.56              |
| 3:3:572:PRO:HD2  | 3:3:577:LEU:HD21 | 1.87                     | 0.56              |
| 4:4:240:ARG:HG3  | 4:4:265:PRO:O    | 2.06                     | 0.56              |
| 6:6:138:PRO:CG   | 7:9:121:MET:HG3  | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:81:GLN:HB3   | 2:B:122:VAL:CG2  | 2.35                     | 0.56              |
| 3:C:373:GLY:HA3  | 3:C:538:ALA:HB2  | 1.87                     | 0.56              |
| 3:C:693:TYR:HB3  | 3:C:759:TYR:CD2  | 2.41                     | 0.56              |
| 4:D:363:SER:HB2  | 5:E:174:LEU:H    | 1.69                     | 0.56              |
| 8:H:37:PHE:HD1   | 8:H:53:THR:O     | 1.88                     | 0.56              |
| 3:L:473:GLU:O    | 3:L:477:LEU:HD13 | 2.04                     | 0.56              |
| 4:M:409:ARG:O    | 4:M:409:ARG:HG2  | 2.05                     | 0.56              |
| 7:P:33:LEU:HD11  | 7:P:161:TYR:CB   | 2.33                     | 0.56              |
| 3:U:46:ARG:O     | 3:U:107:MET:HG2  | 2.05                     | 0.56              |
| 3:U:571:VAL:CG2  | 3:U:587:LEU:HD11 | 2.35                     | 0.56              |
| 5:W:134:LYS:HD3  | 5:W:137:THR:OG1  | 2.04                     | 0.56              |
| 7:9:30:PRO:HB2   | 7:9:162:VAL:HG13 | 1.87                     | 0.56              |
| 7:9:96:LEU:HD21  | 7:9:129:LEU:HD12 | 1.87                     | 0.56              |
| 3:C:94:ASP:OD2   | 3:C:97:SER:HB2   | 2.06                     | 0.56              |
| 4:D:254:TYR:HE2  | 4:D:346:THR:HA   | 1.67                     | 0.56              |
| 8:H:8:GLU:HG2    | 8:H:97:TYR:CZ    | 2.41                     | 0.56              |
| 4:M:40:VAL:HG23  | 6:O:88:MET:CE    | 2.36                     | 0.56              |
| 1:S:64:GLY:HA3   | 10:S:440:FMN:O1P | 2.05                     | 0.56              |
| 1:S:92:ASN:ND2   | 10:S:440:FMN:O3' | 2.38                     | 0.56              |
| 3:U:208:HIS:HB3  | 8:Z:85:ARG:NH2   | 2.20                     | 0.56              |
| 3:U:572:PRO:HD2  | 3:U:577:LEU:HD21 | 1.87                     | 0.56              |
| 4:V:115:THR:CG2  | 4:V:297:LEU:HD23 | 2.36                     | 0.56              |
| 8:Z:37:PHE:HD1   | 8:Z:53:THR:O     | 1.87                     | 0.56              |
| 2:2:114:ASP:OD2  | 2:2:116:LEU:HD21 | 2.06                     | 0.56              |
| 3:3:281:GLU:HG2  | 3:3:283:PRO:HD3  | 1.86                     | 0.56              |
| 3:3:701:ALA:HB2  | 3:3:763:LEU:HB2  | 1.86                     | 0.56              |
| 6:6:107:SER:O    | 6:6:137:VAL:HG12 | 2.06                     | 0.56              |
| 3:C:688:ARG:HB3  | 3:C:770:ARG:HD3  | 1.87                     | 0.56              |
| 6:F:16:ARG:HG2   | 6:F:21:PHE:HE2   | 1.70                     | 0.56              |
| 1:J:104:ARG:HH21 | 2:K:127:SER:HB2  | 1.70                     | 0.56              |
| 3:L:326:PHE:CE2  | 3:L:330:LYS:HE3  | 2.40                     | 0.56              |
| 3:L:469:ARG:HA   | 3:L:754:PRO:HG3  | 1.87                     | 0.56              |
| 4:M:213:ILE:CG2  | 4:M:217:ARG:HH11 | 2.18                     | 0.56              |
| 4:M:252:TYR:HE2  | 5:N:87:ARG:NH2   | 2.04                     | 0.56              |
| 6:O:43:LEU:HD13  | 6:O:83:ARG:O     | 2.06                     | 0.56              |
| 3:U:54:LEU:N     | 3:U:55:PRO:HD3   | 2.21                     | 0.56              |
| 4:V:167:ARG:HD3  | 6:X:143:ARG:NH1  | 2.20                     | 0.56              |
| 5:W:33:ARG:O     | 5:W:37:GLU:HB2   | 2.05                     | 0.56              |
| 5:W:37:GLU:O     | 5:W:41:TYR:HD1   | 1.88                     | 0.56              |
| 1:1:438:ARG:HD2  | 1:1:438:ARG:N    | 2.21                     | 0.56              |
| 2:2:10:PHE:CZ    | 2:2:33:ARG:HG3   | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:215:TYR:CE2  | 4:4:219:ARG:HG3  | 2.41                     | 0.56              |
| 6:6:78:MET:O     | 6:6:78:MET:HG3   | 2.04                     | 0.56              |
| 7:9:33:LEU:CD1   | 7:9:161:TYR:HB2  | 2.32                     | 0.56              |
| 1:A:259:LYS:HA   | 1:A:284:LEU:HD21 | 1.87                     | 0.56              |
| 6:F:78:MET:O     | 6:F:78:MET:HG3   | 2.05                     | 0.56              |
| 1:J:162:LEU:O    | 1:J:165:THR:HG22 | 2.06                     | 0.56              |
| 1:J:250:LYS:HB3  | 1:J:252:TYR:CE2  | 2.41                     | 0.56              |
| 3:L:333:LEU:HD22 | 3:L:648:LEU:HD21 | 1.88                     | 0.56              |
| 5:N:116:ARG:HG3  | 5:N:129:HIS:CE1  | 2.39                     | 0.56              |
| 5:N:121:LEU:O    | 5:N:144:HIS:HB3  | 2.05                     | 0.56              |
| 6:O:16:ARG:HG2   | 6:O:21:PHE:HE2   | 1.70                     | 0.56              |
| 7:P:33:LEU:CD1   | 7:P:161:TYR:HB2  | 2.31                     | 0.56              |
| 1:S:37:GLY:C     | 1:S:39:GLU:H     | 2.14                     | 0.56              |
| 3:U:94:ASP:OD2   | 3:U:97:SER:HB2   | 2.06                     | 0.56              |
| 4:V:254:TYR:CD1  | 4:V:255:SER:N    | 2.68                     | 0.56              |
| 3:3:571:VAL:CG2  | 3:3:587:LEU:HD11 | 2.35                     | 0.56              |
| 4:4:76:LEU:HD12  | 4:4:76:LEU:O     | 2.06                     | 0.56              |
| 1:A:397:ARG:HG2  | 3:C:49:LEU:HD13  | 1.87                     | 0.56              |
| 3:C:55:PRO:HG3   | 3:C:74:GLN:H     | 1.66                     | 0.56              |
| 3:C:202:PHE:C    | 3:C:203:ILE:HD13 | 2.29                     | 0.56              |
| 3:C:282:VAL:HG22 | 3:C:285:VAL:HG12 | 1.88                     | 0.56              |
| 3:C:629:ILE:HG22 | 3:C:630:GLU:N    | 2.21                     | 0.56              |
| 4:D:247:ASP:OD1  | 4:D:249:ARG:HG3  | 2.05                     | 0.56              |
| 4:M:84:ARG:O     | 6:O:83:ARG:NH2   | 2.39                     | 0.56              |
| 4:M:153:ARG:HG3  | 4:M:153:ARG:NH1  | 2.21                     | 0.56              |
| 7:P:46:HIS:CE1   | 7:P:52:LYS:HG2   | 2.41                     | 0.56              |
| 1:S:303:THR:OG1  | 1:S:306:VAL:HG23 | 2.06                     | 0.56              |
| 4:V:409:ARG:HG2  | 4:V:409:ARG:O    | 2.03                     | 0.56              |
| 1:1:266:LEU:HB3  | 1:1:270:THR:HG21 | 1.88                     | 0.56              |
| 2:2:38:GLU:OE2   | 2:2:45:ARG:NH1   | 2.39                     | 0.56              |
| 4:4:213:ILE:CG2  | 4:4:217:ARG:HH11 | 2.19                     | 0.56              |
| 8:7:37:PHE:HD1   | 8:7:53:THR:O     | 1.88                     | 0.56              |
| 3:C:344:TYR:CD1  | 3:C:568:TYR:CE1  | 2.93                     | 0.56              |
| 3:C:474:ARG:HA   | 3:C:517:ALA:HB2  | 1.88                     | 0.56              |
| 5:E:58:LEU:HD12  | 5:E:58:LEU:O     | 2.05                     | 0.56              |
| 3:L:55:PRO:HG3   | 3:L:74:GLN:H     | 1.66                     | 0.56              |
| 3:L:571:VAL:HG21 | 3:L:591:HIS:CD2  | 2.40                     | 0.56              |
| 4:M:26:MET:N     | 4:M:48:SER:HG    | 2.03                     | 0.56              |
| 4:M:64:THR:HB    | 4:M:66:PHE:HE1   | 1.71                     | 0.56              |
| 1:1:89:LEU:HD23  | 1:1:118:MET:HE3  | 1.88                     | 0.56              |
| 1:1:287:ILE:HG22 | 1:1:302:PHE:CG   | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:357:ALA:HB2  | 3:3:641:LEU:HD11 | 1.88                     | 0.56              |
| 4:4:215:TYR:O    | 4:4:219:ARG:HB2  | 2.05                     | 0.56              |
| 6:6:77:VAL:O     | 6:6:77:VAL:HG12  | 2.06                     | 0.56              |
| 3:C:357:ALA:HB2  | 3:C:641:LEU:HD11 | 1.88                     | 0.56              |
| 3:C:469:ARG:HA   | 3:C:754:PRO:HG3  | 1.88                     | 0.56              |
| 7:G:123:ASP:HB2  | 7:G:129:LEU:HD21 | 1.87                     | 0.56              |
| 1:J:316:LEU:HD12 | 1:J:323:LEU:HB2  | 1.88                     | 0.56              |
| 3:L:285:VAL:HG22 | 3:L:286:ASN:H    | 1.70                     | 0.56              |
| 1:S:238:PHE:HE1  | 1:S:249:MET:CE   | 2.19                     | 0.56              |
| 2:T:38:GLU:OE2   | 2:T:45:ARG:NH1   | 2.38                     | 0.56              |
| 3:U:205:ARG:C    | 3:U:209:THR:HG22 | 2.31                     | 0.56              |
| 4:V:116:ILE:HD11 | 4:V:182:LEU:HG   | 1.86                     | 0.56              |
| 4:V:332:THR:O    | 5:W:172:ALA:HB3  | 2.06                     | 0.56              |
| 6:X:78:MET:HG3   | 6:X:78:MET:O     | 2.06                     | 0.56              |
| 1:1:357:THR:N    | 1:1:358:PRO:HD2  | 2.21                     | 0.55              |
| 3:3:546:ALA:C    | 3:3:547:MET:HE2  | 2.30                     | 0.55              |
| 4:4:211:SER:HB2  | 4:4:214:PHE:HB3  | 1.89                     | 0.55              |
| 5:5:58:LEU:HD12  | 5:5:58:LEU:O     | 2.06                     | 0.55              |
| 6:6:152:MET:HE2  | 6:6:156:LYS:HE2  | 1.88                     | 0.55              |
| 3:C:227:THR:HG21 | 3:C:237:ASP:HB2  | 1.88                     | 0.55              |
| 3:C:398:VAL:HG21 | 3:C:448:MET:HE2  | 1.87                     | 0.55              |
| 3:C:400:GLY:O    | 3:C:402:PRO:HD3  | 2.06                     | 0.55              |
| 3:C:695:ARG:NH1  | 3:C:715:GLU:OE1  | 2.39                     | 0.55              |
| 7:G:30:PRO:HB2   | 7:G:162:VAL:HG13 | 1.88                     | 0.55              |
| 3:L:54:LEU:N     | 3:L:55:PRO:HD3   | 2.20                     | 0.55              |
| 3:L:373:GLY:HA3  | 3:L:538:ALA:HB2  | 1.87                     | 0.55              |
| 4:M:52:VAL:HG23  | 4:M:388:GLU:O    | 2.06                     | 0.55              |
| 5:N:20:ASN:HD21  | 5:N:24:ASN:HB2   | 1.70                     | 0.55              |
| 3:U:399:LEU:HD12 | 3:U:399:LEU:N    | 2.21                     | 0.55              |
| 4:V:262:PHE:HD1  | 4:V:289:ILE:HD11 | 1.72                     | 0.55              |
| 8:Z:13:TRP:CE2   | 8:Z:17:LEU:HD11  | 2.41                     | 0.55              |
| 6:6:115:GLY:HA3  | 6:6:125:GLN:OE1  | 2.06                     | 0.55              |
| 1:A:29:LEU:CD1   | 1:A:155:ARG:HG3  | 2.37                     | 0.55              |
| 1:A:186:THR:HG23 | 1:A:200:ARG:H    | 1.71                     | 0.55              |
| 2:B:7:LYS:HD2    | 2:B:7:LYS:N      | 2.18                     | 0.55              |
| 2:B:61:MET:HE2   | 3:C:214:MET:HG2  | 1.87                     | 0.55              |
| 5:E:1:MET:C      | 5:E:3:LEU:H      | 2.14                     | 0.55              |
| 8:H:37:PHE:CD1   | 8:H:55:MET:HB2   | 2.42                     | 0.55              |
| 3:L:94:ASP:OD2   | 3:L:97:SER:HB2   | 2.07                     | 0.55              |
| 3:L:583:VAL:CG2  | 3:L:598:ALA:HA   | 2.36                     | 0.55              |
| 5:N:59:THR:O     | 5:N:59:THR:HG22  | 2.05                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:N:125:VAL:HG12 | 5:N:126:PHE:N    | 2.21                     | 0.55              |
| 1:S:363:VAL:HA   | 1:S:367:MET:HB2  | 1.89                     | 0.55              |
| 6:X:16:ARG:HG2   | 6:X:21:PHE:HE2   | 1.69                     | 0.55              |
| 1:1:160:LYS:HG3  | 1:1:161:ASN:H    | 1.71                     | 0.55              |
| 3:3:227:THR:HG21 | 3:3:237:ASP:HB2  | 1.88                     | 0.55              |
| 3:3:477:LEU:HD22 | 3:3:517:ALA:HB1  | 1.87                     | 0.55              |
| 4:4:148:TYR:CB   | 4:4:200:ARG:HH12 | 2.18                     | 0.55              |
| 4:4:367:ARG:HE   | 5:5:122:PHE:HZ   | 1.54                     | 0.55              |
| 1:A:265:GLU:O    | 1:A:266:LEU:HG   | 2.06                     | 0.55              |
| 4:D:85:MET:HE3   | 4:D:409:ARG:CG   | 2.36                     | 0.55              |
| 4:D:381:LEU:HD11 | 4:D:397:ILE:HG12 | 1.87                     | 0.55              |
| 1:J:37:GLY:C     | 1:J:39:GLU:H     | 2.14                     | 0.55              |
| 1:J:41:ALA:HB2   | 1:J:116:GLU:HG3  | 1.89                     | 0.55              |
| 3:L:330:LYS:HA   | 3:L:647:ALA:HB1  | 1.88                     | 0.55              |
| 3:L:456:ALA:HB3  | 3:L:459:MET:HE3  | 1.89                     | 0.55              |
| 1:S:18:TYR:OH    | 1:S:105:TYR:HB2  | 2.06                     | 0.55              |
| 3:U:112:LEU:CD2  | 3:U:130:LEU:HD11 | 2.37                     | 0.55              |
| 3:U:185:LYS:HG3  | 3:U:202:PHE:HE2  | 1.71                     | 0.55              |
| 3:U:341:VAL:HG21 | 3:U:364:LEU:HD11 | 1.87                     | 0.55              |
| 4:V:252:TYR:CE2  | 5:W:87:ARG:NH2   | 2.74                     | 0.55              |
| 4:4:74:THR:HB    | 4:4:77:GLN:H     | 1.71                     | 0.55              |
| 1:A:238:PHE:HE1  | 1:A:249:MET:HE1  | 1.72                     | 0.55              |
| 3:C:341:VAL:HG21 | 3:C:364:LEU:HD11 | 1.87                     | 0.55              |
| 7:G:46:HIS:CE1   | 7:G:52:LYS:HG2   | 2.41                     | 0.55              |
| 3:L:227:THR:HG21 | 3:L:237:ASP:HB2  | 1.88                     | 0.55              |
| 1:S:63:ARG:HD3   | 1:S:313:TYR:HD2  | 1.71                     | 0.55              |
| 2:T:139:GLU:CB   | 2:T:140:PRO:CD   | 2.83                     | 0.55              |
| 3:U:671:GLU:HA   | 3:U:671:GLU:OE2  | 2.07                     | 0.55              |
| 3:U:722:THR:HG21 | 3:U:756:GLY:N    | 2.20                     | 0.55              |
| 8:Z:37:PHE:CD1   | 8:Z:55:MET:HB2   | 2.41                     | 0.55              |
| 1:1:265:GLU:O    | 1:1:266:LEU:HG   | 2.07                     | 0.55              |
| 6:6:16:ARG:O     | 6:6:21:PHE:HD2   | 1.89                     | 0.55              |
| 6:6:163:TYR:CD2  | 6:6:169:ARG:HA   | 2.34                     | 0.55              |
| 1:A:97:GLU:O     | 1:A:100:SER:HB3  | 2.06                     | 0.55              |
| 1:A:109:ASP:C    | 1:A:111:PRO:HD3  | 2.32                     | 0.55              |
| 1:A:274:GLU:HG2  | 1:A:279:TRP:HE1  | 1.72                     | 0.55              |
| 3:C:458:LEU:H    | 3:C:458:LEU:HD12 | 1.72                     | 0.55              |
| 1:J:239:ALA:C    | 1:J:241:MET:H    | 2.15                     | 0.55              |
| 3:L:185:LYS:HG2  | 3:L:188:VAL:HG22 | 1.88                     | 0.55              |
| 3:L:440:ARG:CG   | 3:L:440:ARG:NH1  | 2.70                     | 0.55              |
| 4:M:96:ALA:HB2   | 4:M:346:THR:HG21 | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:266:LEU:HB3  | 1:S:270:THR:HG21 | 1.89                     | 0.55              |
| 6:X:36:LEU:HD22  | 6:X:77:VAL:HG21  | 1.87                     | 0.55              |
| 6:X:152:MET:HE2  | 6:X:156:LYS:HE2  | 1.88                     | 0.55              |
| 6:6:16:ARG:HG2   | 6:6:21:PHE:HE2   | 1.70                     | 0.55              |
| 6:6:77:VAL:HA    | 6:6:104:TRP:O    | 2.06                     | 0.55              |
| 2:B:77:LYS:H     | 2:B:116:LEU:HA   | 1.72                     | 0.55              |
| 6:F:41:PHE:CZ    | 6:F:92:MET:HB2   | 2.41                     | 0.55              |
| 6:F:138:PRO:HG2  | 7:G:121:MET:HG3  | 1.89                     | 0.55              |
| 1:J:186:THR:HG23 | 1:J:200:ARG:H    | 1.71                     | 0.55              |
| 4:M:240:ARG:HG3  | 4:M:265:PRO:O    | 2.07                     | 0.55              |
| 4:M:318:GLU:HB2  | 8:Q:39:ASP:HA    | 1.89                     | 0.55              |
| 1:S:356:CYS:HB3  | 1:S:358:PRO:HG2  | 1.88                     | 0.55              |
| 4:V:64:THR:OG1   | 6:X:83:ARG:NH1   | 2.39                     | 0.55              |
| 4:V:148:TYR:CB   | 4:V:200:ARG:HH12 | 2.19                     | 0.55              |
| 4:V:213:ILE:HG22 | 4:V:217:ARG:HG3  | 1.89                     | 0.55              |
| 7:Y:44:THR:OG1   | 7:Y:52:LYS:HD2   | 2.07                     | 0.55              |
| 1:I:109:ASP:C    | 1:I:111:PRO:HD3  | 2.32                     | 0.55              |
| 3:3:216:PHE:CZ   | 8:7:128:PHE:HD2  | 2.20                     | 0.55              |
| 3:3:413:LEU:HA   | 3:3:416:PHE:HB3  | 1.88                     | 0.55              |
| 3:C:54:LEU:N     | 3:C:55:PRO:HD3   | 2.22                     | 0.55              |
| 1:J:357:THR:N    | 1:J:358:PRO:HD2  | 2.21                     | 0.55              |
| 3:L:398:VAL:HG21 | 3:L:448:MET:HE2  | 1.89                     | 0.55              |
| 3:L:701:ALA:HB2  | 3:L:763:LEU:HB2  | 1.87                     | 0.55              |
| 1:S:145:LEU:O    | 1:S:149:ILE:HG13 | 2.06                     | 0.55              |
| 3:U:309:PRO:HG2  | 3:U:320:ALA:O    | 2.07                     | 0.55              |
| 3:U:483:ASP:O    | 3:U:484:LYS:HG2  | 2.07                     | 0.55              |
| 1:I:397:ARG:HE   | 3:3:79:LEU:CD1   | 2.19                     | 0.55              |
| 5:5:35:LYS:HD3   | 5:5:102:PRO:HB2  | 1.87                     | 0.55              |
| 5:5:116:ARG:HB3  | 5:5:135:ILE:HG13 | 1.87                     | 0.55              |
| 6:6:36:LEU:HD22  | 6:6:77:VAL:HG21  | 1.89                     | 0.55              |
| 7:9:134:GLU:CD   | 7:9:134:GLU:H    | 2.14                     | 0.55              |
| 1:A:162:LEU:O    | 1:A:165:THR:HG22 | 2.06                     | 0.55              |
| 3:C:200:LEU:O    | 3:C:201:ASP:HB2  | 2.07                     | 0.55              |
| 3:C:309:PRO:HG2  | 3:C:320:ALA:O    | 2.06                     | 0.55              |
| 1:J:265:GLU:O    | 1:J:266:LEU:HG   | 2.07                     | 0.55              |
| 4:M:70:MET:HG2   | 4:M:78:ASN:OD1   | 2.07                     | 0.55              |
| 3:U:440:ARG:HH11 | 3:U:440:ARG:CG   | 2.19                     | 0.55              |
| 5:W:42:LYS:CB    | 5:W:107:LEU:HD13 | 2.32                     | 0.55              |
| 3:3:326:PHE:CE2  | 3:3:330:LYS:HE3  | 2.41                     | 0.55              |
| 3:3:689:LYS:HE3  | 3:3:771:VAL:HG13 | 1.88                     | 0.55              |
| 4:D:148:TYR:CB   | 4:D:200:ARG:HH12 | 2.19                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:10:PHE:CZ    | 2:K:33:ARG:HG3   | 2.42                     | 0.55              |
| 3:L:141:GLU:OE2  | 3:L:143:TYR:HE1  | 1.90                     | 0.55              |
| 3:L:305:ARG:HG2  | 3:L:588:SER:O    | 2.07                     | 0.55              |
| 4:M:250:LYS:CE   | 4:M:262:PHE:HB3  | 2.37                     | 0.55              |
| 6:O:57:ARG:C     | 6:O:57:ARG:NE    | 2.65                     | 0.55              |
| 6:O:115:GLY:HA3  | 6:O:125:GLN:OE1  | 2.07                     | 0.55              |
| 1:S:397:ARG:HG2  | 3:U:49:LEU:HD13  | 1.89                     | 0.55              |
| 3:U:141:GLU:OE2  | 3:U:143:TYR:HE1  | 1.90                     | 0.55              |
| 3:U:497:TRP:O    | 3:U:528:LYS:HE3  | 2.06                     | 0.55              |
| 3:U:497:TRP:O    | 3:U:500:ALA:HB3  | 2.06                     | 0.55              |
| 5:5:20:ASN:HD21  | 5:5:24:ASN:HB2   | 1.72                     | 0.55              |
| 5:5:66:GLU:HG2   | 5:5:95:PRO:HA    | 1.88                     | 0.55              |
| 8:7:60:SER:HA    | 8:7:66:PRO:HA    | 1.89                     | 0.55              |
| 1:A:189:MET:O    | 1:A:193:GLU:HB2  | 2.07                     | 0.55              |
| 5:E:20:ASN:HD21  | 5:E:24:ASN:HB2   | 1.72                     | 0.55              |
| 8:H:121:ARG:HG3  | 8:H:121:ARG:NH1  | 2.22                     | 0.55              |
| 2:K:38:GLU:OE2   | 2:K:45:ARG:NH1   | 2.40                     | 0.55              |
| 2:K:139:GLU:HB2  | 2:K:140:PRO:CD   | 2.35                     | 0.55              |
| 3:L:112:LEU:HD12 | 4:M:322:GLU:HG3  | 1.88                     | 0.55              |
| 3:L:497:TRP:O    | 3:L:528:LYS:HE3  | 2.06                     | 0.55              |
| 4:M:85:MET:HE3   | 4:M:409:ARG:CG   | 2.37                     | 0.55              |
| 4:M:115:THR:CG2  | 4:M:297:LEU:HD23 | 2.37                     | 0.55              |
| 4:4:70:MET:HG2   | 4:4:78:ASN:OD1   | 2.08                     | 0.54              |
| 5:5:59:THR:O     | 5:5:59:THR:HG22  | 2.06                     | 0.54              |
| 4:D:153:ARG:HG3  | 4:D:153:ARG:NH1  | 2.21                     | 0.54              |
| 4:D:213:ILE:CG2  | 4:D:217:ARG:HH11 | 2.19                     | 0.54              |
| 6:F:57:ARG:C     | 6:F:57:ARG:NE    | 2.65                     | 0.54              |
| 3:L:281:GLU:HG2  | 3:L:283:PRO:HD3  | 1.88                     | 0.54              |
| 3:L:413:LEU:HA   | 3:L:416:PHE:HB3  | 1.87                     | 0.54              |
| 4:M:381:LEU:H    | 4:M:382:PRO:HD2  | 1.72                     | 0.54              |
| 3:U:115:HIS:CD2  | 3:U:116:PRO:HD2  | 2.41                     | 0.54              |
| 3:U:501:LYS:H    | 3:U:501:LYS:CD   | 2.03                     | 0.54              |
| 5:W:92:VAL:HG23  | 5:W:92:VAL:O     | 2.07                     | 0.54              |
| 2:2:110:GLU:HA   | 8:7:121:ARG:NH1  | 2.21                     | 0.54              |
| 3:3:54:LEU:N     | 3:3:55:PRO:HD3   | 2.22                     | 0.54              |
| 1:A:104:ARG:HH21 | 2:B:127:SER:HB2  | 1.71                     | 0.54              |
| 1:A:438:ARG:HD2  | 1:A:438:ARG:N    | 2.22                     | 0.54              |
| 3:C:399:LEU:HD12 | 3:C:399:LEU:N    | 2.23                     | 0.54              |
| 3:C:572:PRO:HD2  | 3:C:577:LEU:HD21 | 1.89                     | 0.54              |
| 4:D:248:VAL:HB   | 4:D:347:GLU:HB2  | 1.89                     | 0.54              |
| 7:G:134:GLU:H    | 7:G:134:GLU:CD   | 2.14                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:72:THR:HG21  | 1:J:223:THR:HG21 | 1.90                     | 0.54              |
| 1:J:438:ARG:HD2  | 1:J:438:ARG:N    | 2.23                     | 0.54              |
| 3:L:18:SER:HB2   | 3:L:433:ALA:O    | 2.06                     | 0.54              |
| 3:L:125:GLY:HA3  | 3:L:246:ASN:HD22 | 1.72                     | 0.54              |
| 3:L:329:LEU:HD21 | 3:L:644:LEU:HA   | 1.89                     | 0.54              |
| 3:L:477:LEU:HD22 | 3:L:517:ALA:HB1  | 1.87                     | 0.54              |
| 4:M:85:MET:HE1   | 4:M:370:VAL:HG11 | 1.89                     | 0.54              |
| 5:N:1:MET:C      | 5:N:3:LEU:H      | 2.14                     | 0.54              |
| 1:S:238:PHE:HE1  | 1:S:249:MET:HE1  | 1.72                     | 0.54              |
| 1:S:391:LEU:HD22 | 1:S:407:VAL:HB   | 1.90                     | 0.54              |
| 3:U:117:LEU:H    | 4:V:321:MET:CE   | 2.16                     | 0.54              |
| 3:U:469:ARG:HA   | 3:U:754:PRO:HG3  | 1.88                     | 0.54              |
| 3:U:715:GLU:HB3  | 3:U:746:ARG:NH1  | 2.22                     | 0.54              |
| 3:3:282:VAL:HG22 | 3:3:285:VAL:HG12 | 1.90                     | 0.54              |
| 4:4:84:ARG:O     | 6:6:83:ARG:NH2   | 2.40                     | 0.54              |
| 4:4:363:SER:CB   | 5:5:174:LEU:H    | 2.19                     | 0.54              |
| 1:A:196:ARG:NH2  | 3:C:204:GLU:O    | 2.41                     | 0.54              |
| 3:C:20:MET:HE2   | 3:C:433:ALA:HB2  | 1.90                     | 0.54              |
| 3:C:402:PRO:CB   | 3:C:535:MET:HE1  | 2.37                     | 0.54              |
| 1:J:53:VAL:O     | 1:J:57:VAL:HG23  | 2.06                     | 0.54              |
| 1:J:197:ALA:HB3  | 2:K:66:PHE:CE1   | 2.43                     | 0.54              |
| 3:L:184:CYS:O    | 9:L:785:SF4:S4   | 2.66                     | 0.54              |
| 3:L:344:TYR:CD1  | 3:L:568:TYR:CE1  | 2.96                     | 0.54              |
| 6:O:115:GLY:HA2  | 6:O:125:GLN:HA   | 1.89                     | 0.54              |
| 8:Q:89:ALA:O     | 8:Q:91:ILE:HG13  | 2.08                     | 0.54              |
| 2:T:10:PHE:CZ    | 2:T:33:ARG:HG3   | 2.42                     | 0.54              |
| 1:1:341:MET:HE2  | 1:1:409:PRO:O    | 2.08                     | 0.54              |
| 4:4:43:LEU:HD11  | 4:4:397:ILE:CD1  | 2.38                     | 0.54              |
| 4:4:83:PRO:HB2   | 4:4:169:HIS:HA   | 1.89                     | 0.54              |
| 4:4:119:ILE:O    | 4:4:123:LEU:HB2  | 2.07                     | 0.54              |
| 4:4:240:ARG:NH2  | 4:4:347:GLU:OE2  | 2.39                     | 0.54              |
| 4:4:287:VAL:O    | 4:4:291:LYS:HG3  | 2.07                     | 0.54              |
| 1:A:287:ILE:HG22 | 1:A:302:PHE:CG   | 2.42                     | 0.54              |
| 5:E:25:LEU:N     | 5:E:25:LEU:CD2   | 2.71                     | 0.54              |
| 4:M:404:MET:HA   | 4:M:407:VAL:CG1  | 2.38                     | 0.54              |
| 1:S:41:ALA:HB2   | 1:S:116:GLU:HG3  | 1.90                     | 0.54              |
| 4:V:74:THR:HB    | 4:V:77:GLN:HG3   | 1.88                     | 0.54              |
| 4:V:241:ALA:CA   | 4:V:278:VAL:HG21 | 2.37                     | 0.54              |
| 5:W:1:MET:C      | 5:W:3:LEU:H      | 2.15                     | 0.54              |
| 1:1:63:ARG:HD3   | 1:1:313:TYR:HD2  | 1.73                     | 0.54              |
| 2:2:139:GLU:CB   | 2:2:140:PRO:CD   | 2.84                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:683:LEU:N    | 3:3:683:LEU:HD23 | 2.23                     | 0.54              |
| 4:4:161:GLU:OE1  | 7:9:34:LYS:HG2   | 2.07                     | 0.54              |
| 5:5:84:ASP:OD1   | 5:5:84:ASP:N     | 2.39                     | 0.54              |
| 6:6:57:ARG:C     | 6:6:57:ARG:NE    | 2.66                     | 0.54              |
| 1:A:342:TRP:O    | 1:A:342:TRP:HE3  | 1.90                     | 0.54              |
| 3:C:282:VAL:HG22 | 3:C:282:VAL:O    | 2.06                     | 0.54              |
| 3:C:330:LYS:HA   | 3:C:647:ALA:HB1  | 1.90                     | 0.54              |
| 3:C:440:ARG:HH11 | 3:C:440:ARG:CG   | 2.19                     | 0.54              |
| 1:J:186:THR:HA   | 1:J:189:MET:HE2  | 1.89                     | 0.54              |
| 1:J:303:THR:OG1  | 1:J:306:VAL:HG23 | 2.07                     | 0.54              |
| 3:L:112:LEU:HD21 | 3:L:130:LEU:HD11 | 1.88                     | 0.54              |
| 3:L:515:THR:HG23 | 3:L:683:LEU:CD1  | 2.35                     | 0.54              |
| 3:L:688:ARG:HB3  | 3:L:770:ARG:HD3  | 1.89                     | 0.54              |
| 4:M:342:VAL:HG22 | 4:M:343:TYR:H    | 1.73                     | 0.54              |
| 3:U:414:SER:O    | 3:U:418:ARG:HG3  | 2.08                     | 0.54              |
| 4:V:249:ARG:HD2  | 4:V:257:TYR:CE1  | 2.43                     | 0.54              |
| 5:W:20:ASN:HD21  | 5:W:24:ASN:HB2   | 1.73                     | 0.54              |
| 5:W:174:LEU:HD22 | 5:W:180:GLY:HA2  | 1.90                     | 0.54              |
| 1:1:92:ASN:ND2   | 10:1:440:FMN:O3' | 2.41                     | 0.54              |
| 3:3:94:ASP:OD2   | 3:3:97:SER:HB2   | 2.08                     | 0.54              |
| 3:3:694:LEU:HB3  | 3:3:762:ALA:CB   | 2.34                     | 0.54              |
| 1:A:360:ARG:O    | 1:A:364:ALA:HB3  | 2.07                     | 0.54              |
| 3:C:241:ARG:HH11 | 7:G:74:GLU:CD    | 2.15                     | 0.54              |
| 4:D:74:THR:HB    | 4:D:77:GLN:HG3   | 1.90                     | 0.54              |
| 5:E:1:MET:SD     | 8:Z:113:GLU:OE2  | 2.65                     | 0.54              |
| 7:G:128:ASP:O    | 7:G:144:LYS:HD3  | 2.07                     | 0.54              |
| 2:K:77:LYS:H     | 2:K:116:LEU:HA   | 1.72                     | 0.54              |
| 2:K:81:GLN:HB3   | 2:K:122:VAL:CG2  | 2.37                     | 0.54              |
| 4:M:59:ILE:HD13  | 4:M:59:ILE:H     | 1.71                     | 0.54              |
| 3:U:333:LEU:HD22 | 3:U:648:LEU:HD21 | 1.90                     | 0.54              |
| 3:U:402:PRO:HD2  | 3:U:458:LEU:HD13 | 1.89                     | 0.54              |
| 3:U:409:LEU:HD12 | 3:U:535:MET:CE   | 2.37                     | 0.54              |
| 4:V:215:TYR:CE2  | 4:V:219:ARG:HG3  | 2.43                     | 0.54              |
| 5:W:116:ARG:HB3  | 5:W:135:ILE:HG13 | 1.88                     | 0.54              |
| 5:W:175:THR:CG2  | 5:W:178:ASP:HB2  | 2.32                     | 0.54              |
| 6:X:115:GLY:HA2  | 6:X:125:GLN:HA   | 1.88                     | 0.54              |
| 1:1:274:GLU:HG2  | 1:1:279:TRP:HE1  | 1.72                     | 0.54              |
| 1:1:363:VAL:HA   | 1:1:367:MET:HB2  | 1.89                     | 0.54              |
| 3:3:400:GLY:O    | 3:3:402:PRO:HD3  | 2.07                     | 0.54              |
| 3:3:688:ARG:HB3  | 3:3:770:ARG:HD3  | 1.88                     | 0.54              |
| 4:4:84:ARG:HG2   | 9:6:182:SF4:S2   | 2.47                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:167:ARG:HD3  | 6:6:143:ARG:HH12 | 1.73                     | 0.54              |
| 4:4:252:TYR:CE2  | 5:5:87:ARG:NH2   | 2.75                     | 0.54              |
| 4:4:265:PRO:HG2  | 4:4:282:GLU:HG2  | 1.89                     | 0.54              |
| 4:D:119:ILE:O    | 4:D:123:LEU:HB2  | 2.08                     | 0.54              |
| 3:L:341:VAL:HG21 | 3:L:364:LEU:HD11 | 1.88                     | 0.54              |
| 3:L:586:HIS:NE2  | 3:L:604:ALA:HB2  | 2.23                     | 0.54              |
| 6:O:155:GLN:O    | 6:O:158:VAL:HG22 | 2.08                     | 0.54              |
| 3:U:192:GLU:OE2  | 3:U:440:ARG:HA   | 2.08                     | 0.54              |
| 3:U:281:GLU:HG2  | 3:U:283:PRO:HD3  | 1.88                     | 0.54              |
| 4:V:69:THR:HG21  | 6:X:120:ASN:HD22 | 1.71                     | 0.54              |
| 4:V:85:MET:HE3   | 4:V:409:ARG:CG   | 2.37                     | 0.54              |
| 4:V:283:MET:O    | 4:V:287:VAL:HG23 | 2.08                     | 0.54              |
| 6:X:117:MET:HB3  | 7:Y:99:ILE:HD13  | 1.89                     | 0.54              |
| 8:Z:8:GLU:HG2    | 8:Z:97:TYR:CZ    | 2.43                     | 0.54              |
| 1:1:274:GLU:HA   | 1:1:278:GLU:HG2  | 1.90                     | 0.54              |
| 5:5:33:ARG:O     | 5:5:37:GLU:HB2   | 2.07                     | 0.54              |
| 7:9:33:LEU:HD11  | 7:9:161:TYR:CB   | 2.34                     | 0.54              |
| 3:C:414:SER:O    | 3:C:418:ARG:HG3  | 2.08                     | 0.54              |
| 3:C:701:ALA:HB2  | 3:C:763:LEU:HB2  | 1.90                     | 0.54              |
| 3:C:734:VAL:CG1  | 3:C:775:VAL:HG13 | 2.37                     | 0.54              |
| 4:D:59:ILE:H     | 4:D:59:ILE:HD13  | 1.71                     | 0.54              |
| 1:J:341:MET:HE2  | 1:J:409:PRO:O    | 2.08                     | 0.54              |
| 3:L:216:PHE:CZ   | 8:Q:128:PHE:HD2  | 2.20                     | 0.54              |
| 7:P:48:ASN:CB    | 7:P:50:LEU:HD23  | 2.36                     | 0.54              |
| 8:Q:13:TRP:CZ2   | 8:Q:17:LEU:HD11  | 2.42                     | 0.54              |
| 6:X:43:LEU:HD11  | 6:X:84:LEU:HD23  | 1.89                     | 0.54              |
| 1:A:201:LEU:HG   | 1:A:203:PRO:HD2  | 1.90                     | 0.54              |
| 1:A:366:PHE:HD1  | 1:A:370:LEU:HD21 | 1.72                     | 0.54              |
| 1:A:436:LEU:HD23 | 2:B:90:LEU:HA    | 1.90                     | 0.54              |
| 4:D:84:ARG:NE    | 6:F:117:MET:HE1  | 2.22                     | 0.54              |
| 4:D:112:ARG:HH21 | 4:D:297:LEU:HD11 | 1.72                     | 0.54              |
| 4:D:162:TRP:CE2  | 7:G:34:LYS:HD2   | 2.41                     | 0.54              |
| 5:E:33:ARG:O     | 5:E:37:GLU:HB2   | 2.08                     | 0.54              |
| 6:F:93:ARG:NH1   | 6:F:96:TRP:CZ3   | 2.76                     | 0.54              |
| 1:J:397:ARG:HE   | 3:L:79:LEU:CD1   | 2.19                     | 0.54              |
| 2:K:7:LYS:HD2    | 2:K:7:LYS:N      | 2.20                     | 0.54              |
| 3:L:400:GLY:O    | 3:L:402:PRO:HD3  | 2.08                     | 0.54              |
| 3:U:478:LEU:CD2  | 3:U:483:ASP:HB2  | 2.38                     | 0.54              |
| 4:V:106:GLY:O    | 5:W:194:SER:HB3  | 2.08                     | 0.54              |
| 4:V:363:SER:CB   | 5:W:174:LEU:H    | 2.21                     | 0.54              |
| 6:X:57:ARG:C     | 6:X:57:ARG:NE    | 2.65                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:X:145:GLU:CG   | 7:Y:31:VAL:HG21  | 2.20                     | 0.54              |
| 3:3:185:LYS:HG2  | 3:3:188:VAL:HG22 | 1.89                     | 0.54              |
| 3:3:341:VAL:HG11 | 3:3:364:LEU:HD21 | 1.89                     | 0.54              |
| 4:4:247:ASP:OD1  | 4:4:249:ARG:HG3  | 2.07                     | 0.54              |
| 1:A:274:GLU:HG3  | 1:A:278:GLU:HG3  | 1.90                     | 0.54              |
| 1:A:332:PRO:CD   | 2:B:90:LEU:HD23  | 2.38                     | 0.54              |
| 2:K:139:GLU:CB   | 2:K:140:PRO:CD   | 2.85                     | 0.54              |
| 3:L:269:THR:HG22 | 3:L:274:LEU:HA   | 1.90                     | 0.54              |
| 4:M:241:ALA:CA   | 4:M:278:VAL:HG21 | 2.38                     | 0.54              |
| 3:U:357:ALA:HB2  | 3:U:641:LEU:HD11 | 1.90                     | 0.54              |
| 4:V:74:THR:HB    | 4:V:77:GLN:H     | 1.73                     | 0.54              |
| 4:V:84:ARG:HG2   | 9:X:182:SF4:S2   | 2.48                     | 0.54              |
| 4:V:393:MET:O    | 4:V:396:ILE:HG22 | 2.07                     | 0.54              |
| 6:X:107:SER:O    | 6:X:137:VAL:HG12 | 2.07                     | 0.54              |
| 1:1:356:CYS:HB3  | 1:1:358:PRO:HG2  | 1.89                     | 0.53              |
| 3:3:192:GLU:OE2  | 3:3:440:ARG:HA   | 2.08                     | 0.53              |
| 4:4:74:THR:HB    | 4:4:77:GLN:HG3   | 1.88                     | 0.53              |
| 4:4:85:MET:HE3   | 4:4:409:ARG:CG   | 2.38                     | 0.53              |
| 4:M:116:ILE:HD11 | 4:M:182:LEU:HG   | 1.90                     | 0.53              |
| 4:M:148:TYR:CB   | 4:M:200:ARG:HH12 | 2.21                     | 0.53              |
| 4:M:254:TYR:CD2  | 4:M:346:THR:HA   | 2.42                     | 0.53              |
| 5:N:84:ASP:OD1   | 5:N:84:ASP:N     | 2.40                     | 0.53              |
| 5:N:116:ARG:HB3  | 5:N:135:ILE:HG13 | 1.89                     | 0.53              |
| 8:Q:86:LEU:HD12  | 8:Q:91:ILE:HD12  | 1.90                     | 0.53              |
| 1:S:301:PRO:O    | 1:S:306:VAL:HG21 | 2.08                     | 0.53              |
| 2:T:61:MET:HE2   | 3:U:214:MET:HG2  | 1.89                     | 0.53              |
| 3:U:473:GLU:O    | 3:U:477:LEU:HD13 | 2.08                     | 0.53              |
| 6:X:138:PRO:HG2  | 7:Y:121:MET:HG3  | 1.89                     | 0.53              |
| 3:3:402:PRO:HD2  | 3:3:458:LEU:HD13 | 1.90                     | 0.53              |
| 3:3:583:VAL:CG2  | 3:3:598:ALA:HA   | 2.38                     | 0.53              |
| 4:4:123:LEU:HD21 | 4:4:159:LEU:HD12 | 1.90                     | 0.53              |
| 4:4:404:MET:HA   | 4:4:407:VAL:CG1  | 2.38                     | 0.53              |
| 5:5:37:GLU:O     | 5:5:41:TYR:HD1   | 1.90                     | 0.53              |
| 5:E:26:TRP:HE1   | 5:E:91:ARG:HH21  | 1.53                     | 0.53              |
| 1:J:266:LEU:HB3  | 1:J:270:THR:HG21 | 1.90                     | 0.53              |
| 3:L:46:ARG:O     | 3:L:107:MET:HG2  | 2.08                     | 0.53              |
| 4:M:342:VAL:HG22 | 4:M:343:TYR:N    | 2.24                     | 0.53              |
| 8:Q:37:PHE:CE2   | 8:Q:74:PRO:HA    | 2.43                     | 0.53              |
| 3:U:24:PHE:CE1   | 3:U:29:ASP:HA    | 2.42                     | 0.53              |
| 3:U:501:LYS:HD2  | 3:U:501:LYS:N    | 2.08                     | 0.53              |
| 8:Z:117:ALA:O    | 8:Z:121:ARG:HG2  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:185:LYS:HG3  | 3:3:202:PHE:CE2  | 2.43                     | 0.53              |
| 3:3:473:GLU:O    | 3:3:477:LEU:HD13 | 2.08                     | 0.53              |
| 4:4:254:TYR:CD1  | 4:4:255:SER:N    | 2.70                     | 0.53              |
| 3:C:413:LEU:HA   | 3:C:416:PHE:HB3  | 1.89                     | 0.53              |
| 3:C:670:PRO:HD2  | 3:C:676:LEU:HD23 | 1.90                     | 0.53              |
| 5:E:37:GLU:O     | 5:E:41:TYR:HD1   | 1.91                     | 0.53              |
| 3:L:474:ARG:HA   | 3:L:517:ALA:HB2  | 1.91                     | 0.53              |
| 3:L:583:VAL:HG23 | 3:L:599:HIS:H    | 1.73                     | 0.53              |
| 4:M:119:ILE:O    | 4:M:123:LEU:HB2  | 2.08                     | 0.53              |
| 4:M:374:SER:HB2  | 4:M:406:ASP:HB3  | 1.90                     | 0.53              |
| 5:N:71:VAL:CG1   | 5:N:89:PHE:HD2   | 2.21                     | 0.53              |
| 1:S:398:SER:HA   | 3:U:46:ARG:HD2   | 1.89                     | 0.53              |
| 3:U:173:PHE:HB3  | 3:U:296:PHE:CZ   | 2.43                     | 0.53              |
| 3:U:341:VAL:HG11 | 3:U:364:LEU:HD21 | 1.90                     | 0.53              |
| 4:V:187:VAL:N    | 4:V:188:PRO:HD2  | 2.24                     | 0.53              |
| 5:W:121:LEU:O    | 5:W:144:HIS:HB3  | 2.08                     | 0.53              |
| 3:3:402:PRO:CG   | 3:3:535:MET:HE1  | 2.39                     | 0.53              |
| 4:4:342:VAL:HG22 | 4:4:343:TYR:H    | 1.73                     | 0.53              |
| 5:5:1:MET:C      | 5:5:3:LEU:H      | 2.15                     | 0.53              |
| 1:A:37:GLY:C     | 1:A:39:GLU:H     | 2.17                     | 0.53              |
| 3:C:24:PHE:CE1   | 3:C:29:ASP:HA    | 2.43                     | 0.53              |
| 4:D:404:MET:HA   | 4:D:407:VAL:CG1  | 2.39                     | 0.53              |
| 1:J:270:THR:O    | 1:J:311:MET:HG3  | 2.08                     | 0.53              |
| 1:J:437:TRP:CZ3  | 2:K:96:LEU:HB2   | 2.44                     | 0.53              |
| 3:L:192:GLU:OE2  | 3:L:440:ARG:HA   | 2.09                     | 0.53              |
| 4:M:123:LEU:HD21 | 4:M:159:LEU:HD12 | 1.91                     | 0.53              |
| 4:M:187:VAL:N    | 4:M:188:PRO:HD2  | 2.23                     | 0.53              |
| 3:U:750:ARG:HB3  | 3:U:752:ASP:OD1  | 2.07                     | 0.53              |
| 4:V:254:TYR:CE2  | 4:V:346:THR:CA   | 2.87                     | 0.53              |
| 1:1:341:MET:CE   | 1:1:409:PRO:HB2  | 2.38                     | 0.53              |
| 3:3:305:ARG:HG2  | 3:3:588:SER:O    | 2.08                     | 0.53              |
| 3:3:557:SER:H    | 3:3:560:GLU:HB2  | 1.74                     | 0.53              |
| 4:4:73:ARG:HG3   | 4:4:77:GLN:OE1   | 2.08                     | 0.53              |
| 8:7:82:ILE:HG23  | 8:7:95:ALA:HB3   | 1.90                     | 0.53              |
| 1:A:92:ASN:ND2   | 10:A:440:FMN:N1  | 2.57                     | 0.53              |
| 3:C:456:ALA:HB3  | 3:C:459:MET:HE3  | 1.90                     | 0.53              |
| 3:C:515:THR:HG23 | 3:C:683:LEU:CD1  | 2.35                     | 0.53              |
| 4:D:84:ARG:HD3   | 6:F:117:MET:HE1  | 1.90                     | 0.53              |
| 6:F:36:LEU:HD22  | 6:F:77:VAL:HG21  | 1.89                     | 0.53              |
| 6:F:155:GLN:O    | 6:F:158:VAL:HG22 | 2.09                     | 0.53              |
| 2:K:101:THR:HG23 | 2:K:106:ILE:O    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:694:LEU:CB   | 3:L:762:ALA:HB2  | 2.35                     | 0.53              |
| 6:O:163:TYR:CD2  | 6:O:169:ARG:HA   | 2.36                     | 0.53              |
| 5:W:66:GLU:HG2   | 5:W:95:PRO:HA    | 1.91                     | 0.53              |
| 6:X:41:PHE:CZ    | 6:X:92:MET:HB2   | 2.43                     | 0.53              |
| 1:1:49:THR:OG1   | 1:1:52:GLU:HG3   | 2.09                     | 0.53              |
| 3:3:161:ARG:HG2  | 3:3:161:ARG:HH11 | 1.74                     | 0.53              |
| 3:3:474:ARG:HA   | 3:3:517:ALA:HB2  | 1.91                     | 0.53              |
| 4:4:120:LEU:HD13 | 4:4:160:PHE:CE1  | 2.39                     | 0.53              |
| 5:5:167:PRO:HB3  | 7:9:66:TYR:CE2   | 2.44                     | 0.53              |
| 3:C:268:ASP:OD2  | 3:C:278:ARG:NH1  | 2.41                     | 0.53              |
| 3:C:341:VAL:HG11 | 3:C:364:LEU:HD21 | 1.91                     | 0.53              |
| 5:E:157:THR:C    | 5:E:158:LEU:HD23 | 2.34                     | 0.53              |
| 6:F:99:MET:CG    | 6:F:100:PRO:HD2  | 2.36                     | 0.53              |
| 2:K:106:ILE:HG22 | 2:K:110:GLU:HB2  | 1.91                     | 0.53              |
| 3:L:194:VAL:HG12 | 3:L:411:LEU:HD22 | 1.90                     | 0.53              |
| 3:L:341:VAL:HG11 | 3:L:364:LEU:HD21 | 1.89                     | 0.53              |
| 3:L:683:LEU:N    | 3:L:683:LEU:HD23 | 2.24                     | 0.53              |
| 5:N:134:LYS:HD3  | 5:N:137:THR:OG1  | 2.07                     | 0.53              |
| 8:Q:37:PHE:HD1   | 8:Q:53:THR:O     | 1.90                     | 0.53              |
| 8:Q:60:SER:HA    | 8:Q:66:PRO:HA    | 1.90                     | 0.53              |
| 1:S:342:TRP:O    | 1:S:342:TRP:HE3  | 1.92                     | 0.53              |
| 2:T:86:LEU:O     | 2:T:90:LEU:HD12  | 2.08                     | 0.53              |
| 4:V:248:VAL:HB   | 4:V:347:GLU:HB2  | 1.91                     | 0.53              |
| 8:Z:70:ALA:HA    | 8:Z:83:GLY:O     | 2.09                     | 0.53              |
| 4:4:187:VAL:N    | 4:4:188:PRO:HD2  | 2.23                     | 0.53              |
| 5:5:141:LEU:HD11 | 5:5:150:TYR:OH   | 2.09                     | 0.53              |
| 4:D:338:PRO:HG3  | 5:E:192:TYR:O    | 2.09                     | 0.53              |
| 4:M:219:ARG:NH1  | 4:M:273:PHE:CD2  | 2.77                     | 0.53              |
| 2:T:130:THR:HB   | 2:T:144:CYS:SG   | 2.49                     | 0.53              |
| 3:U:684:ARG:HG2  | 3:U:684:ARG:NH1  | 2.22                     | 0.53              |
| 3:3:55:PRO:HG3   | 3:3:74:GLN:H     | 1.68                     | 0.53              |
| 3:3:372:GLN:O    | 3:3:558:TRP:CE2  | 2.62                     | 0.53              |
| 6:6:93:ARG:NH1   | 6:6:96:TRP:CZ3   | 2.76                     | 0.53              |
| 1:A:357:THR:N    | 1:A:358:PRO:HD2  | 2.24                     | 0.53              |
| 3:C:583:VAL:HG23 | 3:C:599:HIS:H    | 1.73                     | 0.53              |
| 3:C:612:GLY:O    | 3:C:624:LEU:HB2  | 2.09                     | 0.53              |
| 4:D:74:THR:HB    | 4:D:77:GLN:H     | 1.73                     | 0.53              |
| 6:F:77:VAL:HA    | 6:F:104:TRP:O    | 2.08                     | 0.53              |
| 3:L:497:TRP:O    | 3:L:500:ALA:HB3  | 2.09                     | 0.53              |
| 6:O:117:MET:HE2  | 7:P:99:ILE:HG12  | 1.91                     | 0.53              |
| 1:S:270:THR:O    | 1:S:311:MET:HG3  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:120:PRO:HG2  | 8:Z:42:TYR:OH    | 2.09                     | 0.53              |
| 4:V:61:TYR:CZ    | 6:X:87:LYS:HE2   | 2.44                     | 0.53              |
| 3:3:330:LYS:HA   | 3:3:647:ALA:HB1  | 1.89                     | 0.53              |
| 3:3:333:LEU:HD22 | 3:3:648:LEU:HD21 | 1.91                     | 0.53              |
| 1:A:81:LYS:HA    | 1:A:81:LYS:CE    | 2.39                     | 0.53              |
| 1:J:145:LEU:O    | 1:J:149:ILE:HG13 | 2.09                     | 0.53              |
| 3:U:413:LEU:HA   | 3:U:416:PHE:HB3  | 1.89                     | 0.53              |
| 3:U:693:TYR:HB3  | 3:U:759:TYR:CD2  | 2.44                     | 0.53              |
| 3:3:282:VAL:HG22 | 3:3:282:VAL:O    | 2.10                     | 0.53              |
| 3:3:382:PHE:CD1  | 3:3:382:PHE:N    | 2.76                     | 0.53              |
| 5:5:116:ARG:HG3  | 5:5:129:HIS:CE1  | 2.43                     | 0.53              |
| 1:A:145:LEU:O    | 1:A:149:ILE:HG13 | 2.09                     | 0.53              |
| 3:C:18:SER:HB3   | 3:C:21:ASP:OD1   | 2.08                     | 0.53              |
| 3:C:45:CYS:O     | 3:C:46:ARG:HB2   | 2.07                     | 0.53              |
| 3:C:333:LEU:HD22 | 3:C:648:LEU:HD21 | 1.91                     | 0.53              |
| 3:L:18:SER:HB3   | 3:L:21:ASP:OD1   | 2.08                     | 0.53              |
| 3:L:399:LEU:HD12 | 3:L:399:LEU:N    | 2.24                     | 0.53              |
| 3:L:458:LEU:H    | 3:L:458:LEU:HD12 | 1.73                     | 0.53              |
| 8:Q:121:ARG:HG3  | 8:Q:121:ARG:NH1  | 2.24                     | 0.53              |
| 2:T:40:TRP:CD1   | 2:T:74:PRO:HA    | 2.43                     | 0.53              |
| 3:U:550:LEU:HD23 | 3:U:684:ARG:NH2  | 2.24                     | 0.53              |
| 3:U:583:VAL:CG2  | 3:U:598:ALA:HA   | 2.39                     | 0.53              |
| 3:U:695:ARG:NH1  | 3:U:715:GLU:OE1  | 2.40                     | 0.53              |
| 4:V:52:VAL:HG23  | 4:V:388:GLU:O    | 2.08                     | 0.53              |
| 1:1:29:LEU:CD1   | 1:1:155:ARG:HG3  | 2.38                     | 0.52              |
| 1:1:189:MET:O    | 1:1:193:GLU:HB2  | 2.08                     | 0.52              |
| 3:3:112:LEU:HD21 | 3:3:130:LEU:HD11 | 1.89                     | 0.52              |
| 3:3:269:THR:HG22 | 3:3:274:LEU:HA   | 1.92                     | 0.52              |
| 3:3:693:TYR:HB3  | 3:3:759:TYR:HD2  | 1.73                     | 0.52              |
| 4:4:64:THR:HB    | 4:4:66:PHE:HE1   | 1.74                     | 0.52              |
| 4:4:168:PHE:HE1  | 6:6:141:PRO:HG3  | 1.74                     | 0.52              |
| 1:A:89:LEU:HD23  | 1:A:118:MET:HE3  | 1.90                     | 0.52              |
| 1:A:301:PRO:O    | 1:A:306:VAL:HG21 | 2.08                     | 0.52              |
| 1:A:437:TRP:CZ3  | 2:B:96:LEU:HB2   | 2.44                     | 0.52              |
| 3:C:269:THR:HG22 | 3:C:274:LEU:HA   | 1.91                     | 0.52              |
| 3:C:326:PHE:CE2  | 3:C:330:LYS:HE3  | 2.43                     | 0.52              |
| 4:D:254:TYR:CD2  | 4:D:346:THR:HA   | 2.44                     | 0.52              |
| 4:D:363:SER:CB   | 5:E:174:LEU:H    | 2.22                     | 0.52              |
| 6:O:84:LEU:O     | 6:O:124:VAL:HG23 | 2.09                     | 0.52              |
| 6:O:93:ARG:NH1   | 6:O:96:TRP:CZ3   | 2.76                     | 0.52              |
| 6:O:108:MET:HA   | 6:O:137:VAL:CG1  | 2.39                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:189:MET:O    | 1:S:193:GLU:HB2  | 2.09                     | 0.52              |
| 3:U:245:ARG:NH1  | 7:Y:56:CYS:O     | 2.41                     | 0.52              |
| 2:2:129:HIS:CD2  | 2:2:130:THR:HG23 | 2.43                     | 0.52              |
| 1:A:274:GLU:HA   | 1:A:278:GLU:HG2  | 1.90                     | 0.52              |
| 5:E:167:PRO:HB3  | 7:G:66:TYR:CE2   | 2.44                     | 0.52              |
| 1:J:274:GLU:HG2  | 1:J:279:TRP:HE1  | 1.73                     | 0.52              |
| 1:J:366:PHE:CE1  | 1:J:370:LEU:HD21 | 2.44                     | 0.52              |
| 4:M:74:THR:HB    | 4:M:77:GLN:H     | 1.73                     | 0.52              |
| 7:P:128:ASP:O    | 7:P:144:LYS:HD3  | 2.10                     | 0.52              |
| 3:U:18:SER:HB3   | 3:U:21:ASP:OD1   | 2.08                     | 0.52              |
| 4:V:247:ASP:OD1  | 4:V:249:ARG:HG3  | 2.08                     | 0.52              |
| 1:1:40:THR:O     | 1:1:44:VAL:HG23  | 2.09                     | 0.52              |
| 3:3:546:ALA:O    | 3:3:547:MET:HE2  | 2.09                     | 0.52              |
| 4:4:367:ARG:HH12 | 4:4:369:LYS:CA   | 2.21                     | 0.52              |
| 7:9:128:ASP:O    | 7:9:144:LYS:HD3  | 2.10                     | 0.52              |
| 1:A:40:THR:O     | 1:A:44:VAL:HG23  | 2.09                     | 0.52              |
| 2:B:136:VAL:HG12 | 2:B:137:ASN:N    | 2.23                     | 0.52              |
| 3:C:185:LYS:HG3  | 3:C:202:PHE:HE2  | 1.74                     | 0.52              |
| 8:H:82:ILE:HG23  | 8:H:95:ALA:HB3   | 1.91                     | 0.52              |
| 3:L:506:ILE:CG2  | 3:L:535:MET:HE3  | 2.39                     | 0.52              |
| 1:S:186:THR:HG23 | 1:S:199:PRO:HA   | 1.92                     | 0.52              |
| 1:S:267:PRO:HG2  | 1:S:270:THR:HG22 | 1.90                     | 0.52              |
| 1:S:274:GLU:HA   | 1:S:278:GLU:HG2  | 1.91                     | 0.52              |
| 3:U:165:ASP:HB3  | 3:U:178:ARG:HD2  | 1.89                     | 0.52              |
| 3:U:305:ARG:HG2  | 3:U:588:SER:O    | 2.08                     | 0.52              |
| 4:4:144:THR:N    | 4:4:145:PRO:CD   | 2.72                     | 0.52              |
| 5:5:26:TRP:HE1   | 5:5:91:ARG:HH21  | 1.55                     | 0.52              |
| 3:C:46:ARG:HH11  | 3:C:46:ARG:CG    | 1.96                     | 0.52              |
| 4:D:187:VAL:N    | 4:D:188:PRO:HD2  | 2.24                     | 0.52              |
| 8:H:60:SER:HA    | 8:H:66:PRO:HA    | 1.90                     | 0.52              |
| 1:J:358:PRO:O    | 1:J:362:GLY:HA3  | 2.10                     | 0.52              |
| 3:L:115:HIS:CD2  | 3:L:116:PRO:HD2  | 2.45                     | 0.52              |
| 3:L:120:PRO:HG2  | 8:Q:42:TYR:OH    | 2.09                     | 0.52              |
| 3:L:372:GLN:O    | 3:L:558:TRP:CE2  | 2.62                     | 0.52              |
| 6:O:77:VAL:O     | 6:O:77:VAL:HG12  | 2.09                     | 0.52              |
| 8:Q:29:VAL:HG22  | 8:Q:60:SER:O     | 2.08                     | 0.52              |
| 4:V:219:ARG:NH1  | 4:V:273:PHE:CD2  | 2.78                     | 0.52              |
| 4:V:376:VAL:O    | 4:V:379:GLN:HG3  | 2.09                     | 0.52              |
| 5:W:71:VAL:CG1   | 5:W:89:PHE:HD2   | 2.22                     | 0.52              |
| 1:1:37:GLY:C     | 1:1:39:GLU:H     | 2.18                     | 0.52              |
| 1:1:197:ALA:HB3  | 2:2:66:PHE:CZ    | 2.44                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:734:VAL:CG1  | 3:3:775:VAL:HG13 | 2.38                     | 0.52              |
| 3:3:750:ARG:HB3  | 3:3:752:ASP:OD1  | 2.10                     | 0.52              |
| 4:4:316:LEU:C    | 4:4:318:GLU:H    | 2.17                     | 0.52              |
| 1:A:139:ARG:CG   | 2:B:140:PRO:HD3  | 2.38                     | 0.52              |
| 2:B:33:ARG:HH21  | 2:B:37:GLU:CG    | 2.22                     | 0.52              |
| 3:C:683:LEU:N    | 3:C:683:LEU:HD23 | 2.24                     | 0.52              |
| 4:D:123:LEU:HD21 | 4:D:159:LEU:HD12 | 1.90                     | 0.52              |
| 1:J:274:GLU:HA   | 1:J:278:GLU:HG2  | 1.92                     | 0.52              |
| 5:N:26:TRP:HE1   | 5:N:91:ARG:HH21  | 1.55                     | 0.52              |
| 6:O:152:MET:HE2  | 6:O:156:LYS:HE2  | 1.91                     | 0.52              |
| 1:S:293:GLY:HA3  | 1:S:324:GLY:N    | 2.08                     | 0.52              |
| 4:V:96:ALA:HB2   | 4:V:346:THR:HG21 | 1.91                     | 0.52              |
| 6:X:146:ALA:HB2  | 7:Y:119:PHE:HD1  | 1.74                     | 0.52              |
| 2:2:7:LYS:HD2    | 2:2:7:LYS:N      | 2.22                     | 0.52              |
| 2:B:38:GLU:OE2   | 2:B:45:ARG:NH1   | 2.43                     | 0.52              |
| 4:D:249:ARG:HD2  | 4:D:257:TYR:CE1  | 2.45                     | 0.52              |
| 3:L:186:ARG:HD2  | 3:L:231:PRO:HD3  | 1.91                     | 0.52              |
| 1:S:250:LYS:HB3  | 1:S:252:TYR:CE2  | 2.45                     | 0.52              |
| 1:S:265:GLU:O    | 1:S:266:LEU:HG   | 2.09                     | 0.52              |
| 3:U:186:ARG:HD2  | 3:U:231:PRO:HD3  | 1.91                     | 0.52              |
| 4:V:168:PHE:N    | 4:V:168:PHE:CD1  | 2.78                     | 0.52              |
| 3:3:232:VAL:HB   | 9:3:784:SF4:S2   | 2.50                     | 0.52              |
| 3:3:385:ALA:HB2  | 3:3:531:LYS:HB3  | 1.90                     | 0.52              |
| 3:3:488:GLU:O    | 3:3:491:ALA:HB3  | 2.10                     | 0.52              |
| 3:3:513:GLN:HG2  | 3:3:769:LEU:HD23 | 1.91                     | 0.52              |
| 3:3:715:GLU:HB3  | 3:3:746:ARG:NH1  | 2.24                     | 0.52              |
| 4:4:385:CYS:HB3  | 4:4:396:ILE:HG12 | 1.90                     | 0.52              |
| 1:A:211:LEU:H    | 1:A:216:THR:HG21 | 1.73                     | 0.52              |
| 2:B:42:ARG:HB2   | 2:B:45:ARG:HG2   | 1.91                     | 0.52              |
| 3:L:385:ALA:HB3  | 3:L:533:LEU:CD2  | 2.40                     | 0.52              |
| 3:L:501:LYS:HD2  | 3:L:501:LYS:N    | 2.10                     | 0.52              |
| 1:S:274:GLU:HG3  | 1:S:278:GLU:HG3  | 1.91                     | 0.52              |
| 1:S:357:THR:N    | 1:S:358:PRO:HD2  | 2.25                     | 0.52              |
| 3:U:2:VAL:HG13   | 3:U:89:ASP:HA    | 1.90                     | 0.52              |
| 3:U:185:LYS:HG3  | 3:U:202:PHE:CE2  | 2.44                     | 0.52              |
| 5:W:141:LEU:HD11 | 5:W:150:TYR:OH   | 2.10                     | 0.52              |
| 6:X:163:TYR:CD2  | 6:X:169:ARG:HA   | 2.35                     | 0.52              |
| 8:Z:37:PHE:CE2   | 8:Z:74:PRO:HA    | 2.45                     | 0.52              |
| 1:1:104:ARG:HH21 | 2:2:127:SER:HB2  | 1.74                     | 0.52              |
| 1:1:118:MET:HG2  | 1:1:224:LEU:HD13 | 1.91                     | 0.52              |
| 1:1:239:ALA:C    | 1:1:241:MET:H    | 2.18                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:409:LEU:HD12 | 3:3:535:MET:CE   | 2.39                     | 0.52              |
| 8:7:16:LEU:HG    | 8:7:82:ILE:HD11  | 1.92                     | 0.52              |
| 1:A:63:ARG:HD3   | 1:A:313:TYR:HD2  | 1.75                     | 0.52              |
| 3:C:141:GLU:OE2  | 3:C:143:TYR:HE1  | 1.92                     | 0.52              |
| 5:E:53:VAL:HG22  | 5:E:55:LEU:CD1   | 2.40                     | 0.52              |
| 5:E:174:LEU:HD22 | 5:E:180:GLY:HA2  | 1.91                     | 0.52              |
| 2:K:33:ARG:HH21  | 2:K:37:GLU:CG    | 2.23                     | 0.52              |
| 4:M:240:ARG:NH2  | 4:M:347:GLU:OE2  | 2.40                     | 0.52              |
| 4:M:254:TYR:CE2  | 4:M:346:THR:CA   | 2.91                     | 0.52              |
| 4:M:363:SER:HB3  | 5:N:173:ALA:HB1  | 1.91                     | 0.52              |
| 5:N:53:VAL:HG22  | 5:N:55:LEU:CD1   | 2.40                     | 0.52              |
| 1:S:110:VAL:HG23 | 1:S:110:VAL:O    | 2.10                     | 0.52              |
| 2:T:7:LYS:HD2    | 2:T:7:LYS:N      | 2.23                     | 0.52              |
| 8:Z:20:MET:HE3   | 8:Z:59:LEU:HG    | 1.91                     | 0.52              |
| 5:5:2:ARG:NH1    | 5:5:45:GLY:HA3   | 2.25                     | 0.52              |
| 2:B:33:ARG:HH21  | 2:B:37:GLU:HG3   | 1.75                     | 0.52              |
| 1:J:49:THR:OG1   | 1:J:52:GLU:HG3   | 2.10                     | 0.52              |
| 4:M:144:THR:N    | 4:M:145:PRO:CD   | 2.73                     | 0.52              |
| 6:O:165:GLU:HG2  | 7:P:148:ARG:NH1  | 2.25                     | 0.52              |
| 8:Q:8:GLU:HG2    | 8:Q:97:TYR:CZ    | 2.45                     | 0.52              |
| 1:S:109:ASP:C    | 1:S:111:PRO:HD3  | 2.34                     | 0.52              |
| 3:3:83:CYS:SG    | 3:3:84:VAL:HG13  | 2.50                     | 0.52              |
| 4:4:241:ALA:CA   | 4:4:278:VAL:HG21 | 2.40                     | 0.52              |
| 5:5:121:LEU:O    | 5:5:144:HIS:HB3  | 2.09                     | 0.52              |
| 7:9:48:ASN:CB    | 7:9:50:LEU:HD23  | 2.39                     | 0.52              |
| 1:A:41:ALA:HA    | 1:A:120:LEU:HD21 | 1.92                     | 0.52              |
| 1:A:183:GLY:O    | 10:A:440:FMN:H2' | 2.10                     | 0.52              |
| 4:D:43:LEU:HD11  | 4:D:397:ILE:CD1  | 2.40                     | 0.52              |
| 5:E:125:VAL:HG12 | 5:E:126:PHE:N    | 2.24                     | 0.52              |
| 6:F:93:ARG:NH1   | 6:F:96:TRP:CE3   | 2.78                     | 0.52              |
| 4:M:393:MET:C    | 4:M:396:ILE:HG22 | 2.35                     | 0.52              |
| 1:S:29:LEU:CD1   | 1:S:155:ARG:HG3  | 2.39                     | 0.52              |
| 1:S:89:LEU:HD23  | 1:S:118:MET:HE3  | 1.91                     | 0.52              |
| 1:S:116:GLU:HG2  | 1:S:228:VAL:HG22 | 1.92                     | 0.52              |
| 1:S:118:MET:HG2  | 1:S:224:LEU:HD13 | 1.91                     | 0.52              |
| 3:U:125:GLY:HA3  | 3:U:246:ASN:ND2  | 2.23                     | 0.52              |
| 6:X:20:LEU:O     | 6:X:24:LEU:HD13  | 2.10                     | 0.52              |
| 1:1:397:ARG:NE   | 3:3:79:LEU:HD12  | 2.23                     | 0.51              |
| 6:6:40:THR:HB    | 6:6:50:MET:SD    | 2.50                     | 0.51              |
| 3:C:194:VAL:HG12 | 3:C:411:LEU:HD22 | 1.91                     | 0.51              |
| 3:C:372:GLN:O    | 3:C:558:TRP:CE2  | 2.63                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:215:TYR:CE2  | 4:D:219:ARG:HG3  | 2.45                     | 0.51              |
| 5:E:66:GLU:HG2   | 5:E:95:PRO:HA    | 1.92                     | 0.51              |
| 1:J:341:MET:CE   | 1:J:409:PRO:HB2  | 2.39                     | 0.51              |
| 3:L:478:LEU:CD2  | 3:L:483:ASP:HB2  | 2.40                     | 0.51              |
| 3:U:734:VAL:CG1  | 3:U:775:VAL:HG13 | 2.39                     | 0.51              |
| 1:1:110:VAL:O    | 1:1:110:VAL:HG23 | 2.10                     | 0.51              |
| 3:3:24:PHE:CE1   | 3:3:29:ASP:HA    | 2.45                     | 0.51              |
| 4:4:248:VAL:HB   | 4:4:347:GLU:HB2  | 1.92                     | 0.51              |
| 4:4:249:ARG:HD2  | 4:4:257:TYR:CE1  | 2.45                     | 0.51              |
| 4:4:250:LYS:CE   | 4:4:262:PHE:HB3  | 2.41                     | 0.51              |
| 2:B:102:GLU:HA   | 8:H:108:ILE:HD11 | 1.93                     | 0.51              |
| 4:D:168:PHE:N    | 4:D:168:PHE:CD1  | 2.77                     | 0.51              |
| 5:E:59:THR:HG22  | 5:E:59:THR:O     | 2.09                     | 0.51              |
| 5:E:141:LEU:HD11 | 5:E:150:TYR:OH   | 2.10                     | 0.51              |
| 1:J:436:LEU:HD23 | 2:K:90:LEU:HA    | 1.90                     | 0.51              |
| 3:L:385:ALA:HB2  | 3:L:531:LYS:HB3  | 1.91                     | 0.51              |
| 3:L:734:VAL:CG1  | 3:L:775:VAL:HG13 | 2.39                     | 0.51              |
| 4:M:262:PHE:CD1  | 4:M:289:ILE:HD11 | 2.45                     | 0.51              |
| 1:S:239:ALA:C    | 1:S:241:MET:H    | 2.18                     | 0.51              |
| 1:1:366:PHE:HD1  | 1:1:370:LEU:HD21 | 1.76                     | 0.51              |
| 5:5:160:ARG:HG3  | 7:9:130:VAL:HG11 | 1.92                     | 0.51              |
| 6:6:84:LEU:O     | 6:6:124:VAL:HG23 | 2.10                     | 0.51              |
| 7:9:44:THR:HA    | 7:9:138:VAL:HG13 | 1.91                     | 0.51              |
| 8:7:13:TRP:CE2   | 8:7:17:LEU:HD11  | 2.45                     | 0.51              |
| 2:B:101:THR:HG23 | 2:B:106:ILE:O    | 2.10                     | 0.51              |
| 6:F:138:PRO:HG3  | 7:G:121:MET:HG3  | 1.91                     | 0.51              |
| 5:N:174:LEU:CD2  | 5:N:180:GLY:HA2  | 2.39                     | 0.51              |
| 7:P:163:VAL:HB   | 7:P:164:PRO:HD2  | 1.92                     | 0.51              |
| 8:Q:16:LEU:O     | 8:Q:16:LEU:HD13  | 2.09                     | 0.51              |
| 1:S:355:LYS:HD3  | 1:S:399:PHE:CD2  | 2.45                     | 0.51              |
| 3:U:456:ALA:HB3  | 3:U:459:MET:HE3  | 1.93                     | 0.51              |
| 3:U:474:ARG:HA   | 3:U:517:ALA:HB2  | 1.92                     | 0.51              |
| 3:U:497:TRP:CD1  | 3:U:524:LEU:HD11 | 2.46                     | 0.51              |
| 3:U:583:VAL:HG23 | 3:U:599:HIS:H    | 1.75                     | 0.51              |
| 4:V:211:SER:HB2  | 4:V:215:TYR:N    | 2.26                     | 0.51              |
| 4:V:294:LEU:O    | 4:V:294:LEU:HD23 | 2.11                     | 0.51              |
| 8:Z:16:LEU:HG    | 8:Z:82:ILE:HD11  | 1.92                     | 0.51              |
| 1:1:355:LYS:HD3  | 1:1:399:PHE:CD2  | 2.45                     | 0.51              |
| 3:3:115:HIS:CD2  | 3:3:116:PRO:HD2  | 2.45                     | 0.51              |
| 3:3:385:ALA:HB3  | 3:3:533:LEU:CD2  | 2.41                     | 0.51              |
| 3:3:398:VAL:C    | 3:3:399:LEU:HD12 | 2.34                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:629:ILE:HG22 | 3:3:630:GLU:N    | 2.22                     | 0.51              |
| 4:4:219:ARG:NH1  | 4:4:273:PHE:CD2  | 2.79                     | 0.51              |
| 8:7:121:ARG:NH1  | 8:7:121:ARG:CG   | 2.74                     | 0.51              |
| 3:C:402:PRO:CG   | 3:C:535:MET:HE1  | 2.40                     | 0.51              |
| 3:C:715:GLU:HB3  | 3:C:746:ARG:NH1  | 2.26                     | 0.51              |
| 5:E:34:PHE:HE1   | 5:E:38:MET:SD    | 2.33                     | 0.51              |
| 5:E:84:ASP:OD1   | 5:E:84:ASP:N     | 2.42                     | 0.51              |
| 5:E:103:THR:HG23 | 5:E:127:GLU:O    | 2.10                     | 0.51              |
| 7:G:163:VAL:HB   | 7:G:164:PRO:HD2  | 1.92                     | 0.51              |
| 1:J:366:PHE:HD1  | 1:J:370:LEU:HD21 | 1.76                     | 0.51              |
| 3:L:185:LYS:HG3  | 3:L:202:PHE:HE2  | 1.76                     | 0.51              |
| 3:L:188:VAL:CG2  | 3:L:189:ARG:N    | 2.74                     | 0.51              |
| 3:L:513:GLN:HG2  | 3:L:769:LEU:HD23 | 1.91                     | 0.51              |
| 4:M:74:THR:HB    | 4:M:77:GLN:HG3   | 1.90                     | 0.51              |
| 6:O:138:PRO:HG2  | 7:P:121:MET:HG3  | 1.93                     | 0.51              |
| 1:S:201:LEU:HG   | 1:S:203:PRO:HD2  | 1.92                     | 0.51              |
| 3:U:750:ARG:HB2  | 3:U:753:VAL:HG23 | 1.91                     | 0.51              |
| 4:V:85:MET:HE1   | 4:V:370:VAL:HG11 | 1.92                     | 0.51              |
| 4:V:379:GLN:HG2  | 5:W:113:PHE:CD1  | 2.46                     | 0.51              |
| 6:X:115:GLY:HA3  | 6:X:125:GLN:OE1  | 2.09                     | 0.51              |
| 6:X:155:GLN:O    | 6:X:158:VAL:HG22 | 2.11                     | 0.51              |
| 1:1:272:PHE:CE2  | 1:1:311:MET:HE3  | 2.45                     | 0.51              |
| 3:3:285:VAL:HG22 | 3:3:286:ASN:H    | 1.74                     | 0.51              |
| 3:3:309:PRO:HG2  | 3:3:320:ALA:O    | 2.11                     | 0.51              |
| 3:3:695:ARG:NH1  | 3:3:715:GLU:OE1  | 2.42                     | 0.51              |
| 4:4:363:SER:HB3  | 5:5:173:ALA:HB1  | 1.91                     | 0.51              |
| 1:A:316:LEU:HD12 | 1:A:323:LEU:HB2  | 1.91                     | 0.51              |
| 3:C:382:PHE:CD1  | 3:C:382:PHE:N    | 2.79                     | 0.51              |
| 3:C:750:ARG:HB2  | 3:C:753:VAL:HG23 | 1.93                     | 0.51              |
| 4:D:219:ARG:NH1  | 4:D:273:PHE:CD2  | 2.79                     | 0.51              |
| 5:E:121:LEU:O    | 5:E:144:HIS:HB3  | 2.10                     | 0.51              |
| 6:F:84:LEU:O     | 6:F:124:VAL:HG23 | 2.11                     | 0.51              |
| 8:H:121:ARG:HH11 | 8:H:121:ARG:CG   | 2.21                     | 0.51              |
| 1:J:363:VAL:HA   | 1:J:367:MET:HB2  | 1.90                     | 0.51              |
| 3:L:173:PHE:HB3  | 3:L:296:PHE:CZ   | 2.46                     | 0.51              |
| 3:L:695:ARG:NH1  | 3:L:715:GLU:OE1  | 2.42                     | 0.51              |
| 3:L:750:ARG:HB3  | 3:L:752:ASP:OD1  | 2.11                     | 0.51              |
| 5:N:37:GLU:O     | 5:N:41:TYR:HD1   | 1.93                     | 0.51              |
| 7:P:44:THR:HA    | 7:P:138:VAL:HG13 | 1.93                     | 0.51              |
| 8:Q:33:LYS:HD2   | 8:Q:36:ASP:OD1   | 2.11                     | 0.51              |
| 8:Q:82:ILE:HG23  | 8:Q:95:ALA:HB3   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:33:ARG:HH21  | 2:T:37:GLU:HG3   | 1.75                     | 0.51              |
| 2:T:42:ARG:HB2   | 2:T:45:ARG:HG2   | 1.92                     | 0.51              |
| 3:U:478:LEU:HD21 | 3:U:483:ASP:HB2  | 1.92                     | 0.51              |
| 3:U:513:GLN:HG2  | 3:U:769:LEU:HD23 | 1.93                     | 0.51              |
| 4:V:98:ALA:O     | 4:V:102:GLU:HG3  | 2.11                     | 0.51              |
| 1:1:274:GLU:HG3  | 1:1:278:GLU:HG3  | 1.92                     | 0.51              |
| 4:4:115:THR:HG21 | 4:4:297:LEU:HD23 | 1.93                     | 0.51              |
| 4:4:148:TYR:HB3  | 4:4:200:ARG:HH12 | 1.75                     | 0.51              |
| 4:4:254:TYR:CD2  | 4:4:346:THR:HA   | 2.44                     | 0.51              |
| 4:4:381:LEU:H    | 4:4:382:PRO:HD2  | 1.75                     | 0.51              |
| 6:6:114:SER:HB2  | 7:9:97:ARG:CD    | 2.39                     | 0.51              |
| 8:7:37:PHE:CE2   | 8:7:74:PRO:HA    | 2.46                     | 0.51              |
| 1:A:366:PHE:CE1  | 1:A:370:LEU:HD21 | 2.45                     | 0.51              |
| 8:H:40:PHE:HB2   | 8:H:48:TYR:CE2   | 2.45                     | 0.51              |
| 3:L:693:TYR:HB3  | 3:L:759:TYR:HD2  | 1.75                     | 0.51              |
| 4:M:112:ARG:HH21 | 4:M:297:LEU:HD11 | 1.76                     | 0.51              |
| 6:O:93:ARG:NH1   | 6:O:96:TRP:CE3   | 2.78                     | 0.51              |
| 2:T:33:ARG:HH21  | 2:T:37:GLU:CG    | 2.23                     | 0.51              |
| 3:U:116:PRO:O    | 3:U:117:LEU:HB2  | 2.11                     | 0.51              |
| 4:V:153:ARG:HG3  | 4:V:153:ARG:HH11 | 1.75                     | 0.51              |
| 5:W:53:VAL:HG22  | 5:W:55:LEU:CD1   | 2.40                     | 0.51              |
| 8:Z:60:SER:HA    | 8:Z:66:PRO:HA    | 1.92                     | 0.51              |
| 4:4:118:VAL:HB   | 4:4:257:TYR:HE2  | 1.75                     | 0.51              |
| 3:C:2:VAL:HG13   | 3:C:89:ASP:HA    | 1.93                     | 0.51              |
| 3:C:18:SER:HB2   | 3:C:433:ALA:O    | 2.11                     | 0.51              |
| 3:C:173:PHE:HB3  | 3:C:296:PHE:CZ   | 2.45                     | 0.51              |
| 6:F:20:LEU:O     | 6:F:24:LEU:HD13  | 2.10                     | 0.51              |
| 2:K:110:GLU:HA   | 8:Q:121:ARG:NH1  | 2.25                     | 0.51              |
| 3:L:202:PHE:HA   | 3:L:210:PHE:O    | 2.11                     | 0.51              |
| 6:O:113:SER:HB3  | 7:P:96:LEU:HD13  | 1.93                     | 0.51              |
| 7:P:45:ARG:HH21  | 7:P:137:LEU:HD23 | 1.75                     | 0.51              |
| 4:V:93:HIS:HA    | 4:V:353:LEU:HD21 | 1.92                     | 0.51              |
| 4:V:120:LEU:HD13 | 4:V:160:PHE:CE1  | 2.43                     | 0.51              |
| 5:W:58:LEU:HD12  | 5:W:58:LEU:O     | 2.11                     | 0.51              |
| 6:X:82:GLY:HA2   | 9:X:182:SF4:S4   | 2.51                     | 0.51              |
| 7:Y:44:THR:HA    | 7:Y:138:VAL:HG13 | 1.93                     | 0.51              |
| 1:1:359:CYS:O    | 1:1:363:VAL:HG22 | 2.11                     | 0.51              |
| 2:2:101:THR:HG23 | 2:2:106:ILE:O    | 2.10                     | 0.51              |
| 3:3:515:THR:HG23 | 3:3:683:LEU:CD1  | 2.39                     | 0.51              |
| 3:3:750:ARG:HB2  | 3:3:753:VAL:HG23 | 1.91                     | 0.51              |
| 4:4:213:ILE:HG22 | 4:4:217:ARG:HG3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:332:PRO:HD2  | 2:B:90:LEU:HD23  | 1.92                     | 0.51              |
| 3:C:546:ALA:O    | 3:C:547:MET:HE2  | 2.10                     | 0.51              |
| 3:C:557:SER:H    | 3:C:560:GLU:HB2  | 1.76                     | 0.51              |
| 1:S:364:ALA:HB1  | 3:U:207:VAL:HG22 | 1.92                     | 0.51              |
| 4:V:198:PRO:HG3  | 4:V:291:LYS:NZ   | 2.26                     | 0.51              |
| 4:4:261:THR:HB   | 4:4:292:GLN:OE1  | 2.11                     | 0.51              |
| 4:4:332:THR:O    | 5:5:172:ALA:HB3  | 2.11                     | 0.51              |
| 5:5:103:THR:HG23 | 5:5:127:GLU:O    | 2.11                     | 0.51              |
| 8:7:8:GLU:HG2    | 8:7:97:TYR:CZ    | 2.46                     | 0.51              |
| 4:D:252:TYR:CE2  | 5:E:87:ARG:NH2   | 2.77                     | 0.51              |
| 6:F:84:LEU:HD11  | 6:F:89:ALA:HA    | 1.92                     | 0.51              |
| 5:N:2:ARG:NH1    | 5:N:45:GLY:HA3   | 2.26                     | 0.51              |
| 6:O:36:LEU:HD22  | 6:O:77:VAL:HG21  | 1.92                     | 0.51              |
| 8:Q:37:PHE:HE2   | 8:Q:74:PRO:HA    | 1.76                     | 0.51              |
| 8:Q:40:PHE:HB2   | 8:Q:48:TYR:CE2   | 2.46                     | 0.51              |
| 1:S:186:THR:HA   | 1:S:189:MET:HE2  | 1.93                     | 0.51              |
| 2:T:81:GLN:HB3   | 2:T:122:VAL:CG2  | 2.40                     | 0.51              |
| 3:U:372:GLN:O    | 3:U:558:TRP:CE2  | 2.63                     | 0.51              |
| 4:V:218:ALA:HB1  | 4:V:272:VAL:HG22 | 1.93                     | 0.51              |
| 6:X:93:ARG:NH1   | 6:X:96:TRP:CZ3   | 2.79                     | 0.51              |
| 2:2:42:ARG:HB2   | 2:2:45:ARG:HG2   | 1.92                     | 0.51              |
| 4:4:129:HIS:HE1  | 4:4:349:ALA:HB1  | 1.66                     | 0.51              |
| 4:4:379:GLN:HG2  | 5:5:113:PHE:CD1  | 2.46                     | 0.51              |
| 3:C:55:PRO:CG    | 3:C:74:GLN:N     | 2.70                     | 0.51              |
| 3:C:116:PRO:O    | 3:C:117:LEU:HB2  | 2.10                     | 0.51              |
| 3:C:125:GLY:HA3  | 3:C:246:ASN:ND2  | 2.26                     | 0.51              |
| 6:F:107:SER:O    | 6:F:137:VAL:HG12 | 2.11                     | 0.51              |
| 1:J:298:PRO:HD2  | 1:J:321:SER:OG   | 2.11                     | 0.51              |
| 4:M:93:HIS:HA    | 4:M:353:LEU:HD21 | 1.93                     | 0.51              |
| 4:M:210:GLU:O    | 4:M:212:PRO:HD3  | 2.11                     | 0.51              |
| 4:M:287:VAL:O    | 4:M:291:LYS:HG3  | 2.11                     | 0.51              |
| 5:N:141:LEU:HD11 | 5:N:150:TYR:OH   | 2.11                     | 0.51              |
| 6:O:155:GLN:C    | 6:O:157:LYS:H    | 2.19                     | 0.51              |
| 4:V:64:THR:HB    | 4:V:66:PHE:HE1   | 1.74                     | 0.51              |
| 4:V:168:PHE:HE1  | 6:X:141:PRO:HG3  | 1.75                     | 0.51              |
| 7:Y:53:CYS:HB2   | 7:Y:112:ALA:HB1  | 1.93                     | 0.51              |
| 3:3:200:LEU:O    | 3:3:201:ASP:HB2  | 2.09                     | 0.50              |
| 3:3:268:ASP:OD2  | 3:3:278:ARG:NH1  | 2.44                     | 0.50              |
| 3:3:329:LEU:HD21 | 3:3:644:LEU:HA   | 1.93                     | 0.50              |
| 3:C:112:LEU:HD21 | 3:C:130:LEU:HD11 | 1.93                     | 0.50              |
| 3:C:368:HIS:CD2  | 3:C:556:ALA:HB3  | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:750:ARG:HB3  | 3:C:752:ASP:OD1  | 2.11                     | 0.50              |
| 4:D:79:ILE:O     | 4:D:79:ILE:HG22  | 2.11                     | 0.50              |
| 1:J:110:VAL:HG23 | 1:J:110:VAL:O    | 2.11                     | 0.50              |
| 4:M:249:ARG:HD2  | 4:M:257:TYR:CE1  | 2.46                     | 0.50              |
| 6:O:114:SER:HB2  | 7:P:97:ARG:CD    | 2.41                     | 0.50              |
| 4:V:346:THR:HG22 | 4:V:353:LEU:O    | 2.11                     | 0.50              |
| 7:Y:134:GLU:CD   | 7:Y:134:GLU:H    | 2.18                     | 0.50              |
| 3:3:505:LEU:HB3  | 3:3:532:VAL:HG22 | 1.93                     | 0.50              |
| 4:4:85:MET:HE1   | 4:4:370:VAL:HG11 | 1.93                     | 0.50              |
| 4:4:218:ALA:HB1  | 4:4:272:VAL:HG22 | 1.94                     | 0.50              |
| 1:A:288:GLN:HB3  | 1:A:333:GLU:HG2  | 1.93                     | 0.50              |
| 2:B:110:GLU:HA   | 8:H:121:ARG:NH1  | 2.23                     | 0.50              |
| 3:C:185:LYS:HG3  | 3:C:202:PHE:CE2  | 2.47                     | 0.50              |
| 8:H:13:TRP:CE2   | 8:H:17:LEU:HD11  | 2.45                     | 0.50              |
| 2:K:33:ARG:HH21  | 2:K:37:GLU:HG3   | 1.75                     | 0.50              |
| 3:U:18:SER:HB2   | 3:U:433:ALA:O    | 2.11                     | 0.50              |
| 4:V:153:ARG:HG3  | 4:V:153:ARG:NH1  | 2.27                     | 0.50              |
| 4:V:385:CYS:HB3  | 4:V:396:ILE:HG12 | 1.93                     | 0.50              |
| 6:X:117:MET:HE3  | 6:X:118:PHE:CZ   | 2.46                     | 0.50              |
| 1:1:186:THR:HG23 | 1:1:199:PRO:HA   | 1.93                     | 0.50              |
| 1:1:366:PHE:CE1  | 1:1:370:LEU:HD21 | 2.46                     | 0.50              |
| 3:3:132:ASP:O    | 3:3:136:GLU:HG3  | 2.11                     | 0.50              |
| 1:A:64:GLY:HA3   | 10:A:440:FMN:O1P | 2.12                     | 0.50              |
| 3:C:583:VAL:CG2  | 3:C:598:ALA:HA   | 2.41                     | 0.50              |
| 7:G:41:HIS:ND1   | 7:G:95:MET:HE1   | 2.27                     | 0.50              |
| 1:J:189:MET:O    | 1:J:193:GLU:HB2  | 2.10                     | 0.50              |
| 1:J:238:PHE:HE1  | 1:J:249:MET:CE   | 2.25                     | 0.50              |
| 4:M:120:LEU:HD13 | 4:M:160:PHE:CE1  | 2.42                     | 0.50              |
| 1:S:366:PHE:CE1  | 1:S:370:LEU:HD21 | 2.47                     | 0.50              |
| 2:T:77:LYS:H     | 2:T:116:LEU:HA   | 1.75                     | 0.50              |
| 4:V:83:PRO:HB2   | 4:V:169:HIS:HA   | 1.94                     | 0.50              |
| 4:V:144:THR:N    | 4:V:145:PRO:CD   | 2.74                     | 0.50              |
| 4:V:367:ARG:HH12 | 4:V:369:LYS:CA   | 2.25                     | 0.50              |
| 6:X:84:LEU:O     | 6:X:124:VAL:HG23 | 2.11                     | 0.50              |
| 8:Z:121:ARG:HH11 | 8:Z:121:ARG:CG   | 2.20                     | 0.50              |
| 1:1:288:GLN:HB3  | 1:1:333:GLU:HG2  | 1.93                     | 0.50              |
| 3:3:173:PHE:HB3  | 3:3:296:PHE:CZ   | 2.47                     | 0.50              |
| 3:3:456:ALA:HB3  | 3:3:459:MET:HE3  | 1.94                     | 0.50              |
| 3:3:501:LYS:HD2  | 3:3:501:LYS:N    | 2.11                     | 0.50              |
| 4:4:79:ILE:O     | 4:4:79:ILE:HG22  | 2.12                     | 0.50              |
| 1:A:92:ASN:HD21  | 10:A:440:FMN:C2  | 2.23                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:VAL:O    | 1:A:110:VAL:HG23 | 2.11                     | 0.50              |
| 3:C:329:LEU:HD21 | 3:C:644:LEU:HA   | 1.92                     | 0.50              |
| 3:C:478:LEU:CD2  | 3:C:483:ASP:HB2  | 2.41                     | 0.50              |
| 6:F:152:MET:HE2  | 6:F:156:LYS:HE2  | 1.93                     | 0.50              |
| 1:J:391:LEU:HD22 | 1:J:407:VAL:HB   | 1.92                     | 0.50              |
| 3:L:414:SER:O    | 3:L:418:ARG:HG3  | 2.12                     | 0.50              |
| 2:T:112:THR:HG22 | 2:T:116:LEU:H    | 1.77                     | 0.50              |
| 1:1:39:GLU:O     | 1:1:43:ARG:HG3   | 2.12                     | 0.50              |
| 1:1:290:ILE:HG22 | 1:1:330:LEU:HD22 | 1.93                     | 0.50              |
| 1:1:360:ARG:O    | 1:1:364:ALA:HB3  | 2.11                     | 0.50              |
| 6:6:117:MET:HE2  | 7:9:99:ILE:HG12  | 1.94                     | 0.50              |
| 1:A:180:TYR:CE2  | 10:A:440:FMN:H6  | 2.47                     | 0.50              |
| 3:C:305:ARG:HG2  | 3:C:588:SER:O    | 2.11                     | 0.50              |
| 4:D:211:SER:HB2  | 4:D:215:TYR:N    | 2.26                     | 0.50              |
| 3:L:402:PRO:HD2  | 3:L:458:LEU:HD13 | 1.94                     | 0.50              |
| 3:L:409:LEU:HD12 | 3:L:535:MET:CE   | 2.39                     | 0.50              |
| 3:L:505:LEU:HD21 | 3:L:507:LEU:HD23 | 1.94                     | 0.50              |
| 3:L:750:ARG:HB2  | 3:L:753:VAL:HG23 | 1.91                     | 0.50              |
| 4:M:381:LEU:H    | 4:M:382:PRO:CD   | 2.24                     | 0.50              |
| 1:S:87:HIS:HB2   | 1:S:126:ARG:O    | 2.11                     | 0.50              |
| 1:S:183:GLY:O    | 10:S:440:FMN:H2' | 2.11                     | 0.50              |
| 3:U:368:HIS:CD2  | 3:U:556:ALA:HB3  | 2.47                     | 0.50              |
| 3:3:487:SER:OG   | 3:3:490:VAL:HG23 | 2.12                     | 0.50              |
| 3:3:670:PRO:CD   | 3:3:676:LEU:HD23 | 2.42                     | 0.50              |
| 4:4:59:ILE:H     | 4:4:59:ILE:HD13  | 1.75                     | 0.50              |
| 4:4:200:ARG:O    | 4:4:204:TYR:HD1  | 1.94                     | 0.50              |
| 3:C:473:GLU:O    | 3:C:477:LEU:HD13 | 2.11                     | 0.50              |
| 3:C:694:LEU:CB   | 3:C:762:ALA:HB2  | 2.37                     | 0.50              |
| 4:D:210:GLU:O    | 4:D:212:PRO:HD3  | 2.11                     | 0.50              |
| 4:D:213:ILE:HG22 | 4:D:217:ARG:HG3  | 1.92                     | 0.50              |
| 5:E:116:ARG:HB3  | 5:E:135:ILE:HG13 | 1.92                     | 0.50              |
| 3:L:112:LEU:CD2  | 3:L:130:LEU:HD11 | 2.41                     | 0.50              |
| 4:M:76:LEU:O     | 4:M:76:LEU:HD12  | 2.12                     | 0.50              |
| 4:M:294:LEU:HD23 | 4:M:294:LEU:O    | 2.12                     | 0.50              |
| 1:S:39:GLU:O     | 1:S:43:ARG:HG3   | 2.11                     | 0.50              |
| 1:S:395:GLU:HB2  | 1:S:407:VAL:HG21 | 1.92                     | 0.50              |
| 3:U:185:LYS:HG2  | 3:U:188:VAL:CG2  | 2.41                     | 0.50              |
| 6:X:141:PRO:HB3  | 9:X:182:SF4:S1   | 2.52                     | 0.50              |
| 1:1:238:PHE:HE1  | 1:1:249:MET:CE   | 2.25                     | 0.50              |
| 3:3:112:LEU:CD2  | 3:3:130:LEU:HD11 | 2.41                     | 0.50              |
| 3:3:414:SER:O    | 3:3:418:ARG:HG3  | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:583:VAL:HG23 | 3:3:599:HIS:H    | 1.75                     | 0.50              |
| 4:4:168:PHE:N    | 4:4:168:PHE:CD1  | 2.77                     | 0.50              |
| 5:5:71:VAL:CG1   | 5:5:89:PHE:HD2   | 2.24                     | 0.50              |
| 3:C:250:GLU:CD   | 3:C:628:PRO:HG2  | 2.36                     | 0.50              |
| 4:D:93:HIS:HA    | 4:D:353:LEU:HD21 | 1.94                     | 0.50              |
| 5:E:167:PRO:HB3  | 7:G:66:TYR:CD2   | 2.47                     | 0.50              |
| 7:G:39:GLY:O     | 7:G:40:ARG:C     | 2.55                     | 0.50              |
| 2:K:129:HIS:CD2  | 2:K:130:THR:HG23 | 2.45                     | 0.50              |
| 3:L:737:GLU:HB2  | 3:L:776:LEU:HD21 | 1.93                     | 0.50              |
| 4:M:263:ASP:HB2  | 4:M:285:GLU:OE1  | 2.12                     | 0.50              |
| 7:P:93:ILE:HG13  | 7:P:136:MET:HE1  | 1.93                     | 0.50              |
| 7:P:123:ASP:HB2  | 7:P:129:LEU:HD21 | 1.93                     | 0.50              |
| 2:T:129:HIS:CD2  | 2:T:130:THR:HG23 | 2.47                     | 0.50              |
| 3:U:224:GLY:HA3  | 3:U:295:ARG:HD2  | 1.93                     | 0.50              |
| 4:V:210:GLU:O    | 4:V:212:PRO:HD3  | 2.12                     | 0.50              |
| 4:V:381:LEU:H    | 4:V:382:PRO:HD2  | 1.77                     | 0.50              |
| 7:Y:45:ARG:HH21  | 7:Y:137:LEU:HD23 | 1.75                     | 0.50              |
| 1:1:133:TYR:HB2  | 1:1:188:LEU:HD21 | 1.93                     | 0.50              |
| 1:1:270:THR:O    | 1:1:311:MET:HG3  | 2.12                     | 0.50              |
| 1:1:391:LEU:HD22 | 1:1:407:VAL:HB   | 1.94                     | 0.50              |
| 2:2:130:THR:HB   | 2:2:144:CYS:SG   | 2.52                     | 0.50              |
| 6:6:93:ARG:NH1   | 6:6:96:TRP:CE3   | 2.79                     | 0.50              |
| 7:9:99:ILE:HG22  | 7:9:101:CYS:SG   | 2.51                     | 0.50              |
| 8:7:86:LEU:HD12  | 8:7:91:ILE:HD12  | 1.94                     | 0.50              |
| 1:A:98:PRO:HA    | 2:B:124:CYS:SG   | 2.52                     | 0.50              |
| 3:C:46:ARG:O     | 3:C:107:MET:HG2  | 2.11                     | 0.50              |
| 4:D:69:THR:HG21  | 6:F:120:ASN:ND2  | 2.27                     | 0.50              |
| 4:D:240:ARG:HG3  | 4:D:265:PRO:O    | 2.12                     | 0.50              |
| 4:M:350:ARG:NE   | 4:M:403:VAL:CG2  | 2.71                     | 0.50              |
| 4:M:363:SER:CB   | 5:N:174:LEU:H    | 2.23                     | 0.50              |
| 3:U:670:PRO:CD   | 3:U:676:LEU:HD23 | 2.40                     | 0.50              |
| 4:V:114:GLU:O    | 4:V:118:VAL:HG13 | 2.11                     | 0.50              |
| 4:V:226:PRO:HG3  | 4:V:242:SER:O    | 2.11                     | 0.50              |
| 6:X:93:ARG:NH1   | 6:X:96:TRP:CE3   | 2.80                     | 0.50              |
| 1:1:301:PRO:O    | 1:1:306:VAL:HG21 | 2.11                     | 0.50              |
| 4:4:112:ARG:HH21 | 4:4:297:LEU:HD11 | 1.77                     | 0.50              |
| 5:5:53:VAL:HG22  | 5:5:55:LEU:CD1   | 2.42                     | 0.50              |
| 1:A:239:ALA:C    | 1:A:241:MET:H    | 2.20                     | 0.50              |
| 3:C:188:VAL:CG2  | 3:C:189:ARG:N    | 2.74                     | 0.50              |
| 4:D:168:PHE:CE1  | 6:F:141:PRO:HG3  | 2.45                     | 0.50              |
| 4:D:385:CYS:HB3  | 4:D:396:ILE:HG12 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:44:THR:HA    | 7:G:138:VAL:HG13 | 1.93                     | 0.50              |
| 7:G:48:ASN:CB    | 7:G:50:LEU:HD23  | 2.41                     | 0.50              |
| 1:J:29:LEU:CD1   | 1:J:155:ARG:HG3  | 2.41                     | 0.50              |
| 1:J:397:ARG:HG2  | 3:L:49:LEU:HD13  | 1.92                     | 0.50              |
| 3:L:119:CYS:O    | 3:L:120:PRO:C    | 2.53                     | 0.50              |
| 3:L:488:GLU:O    | 3:L:491:ALA:HB3  | 2.12                     | 0.50              |
| 3:U:385:ALA:HB2  | 3:U:531:LYS:CB   | 2.42                     | 0.50              |
| 4:V:148:TYR:HB3  | 4:V:200:ARG:HH12 | 1.75                     | 0.50              |
| 4:V:262:PHE:CD1  | 4:V:289:ILE:HD11 | 2.47                     | 0.50              |
| 6:X:105:VAL:HG11 | 6:X:131:VAL:CG2  | 2.41                     | 0.50              |
| 1:1:293:GLY:HA3  | 1:1:324:GLY:N    | 2.10                     | 0.49              |
| 1:1:398:SER:HA   | 3:3:46:ARG:HD2   | 1.93                     | 0.49              |
| 3:3:131:GLN:O    | 3:3:134:THR:HB   | 2.12                     | 0.49              |
| 4:4:346:THR:HG22 | 4:4:353:LEU:O    | 2.12                     | 0.49              |
| 6:6:20:LEU:O     | 6:6:24:LEU:HD13  | 2.12                     | 0.49              |
| 6:6:117:MET:CE   | 7:9:99:ILE:HG12  | 2.42                     | 0.49              |
| 3:C:269:THR:HG23 | 3:C:274:LEU:HD13 | 1.94                     | 0.49              |
| 3:C:732:ALA:H    | 3:C:747:VAL:CG1  | 2.25                     | 0.49              |
| 4:D:52:VAL:HG23  | 4:D:388:GLU:O    | 2.12                     | 0.49              |
| 4:D:118:VAL:HB   | 4:D:257:TYR:HE2  | 1.77                     | 0.49              |
| 1:J:398:SER:HA   | 3:L:46:ARG:HD2   | 1.93                     | 0.49              |
| 3:L:24:PHE:CE1   | 3:L:29:ASP:HA    | 2.47                     | 0.49              |
| 3:L:550:LEU:HD23 | 3:L:684:ARG:NH2  | 2.27                     | 0.49              |
| 4:M:254:TYR:CD1  | 4:M:255:SER:N    | 2.71                     | 0.49              |
| 6:O:105:VAL:HG11 | 6:O:131:VAL:CG2  | 2.41                     | 0.49              |
| 1:S:397:ARG:HD2  | 1:S:397:ARG:N    | 2.26                     | 0.49              |
| 3:U:20:MET:HE2   | 3:U:433:ALA:HB2  | 1.93                     | 0.49              |
| 3:U:689:LYS:HB2  | 3:U:772:GLU:HG2  | 1.93                     | 0.49              |
| 3:U:694:LEU:CB   | 3:U:762:ALA:HB2  | 2.37                     | 0.49              |
| 4:V:338:PRO:HG3  | 5:W:192:TYR:O    | 2.11                     | 0.49              |
| 6:X:84:LEU:HD11  | 6:X:89:ALA:HA    | 1.93                     | 0.49              |
| 2:2:102:GLU:HA   | 8:7:108:ILE:HD11 | 1.94                     | 0.49              |
| 3:3:202:PHE:HA   | 3:3:210:PHE:O    | 2.12                     | 0.49              |
| 4:4:342:VAL:HG22 | 4:4:343:TYR:N    | 2.27                     | 0.49              |
| 7:9:26:TYR:N     | 7:9:27:PRO:CD    | 2.72                     | 0.49              |
| 2:B:106:ILE:CG2  | 2:B:110:GLU:HB2  | 2.41                     | 0.49              |
| 3:C:474:ARG:CZ   | 3:C:516:VAL:HG21 | 2.36                     | 0.49              |
| 4:D:84:ARG:CD    | 6:F:117:MET:HE1  | 2.42                     | 0.49              |
| 7:G:26:TYR:N     | 7:G:27:PRO:CD    | 2.73                     | 0.49              |
| 8:H:29:VAL:HG22  | 8:H:60:SER:O     | 2.13                     | 0.49              |
| 1:J:18:TYR:OH    | 1:J:105:TYR:HB2  | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:38:TYR:OH    | 1:J:112:HIS:ND1  | 2.37                     | 0.49              |
| 1:J:118:MET:HG2  | 1:J:224:LEU:HD13 | 1.94                     | 0.49              |
| 2:K:116:LEU:N    | 2:K:116:LEU:HD23 | 2.28                     | 0.49              |
| 3:L:629:ILE:HG22 | 3:L:630:GLU:N    | 2.23                     | 0.49              |
| 6:O:43:LEU:HD11  | 6:O:84:LEU:HD23  | 1.92                     | 0.49              |
| 3:U:382:PHE:CD1  | 3:U:382:PHE:N    | 2.79                     | 0.49              |
| 3:U:400:GLY:O    | 3:U:402:PRO:HD3  | 2.13                     | 0.49              |
| 3:U:488:GLU:O    | 3:U:491:ALA:HB3  | 2.12                     | 0.49              |
| 5:W:2:ARG:NH1    | 5:W:45:GLY:HA3   | 2.26                     | 0.49              |
| 1:1:92:ASN:HD21  | 10:1:440:FMN:C2  | 2.25                     | 0.49              |
| 1:1:316:LEU:HD12 | 1:1:323:LEU:HB2  | 1.95                     | 0.49              |
| 3:3:483:ASP:O    | 3:3:484:LYS:HG2  | 2.11                     | 0.49              |
| 3:C:402:PRO:HD2  | 3:C:458:LEU:HD13 | 1.93                     | 0.49              |
| 3:C:478:LEU:HD21 | 3:C:483:ASP:HB2  | 1.94                     | 0.49              |
| 4:D:200:ARG:O    | 4:D:204:TYR:HD1  | 1.95                     | 0.49              |
| 6:F:105:VAL:HG11 | 6:F:131:VAL:CG2  | 2.43                     | 0.49              |
| 6:F:163:TYR:CD2  | 6:F:169:ARG:HA   | 2.36                     | 0.49              |
| 1:J:116:GLU:HG2  | 1:J:228:VAL:HG22 | 1.94                     | 0.49              |
| 2:K:109:GLY:HA2  | 8:Q:91:ILE:HD13  | 1.93                     | 0.49              |
| 4:M:133:LEU:HD21 | 4:M:204:TYR:CE2  | 2.47                     | 0.49              |
| 4:M:248:VAL:HB   | 4:M:347:GLU:HB2  | 1.94                     | 0.49              |
| 8:Q:70:ALA:HA    | 8:Q:83:GLY:O     | 2.13                     | 0.49              |
| 1:S:88:TYR:HB2   | 1:S:216:THR:CG2  | 2.42                     | 0.49              |
| 1:S:203:PRO:HB2  | 1:S:204:PRO:HD3  | 1.93                     | 0.49              |
| 1:S:351:GLU:HA   | 3:U:205:ARG:HH12 | 1.77                     | 0.49              |
| 1:S:366:PHE:HD1  | 1:S:370:LEU:HD21 | 1.77                     | 0.49              |
| 3:U:131:GLN:O    | 3:U:134:THR:HB   | 2.12                     | 0.49              |
| 3:U:402:PRO:CG   | 3:U:535:MET:HE1  | 2.43                     | 0.49              |
| 3:U:694:LEU:C    | 3:U:762:ALA:HB2  | 2.38                     | 0.49              |
| 4:V:188:PRO:O    | 4:V:191:LYS:HB2  | 2.13                     | 0.49              |
| 1:1:41:ALA:HA    | 1:1:120:LEU:HD21 | 1.95                     | 0.49              |
| 2:2:33:ARG:HH21  | 2:2:37:GLU:CG    | 2.26                     | 0.49              |
| 2:2:153:LEU:C    | 2:2:153:LEU:HD13 | 2.37                     | 0.49              |
| 3:3:194:VAL:HG12 | 3:3:411:LEU:HD22 | 1.94                     | 0.49              |
| 3:3:337:ARG:HD2  | 3:3:337:ARG:N    | 2.27                     | 0.49              |
| 4:4:338:PRO:HG3  | 5:5:192:TYR:O    | 2.12                     | 0.49              |
| 6:6:155:GLN:C    | 6:6:157:LYS:H    | 2.20                     | 0.49              |
| 8:7:117:ALA:O    | 8:7:121:ARG:HG2  | 2.12                     | 0.49              |
| 3:C:333:LEU:HD13 | 3:C:648:LEU:HD21 | 1.94                     | 0.49              |
| 3:C:385:ALA:HB2  | 3:C:531:LYS:CB   | 2.42                     | 0.49              |
| 3:C:513:GLN:HG2  | 3:C:769:LEU:HD23 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:115:THR:CG2  | 4:D:297:LEU:HD23 | 2.42                     | 0.49              |
| 5:E:13:LYS:HG2   | 5:E:13:LYS:O     | 2.13                     | 0.49              |
| 1:J:88:TYR:HB2   | 1:J:216:THR:CG2  | 2.42                     | 0.49              |
| 3:L:2:VAL:HG13   | 3:L:89:ASP:HA    | 1.94                     | 0.49              |
| 3:L:185:LYS:HG3  | 3:L:202:PHE:CE2  | 2.48                     | 0.49              |
| 4:M:43:LEU:HD11  | 4:M:397:ILE:CD1  | 2.42                     | 0.49              |
| 4:M:118:VAL:HB   | 4:M:257:TYR:HE2  | 1.77                     | 0.49              |
| 4:M:200:ARG:O    | 4:M:204:TYR:HD1  | 1.94                     | 0.49              |
| 1:S:288:GLN:HB3  | 1:S:333:GLU:HG2  | 1.93                     | 0.49              |
| 1:S:341:MET:HE2  | 1:S:409:PRO:O    | 2.12                     | 0.49              |
| 3:U:2:VAL:CG1    | 3:U:89:ASP:HA    | 2.42                     | 0.49              |
| 4:V:200:ARG:O    | 4:V:204:TYR:HD1  | 1.95                     | 0.49              |
| 1:1:88:TYR:HB2   | 1:1:216:THR:CG2  | 2.42                     | 0.49              |
| 1:1:211:LEU:H    | 1:1:216:THR:HG21 | 1.77                     | 0.49              |
| 2:2:40:TRP:CH2   | 2:2:42:ARG:HG2   | 2.47                     | 0.49              |
| 3:3:118:ASP:O    | 3:3:119:CYS:C    | 2.55                     | 0.49              |
| 3:3:188:VAL:CG2  | 3:3:189:ARG:N    | 2.76                     | 0.49              |
| 3:3:550:LEU:HD23 | 3:3:684:ARG:NH2  | 2.27                     | 0.49              |
| 3:C:361:ALA:HB1  | 3:C:366:THR:CG2  | 2.42                     | 0.49              |
| 4:D:144:THR:N    | 4:D:145:PRO:CD   | 2.75                     | 0.49              |
| 4:D:316:LEU:C    | 4:D:316:LEU:HD12 | 2.36                     | 0.49              |
| 1:J:63:ARG:HD3   | 1:J:313:TYR:HD2  | 1.78                     | 0.49              |
| 4:M:168:PHE:N    | 4:M:168:PHE:CD1  | 2.78                     | 0.49              |
| 5:N:25:LEU:CD2   | 5:N:25:LEU:H     | 2.26                     | 0.49              |
| 3:U:282:VAL:HG22 | 3:U:282:VAL:O    | 2.12                     | 0.49              |
| 3:U:671:GLU:HG3  | 3:U:672:ALA:H    | 1.77                     | 0.49              |
| 4:V:59:ILE:HD13  | 4:V:59:ILE:H     | 1.77                     | 0.49              |
| 4:V:342:VAL:HG22 | 4:V:343:TYR:H    | 1.78                     | 0.49              |
| 1:1:342:TRP:O    | 1:1:342:TRP:HE3  | 1.96                     | 0.49              |
| 4:4:52:VAL:HG23  | 4:4:388:GLU:O    | 2.13                     | 0.49              |
| 4:4:393:MET:C    | 4:4:396:ILE:HG22 | 2.38                     | 0.49              |
| 7:9:163:VAL:HB   | 7:9:164:PRO:HD2  | 1.93                     | 0.49              |
| 1:A:118:MET:HG2  | 1:A:224:LEU:HD13 | 1.95                     | 0.49              |
| 1:A:391:LEU:HD22 | 1:A:407:VAL:HB   | 1.94                     | 0.49              |
| 3:C:49:LEU:HA    | 3:C:80:ALA:O     | 2.12                     | 0.49              |
| 3:C:498:GLU:C    | 3:C:500:ALA:H    | 2.19                     | 0.49              |
| 3:C:693:TYR:HB3  | 3:C:759:TYR:HD2  | 1.76                     | 0.49              |
| 4:D:64:THR:HB    | 4:D:66:PHE:HE1   | 1.75                     | 0.49              |
| 4:D:342:VAL:HG22 | 4:D:343:TYR:H    | 1.78                     | 0.49              |
| 1:J:186:THR:HG23 | 1:J:199:PRO:HA   | 1.94                     | 0.49              |
| 1:J:274:GLU:HG3  | 1:J:278:GLU:HG3  | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:130:THR:HB   | 2:K:144:CYS:SG   | 2.52                     | 0.49              |
| 3:L:381:LEU:HD12 | 3:L:522:ARG:HD3  | 1.94                     | 0.49              |
| 3:L:557:SER:H    | 3:L:560:GLU:HB2  | 1.78                     | 0.49              |
| 3:L:670:PRO:CD   | 3:L:676:LEU:HD23 | 2.43                     | 0.49              |
| 1:S:272:PHE:CE2  | 1:S:311:MET:HE3  | 2.48                     | 0.49              |
| 1:S:358:PRO:O    | 1:S:362:GLY:HA3  | 2.13                     | 0.49              |
| 2:T:102:GLU:HA   | 8:Z:108:ILE:HD11 | 1.95                     | 0.49              |
| 4:V:84:ARG:O     | 6:X:83:ARG:NH2   | 2.46                     | 0.49              |
| 7:Y:163:VAL:HB   | 7:Y:164:PRO:HD2  | 1.95                     | 0.49              |
| 8:Z:40:PHE:HB2   | 8:Z:48:TYR:CE2   | 2.47                     | 0.49              |
| 1:I:163:PHE:C    | 1:I:165:THR:H    | 2.20                     | 0.49              |
| 3:3:497:TRP:CD1  | 3:3:524:LEU:HD11 | 2.47                     | 0.49              |
| 8:7:37:PHE:CE1   | 8:7:55:MET:HB2   | 2.47                     | 0.49              |
| 1:A:398:SER:HA   | 3:C:46:ARG:HD2   | 1.95                     | 0.49              |
| 4:D:122:GLU:OE2  | 4:D:249:ARG:NH1  | 2.42                     | 0.49              |
| 4:D:294:LEU:O    | 4:D:294:LEU:HD23 | 2.13                     | 0.49              |
| 1:J:355:LYS:HD3  | 1:J:399:PHE:CD2  | 2.48                     | 0.49              |
| 3:L:268:ASP:OD2  | 3:L:278:ARG:NH1  | 2.45                     | 0.49              |
| 3:L:326:PHE:CZ   | 3:L:330:LYS:HE3  | 2.48                     | 0.49              |
| 3:L:333:LEU:HD13 | 3:L:648:LEU:HD21 | 1.93                     | 0.49              |
| 3:L:470:PRO:O    | 3:L:471:GLY:C    | 2.55                     | 0.49              |
| 4:M:115:THR:HG22 | 4:M:297:LEU:HD23 | 1.94                     | 0.49              |
| 6:O:138:PRO:HG3  | 7:P:121:MET:HG3  | 1.94                     | 0.49              |
| 1:S:298:PRO:HD2  | 1:S:321:SER:OG   | 2.13                     | 0.49              |
| 3:U:689:LYS:HD2  | 3:U:772:GLU:H    | 1.77                     | 0.49              |
| 4:V:363:SER:HB3  | 5:W:173:ALA:HB1  | 1.94                     | 0.49              |
| 8:Z:13:TRP:CZ2   | 8:Z:17:LEU:HD11  | 2.46                     | 0.49              |
| 4:4:74:THR:HG22  | 4:4:75:TYR:N     | 2.27                     | 0.49              |
| 6:6:138:PRO:HG2  | 7:9:121:MET:HG3  | 1.93                     | 0.49              |
| 1:A:186:THR:HA   | 1:A:189:MET:HE2  | 1.95                     | 0.49              |
| 1:A:272:PHE:O    | 1:A:276:ILE:HG13 | 2.13                     | 0.49              |
| 3:C:237:ASP:OD1  | 3:C:239:THR:HG22 | 2.13                     | 0.49              |
| 4:D:125:ARG:HD2  | 4:D:286:SER:OG   | 2.13                     | 0.49              |
| 4:D:363:SER:HB3  | 5:E:173:ALA:HB1  | 1.95                     | 0.49              |
| 4:D:374:SER:HB2  | 4:D:406:ASP:HB3  | 1.94                     | 0.49              |
| 5:E:71:VAL:CG1   | 5:E:89:PHE:HD2   | 2.25                     | 0.49              |
| 1:J:288:GLN:HB3  | 1:J:333:GLU:HG2  | 1.95                     | 0.49              |
| 3:L:200:LEU:O    | 3:L:201:ASP:HB2  | 2.12                     | 0.49              |
| 4:M:74:THR:HG22  | 4:M:75:TYR:N     | 2.27                     | 0.49              |
| 4:M:224:ILE:HD11 | 4:M:275:ARG:CZ   | 2.43                     | 0.49              |
| 5:N:107:LEU:HD23 | 5:N:107:LEU:HA   | 1.70                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:41:ALA:HA    | 1:S:120:LEU:HD21 | 1.94                     | 0.49              |
| 2:T:116:LEU:N    | 2:T:116:LEU:HD23 | 2.27                     | 0.49              |
| 3:U:19:VAL:HG12  | 3:U:82:SER:HB2   | 1.95                     | 0.49              |
| 4:V:123:LEU:HD21 | 4:V:159:LEU:HD12 | 1.95                     | 0.49              |
| 4:V:125:ARG:HD2  | 4:V:286:SER:OG   | 2.13                     | 0.49              |
| 4:V:261:THR:HB   | 4:V:292:GLN:OE1  | 2.13                     | 0.49              |
| 6:X:128:ASP:HA   | 6:X:131:VAL:O    | 2.12                     | 0.49              |
| 1:1:18:TYR:OH    | 1:1:105:TYR:HB2  | 2.12                     | 0.49              |
| 1:1:358:PRO:O    | 1:1:362:GLY:HA3  | 2.13                     | 0.49              |
| 2:2:85:THR:HG22  | 2:2:86:LEU:N     | 2.28                     | 0.49              |
| 4:4:40:VAL:HG23  | 6:6:88:MET:CE    | 2.43                     | 0.49              |
| 5:5:123:GLY:HA2  | 5:5:144:HIS:CD2  | 2.48                     | 0.49              |
| 3:C:112:LEU:CD2  | 3:C:130:LEU:HD11 | 2.43                     | 0.49              |
| 4:D:69:THR:HG21  | 6:F:120:ASN:HD22 | 1.78                     | 0.49              |
| 4:D:197:LEU:N    | 4:D:198:PRO:HD2  | 2.28                     | 0.49              |
| 1:J:238:PHE:HE1  | 1:J:249:MET:HE1  | 1.78                     | 0.49              |
| 3:L:55:PRO:CG    | 3:L:74:GLN:N     | 2.72                     | 0.49              |
| 6:O:16:ARG:HA    | 6:O:21:PHE:CD2   | 2.47                     | 0.49              |
| 6:O:41:PHE:CZ    | 6:O:92:MET:HB2   | 2.48                     | 0.49              |
| 3:U:385:ALA:HB3  | 3:U:533:LEU:CD2  | 2.43                     | 0.49              |
| 5:W:123:GLY:HA2  | 5:W:144:HIS:CD2  | 2.48                     | 0.49              |
| 5:W:125:VAL:HG12 | 5:W:126:PHE:N    | 2.28                     | 0.49              |
| 8:Z:86:LEU:HD12  | 8:Z:91:ILE:HD12  | 1.94                     | 0.49              |
| 3:3:237:ASP:OD1  | 3:3:239:THR:HG22 | 2.13                     | 0.49              |
| 4:4:210:GLU:O    | 4:4:212:PRO:HD3  | 2.13                     | 0.49              |
| 1:A:397:ARG:HD2  | 1:A:397:ARG:N    | 2.25                     | 0.49              |
| 2:B:116:LEU:HD23 | 2:B:116:LEU:N    | 2.28                     | 0.49              |
| 4:D:85:MET:HE3   | 4:D:409:ARG:CB   | 2.43                     | 0.49              |
| 4:D:212:PRO:HG2  | 4:D:213:ILE:H    | 1.78                     | 0.49              |
| 8:H:49:ASP:OD1   | 8:H:49:ASP:N     | 2.46                     | 0.49              |
| 3:L:655:ARG:HH12 | 3:L:659:GLU:CB   | 2.26                     | 0.49              |
| 4:M:79:ILE:O     | 4:M:79:ILE:HG22  | 2.13                     | 0.49              |
| 2:T:139:GLU:HB2  | 2:T:140:PRO:CD   | 2.33                     | 0.49              |
| 3:U:329:LEU:HD21 | 3:U:644:LEU:HA   | 1.94                     | 0.49              |
| 4:V:69:THR:HG21  | 6:X:120:ASN:ND2  | 2.27                     | 0.49              |
| 4:V:118:VAL:HB   | 4:V:257:TYR:HE2  | 1.77                     | 0.49              |
| 4:V:230:ILE:HD11 | 4:V:244:VAL:CG2  | 2.43                     | 0.49              |
| 8:Z:89:ALA:O     | 8:Z:91:ILE:HG13  | 2.13                     | 0.49              |
| 1:1:72:THR:HG21  | 1:1:223:THR:HG21 | 1.95                     | 0.48              |
| 3:3:478:LEU:CD2  | 3:3:483:ASP:HB2  | 2.43                     | 0.48              |
| 3:3:646:GLU:C    | 3:3:648:LEU:H    | 2.21                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:6:41:PHE:CZ    | 6:6:92:MET:HB2   | 2.48                     | 0.48              |
| 1:A:341:MET:CE   | 1:A:409:PRO:HB2  | 2.42                     | 0.48              |
| 3:C:440:ARG:CG   | 3:C:440:ARG:NH1  | 2.75                     | 0.48              |
| 4:D:104:LEU:HD22 | 4:D:338:PRO:HD2  | 1.95                     | 0.48              |
| 8:H:108:ILE:N    | 8:H:108:ILE:HD12 | 2.28                     | 0.48              |
| 1:J:40:THR:O     | 1:J:44:VAL:HG23  | 2.13                     | 0.48              |
| 1:J:211:LEU:H    | 1:J:216:THR:HG21 | 1.77                     | 0.48              |
| 4:M:84:ARG:HD3   | 6:O:117:MET:HE1  | 1.94                     | 0.48              |
| 4:M:198:PRO:HG3  | 4:M:291:LYS:NZ   | 2.28                     | 0.48              |
| 4:M:393:MET:HA   | 4:M:396:ILE:CG2  | 2.43                     | 0.48              |
| 8:Q:108:ILE:HD12 | 8:Q:108:ILE:N    | 2.27                     | 0.48              |
| 3:U:232:VAL:HB   | 9:U:784:SF4:S2   | 2.53                     | 0.48              |
| 3:U:629:ILE:HG22 | 3:U:630:GLU:N    | 2.25                     | 0.48              |
| 5:W:160:ARG:HG3  | 7:Y:130:VAL:HG11 | 1.95                     | 0.48              |
| 7:Y:96:LEU:HD21  | 7:Y:129:LEU:HD12 | 1.95                     | 0.48              |
| 8:Z:49:ASP:N     | 8:Z:49:ASP:OD1   | 2.46                     | 0.48              |
| 3:3:20:MET:HE2   | 3:3:433:ALA:HB2  | 1.95                     | 0.48              |
| 3:3:117:LEU:H    | 4:4:321:MET:CE   | 2.19                     | 0.48              |
| 3:3:381:LEU:HD12 | 3:3:522:ARG:HD3  | 1.94                     | 0.48              |
| 6:6:108:MET:HA   | 6:6:137:VAL:CG1  | 2.43                     | 0.48              |
| 8:7:40:PHE:HB2   | 8:7:48:TYR:CE2   | 2.49                     | 0.48              |
| 1:A:133:TYR:HB2  | 1:A:188:LEU:HD21 | 1.94                     | 0.48              |
| 2:B:85:THR:HG22  | 2:B:86:LEU:N     | 2.27                     | 0.48              |
| 6:F:114:SER:HB2  | 7:G:97:ARG:CD    | 2.42                     | 0.48              |
| 1:J:334:ARG:O    | 1:J:434:PRO:HG3  | 2.13                     | 0.48              |
| 2:K:85:THR:HG22  | 2:K:86:LEU:N     | 2.28                     | 0.48              |
| 3:L:118:ASP:O    | 3:L:119:CYS:C    | 2.56                     | 0.48              |
| 4:M:366:TYR:CE1  | 5:N:148:LYS:HE3  | 2.48                     | 0.48              |
| 5:N:25:LEU:H     | 5:N:25:LEU:HD23  | 1.78                     | 0.48              |
| 8:Q:16:LEU:HG    | 8:Q:82:ILE:HD11  | 1.95                     | 0.48              |
| 1:S:197:ALA:HB3  | 2:T:66:PHE:CZ    | 2.48                     | 0.48              |
| 4:V:404:MET:HA   | 4:V:407:VAL:CG1  | 2.43                     | 0.48              |
| 3:3:498:GLU:C    | 3:3:500:ALA:H    | 2.21                     | 0.48              |
| 4:4:198:PRO:HG3  | 4:4:291:LYS:NZ   | 2.28                     | 0.48              |
| 6:6:164:ASN:HB2  | 7:9:128:ASP:OD2  | 2.12                     | 0.48              |
| 6:6:165:GLU:HG2  | 7:9:148:ARG:NH1  | 2.28                     | 0.48              |
| 8:7:29:VAL:HG22  | 8:7:60:SER:O     | 2.12                     | 0.48              |
| 1:A:358:PRO:O    | 1:A:362:GLY:HA3  | 2.13                     | 0.48              |
| 3:C:115:HIS:CD2  | 3:C:116:PRO:HD2  | 2.48                     | 0.48              |
| 3:C:184:CYS:O    | 9:C:785:SF4:S4   | 2.72                     | 0.48              |
| 3:C:497:TRP:CD1  | 3:C:524:LEU:HD11 | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:40:VAL:HG23  | 6:F:88:MET:CE    | 2.43                     | 0.48              |
| 4:D:83:PRO:HB2   | 4:D:169:HIS:HA   | 1.94                     | 0.48              |
| 5:E:2:ARG:NH1    | 5:E:45:GLY:HA3   | 2.28                     | 0.48              |
| 6:F:163:TYR:CD1  | 7:G:152:ARG:HD2  | 2.48                     | 0.48              |
| 1:J:133:TYR:HB2  | 1:J:188:LEU:HD21 | 1.93                     | 0.48              |
| 3:L:361:ALA:HB1  | 3:L:366:THR:CG2  | 2.43                     | 0.48              |
| 3:L:583:VAL:HG23 | 3:L:598:ALA:HA   | 1.95                     | 0.48              |
| 4:M:316:LEU:C    | 4:M:318:GLU:H    | 2.22                     | 0.48              |
| 8:Q:68:LEU:HD13  | 8:Q:69:LEU:N     | 2.28                     | 0.48              |
| 4:V:250:LYS:CE   | 4:V:262:PHE:HB3  | 2.43                     | 0.48              |
| 5:W:34:PHE:HE1   | 5:W:38:MET:SD    | 2.35                     | 0.48              |
| 6:X:83:ARG:HD3   | 6:X:111:CYS:SG   | 2.53                     | 0.48              |
| 2:2:58:THR:HG21  | 3:3:200:LEU:N    | 2.27                     | 0.48              |
| 3:3:2:VAL:HG13   | 3:3:89:ASP:HA    | 1.94                     | 0.48              |
| 3:3:31:PRO:HD2   | 3:3:104:GLN:NE2  | 2.27                     | 0.48              |
| 3:3:671:GLU:HG3  | 3:3:672:ALA:H    | 1.79                     | 0.48              |
| 3:3:694:LEU:CB   | 3:3:762:ALA:HB2  | 2.39                     | 0.48              |
| 4:4:222:GLY:HA2  | 4:4:384:ALA:O    | 2.14                     | 0.48              |
| 4:4:224:ILE:HD11 | 4:4:275:ARG:CZ   | 2.43                     | 0.48              |
| 5:5:107:LEU:HA   | 5:5:107:LEU:HD23 | 1.74                     | 0.48              |
| 5:5:125:VAL:HG12 | 5:5:126:PHE:N    | 2.28                     | 0.48              |
| 6:6:155:GLN:O    | 6:6:158:VAL:HG22 | 2.14                     | 0.48              |
| 2:B:66:PHE:CE1   | 3:C:205:ARG:HD3  | 2.48                     | 0.48              |
| 4:D:237:GLY:HA2  | 4:D:240:ARG:NH2  | 2.28                     | 0.48              |
| 1:J:139:ARG:CG   | 2:K:140:PRO:HD3  | 2.39                     | 0.48              |
| 4:M:104:LEU:HD22 | 4:M:338:PRO:HD2  | 1.95                     | 0.48              |
| 6:O:128:ASP:HA   | 6:O:131:VAL:O    | 2.13                     | 0.48              |
| 7:P:41:HIS:ND1   | 7:P:95:MET:HE1   | 2.29                     | 0.48              |
| 1:S:260:ARG:HA   | 2:T:177:HIS:O    | 2.12                     | 0.48              |
| 3:U:269:THR:HG23 | 3:U:274:LEU:HD13 | 1.95                     | 0.48              |
| 3:U:487:SER:OG   | 3:U:490:VAL:HG23 | 2.12                     | 0.48              |
| 3:U:557:SER:H    | 3:U:560:GLU:HB2  | 1.78                     | 0.48              |
| 4:V:168:PHE:HA   | 4:V:170:HIS:CD2  | 2.48                     | 0.48              |
| 5:W:103:THR:HG23 | 5:W:127:GLU:O    | 2.13                     | 0.48              |
| 7:Y:41:HIS:ND1   | 7:Y:95:MET:HE1   | 2.27                     | 0.48              |
| 1:1:201:LEU:HG   | 1:1:203:PRO:HD2  | 1.94                     | 0.48              |
| 3:3:361:ALA:HB1  | 3:3:366:THR:CG2  | 2.44                     | 0.48              |
| 3:3:399:LEU:HD12 | 3:3:399:LEU:N    | 2.28                     | 0.48              |
| 4:4:93:HIS:HA    | 4:4:353:LEU:HD21 | 1.96                     | 0.48              |
| 5:5:25:LEU:CD2   | 5:5:25:LEU:H     | 2.27                     | 0.48              |
| 5:5:25:LEU:H     | 5:5:25:LEU:HD23  | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:6:16:ARG:HA    | 6:6:21:PHE:CD2   | 2.48                     | 0.48              |
| 8:7:16:LEU:HD13  | 8:7:16:LEU:O     | 2.13                     | 0.48              |
| 1:A:186:THR:HG23 | 1:A:199:PRO:HA   | 1.94                     | 0.48              |
| 4:D:218:ALA:HB1  | 4:D:272:VAL:HG22 | 1.95                     | 0.48              |
| 5:E:123:GLY:HA2  | 5:E:144:HIS:CD2  | 2.48                     | 0.48              |
| 1:J:397:ARG:NE   | 3:L:79:LEU:HD12  | 2.25                     | 0.48              |
| 3:L:688:ARG:HD3  | 3:L:688:ARG:HA   | 1.53                     | 0.48              |
| 4:M:367:ARG:HH12 | 4:M:369:LYS:CA   | 2.25                     | 0.48              |
| 1:S:332:PRO:HD2  | 2:T:90:LEU:CD2   | 2.43                     | 0.48              |
| 2:T:11:LEU:O     | 2:T:12:GLU:C     | 2.56                     | 0.48              |
| 3:U:188:VAL:CG2  | 3:U:189:ARG:N    | 2.76                     | 0.48              |
| 3:U:546:ALA:O    | 3:U:547:MET:HE2  | 2.13                     | 0.48              |
| 8:Z:121:ARG:NH1  | 8:Z:121:ARG:CG   | 2.75                     | 0.48              |
| 1:1:87:HIS:HB2   | 1:1:126:ARG:O    | 2.13                     | 0.48              |
| 1:1:104:ARG:HH21 | 2:2:127:SER:CB   | 2.26                     | 0.48              |
| 4:4:188:PRO:O    | 4:4:191:LYS:HB2  | 2.14                     | 0.48              |
| 5:5:167:PRO:HB3  | 7:9:66:TYR:CD2   | 2.48                     | 0.48              |
| 5:E:160:ARG:HD2  | 7:G:92:GLU:OE2   | 2.14                     | 0.48              |
| 4:M:261:THR:HB   | 4:M:292:GLN:OE1  | 2.13                     | 0.48              |
| 3:U:285:VAL:HG22 | 3:U:286:ASN:H    | 1.75                     | 0.48              |
| 3:U:594:ALA:C    | 3:U:596:ARG:H    | 2.22                     | 0.48              |
| 4:V:311:PRO:HD3  | 4:V:330:HIS:CE1  | 2.49                     | 0.48              |
| 5:W:16:PRO:HB2   | 5:W:28:VAL:CG1   | 2.44                     | 0.48              |
| 5:W:52:ILE:CG2   | 5:W:114:LEU:HB3  | 2.40                     | 0.48              |
| 3:3:186:ARG:HD2  | 3:3:231:PRO:HD3  | 1.95                     | 0.48              |
| 1:A:315:HIS:O    | 1:A:319:LYS:HB2  | 2.14                     | 0.48              |
| 5:E:44:MET:HB2   | 5:E:44:MET:HE3   | 1.63                     | 0.48              |
| 6:F:113:SER:HB3  | 7:G:96:LEU:HD13  | 1.95                     | 0.48              |
| 1:J:65:ARG:NH2   | 1:J:268:MET:CE   | 2.75                     | 0.48              |
| 1:J:211:LEU:HB2  | 1:J:216:THR:HG21 | 1.95                     | 0.48              |
| 3:L:385:ALA:HB2  | 3:L:531:LYS:CB   | 2.44                     | 0.48              |
| 4:M:230:ILE:HD11 | 4:M:244:VAL:CG2  | 2.44                     | 0.48              |
| 5:N:16:PRO:HB2   | 5:N:28:VAL:CG1   | 2.44                     | 0.48              |
| 7:P:96:LEU:HD21  | 7:P:129:LEU:HD12 | 1.96                     | 0.48              |
| 1:S:195:LEU:HA   | 2:T:24:ARG:HH21  | 1.78                     | 0.48              |
| 1:S:359:CYS:O    | 1:S:363:VAL:HG22 | 2.13                     | 0.48              |
| 4:V:237:GLY:HA2  | 4:V:240:ARG:NH2  | 2.28                     | 0.48              |
| 5:W:141:LEU:HD21 | 5:W:145:PRO:HD3  | 1.96                     | 0.48              |
| 1:1:116:GLU:HG2  | 1:1:228:VAL:HG22 | 1.95                     | 0.48              |
| 1:1:397:ARG:HD2  | 1:1:397:ARG:N    | 2.27                     | 0.48              |
| 3:3:46:ARG:O     | 3:3:107:MET:HG2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:738:THR:HG22 | 3:C:739:PRO:CD   | 2.37                     | 0.48              |
| 4:D:85:MET:HE1   | 4:D:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:D:161:GLU:OE1  | 7:G:34:LYS:HG2   | 2.13                     | 0.48              |
| 4:D:197:LEU:N    | 4:D:198:PRO:CD   | 2.76                     | 0.48              |
| 4:D:390:VAL:N    | 4:D:391:PRO:CD   | 2.77                     | 0.48              |
| 8:H:17:LEU:HD13  | 8:H:54:ILE:HD13  | 1.96                     | 0.48              |
| 1:J:385:GLU:O    | 1:J:388:GLU:HB3  | 2.13                     | 0.48              |
| 2:K:112:THR:HG22 | 2:K:116:LEU:H    | 1.79                     | 0.48              |
| 3:L:19:VAL:HG23  | 3:L:85:THR:O     | 2.14                     | 0.48              |
| 3:L:282:VAL:HG22 | 3:L:282:VAL:O    | 2.14                     | 0.48              |
| 3:L:546:ALA:C    | 3:L:547:MET:HE2  | 2.38                     | 0.48              |
| 4:M:83:PRO:HB2   | 4:M:169:HIS:HA   | 1.96                     | 0.48              |
| 4:M:168:PHE:HE1  | 6:O:141:PRO:HG3  | 1.79                     | 0.48              |
| 1:S:360:ARG:O    | 1:S:364:ALA:HB3  | 2.14                     | 0.48              |
| 3:U:614:LEU:O    | 3:U:621:VAL:HA   | 2.14                     | 0.48              |
| 4:V:112:ARG:HH21 | 4:V:297:LEU:HD11 | 1.79                     | 0.48              |
| 5:W:84:ASP:OD1   | 5:W:84:ASP:N     | 2.43                     | 0.48              |
| 6:X:37:TRP:HA    | 6:X:37:TRP:CE3   | 2.49                     | 0.48              |
| 6:X:114:SER:HB2  | 7:Y:97:ARG:CD    | 2.39                     | 0.48              |
| 2:2:106:ILE:CG2  | 2:2:110:GLU:HB2  | 2.44                     | 0.48              |
| 3:3:583:VAL:HG23 | 3:3:598:ALA:HA   | 1.95                     | 0.48              |
| 3:3:737:GLU:HB2  | 3:3:776:LEU:HD21 | 1.96                     | 0.48              |
| 4:4:350:ARG:HG3  | 4:4:350:ARG:NH1  | 2.29                     | 0.48              |
| 1:A:72:THR:HG21  | 1:A:223:THR:HG21 | 1.96                     | 0.48              |
| 1:A:264:TYR:CD2  | 1:A:279:TRP:HB3  | 2.49                     | 0.48              |
| 3:C:664:LEU:O    | 3:C:669:VAL:HG12 | 2.13                     | 0.48              |
| 3:C:671:GLU:HG3  | 3:C:672:ALA:H    | 1.79                     | 0.48              |
| 6:F:96:TRP:HA    | 6:F:99:MET:CE    | 2.40                     | 0.48              |
| 6:F:155:GLN:C    | 6:F:157:LYS:H    | 2.22                     | 0.48              |
| 4:M:241:ALA:CB   | 4:M:278:VAL:HG21 | 2.44                     | 0.48              |
| 6:O:84:LEU:HD11  | 6:O:89:ALA:HA    | 1.95                     | 0.48              |
| 3:U:55:PRO:HG3   | 3:U:73:ILE:C     | 2.37                     | 0.48              |
| 3:U:241:ARG:HH11 | 7:Y:74:GLU:CD    | 2.20                     | 0.48              |
| 3:U:646:GLU:C    | 3:U:648:LEU:H    | 2.22                     | 0.48              |
| 4:V:133:LEU:HD21 | 4:V:204:TYR:CE2  | 2.48                     | 0.48              |
| 4:V:223:VAL:O    | 4:V:383:TYR:HE1  | 1.97                     | 0.48              |
| 7:Y:26:TYR:N     | 7:Y:27:PRO:CD    | 2.71                     | 0.48              |
| 3:3:18:SER:HB2   | 3:3:433:ALA:O    | 2.12                     | 0.48              |
| 3:3:119:CYS:O    | 3:3:120:PRO:C    | 2.55                     | 0.48              |
| 3:3:326:PHE:CZ   | 3:3:330:LYS:HE3  | 2.49                     | 0.48              |
| 3:3:398:VAL:CB   | 3:3:450:LEU:HD22 | 2.41                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:211:SER:HB2  | 4:4:215:TYR:N    | 2.28                     | 0.48              |
| 1:A:39:GLU:O     | 1:A:43:ARG:HG3   | 2.14                     | 0.48              |
| 1:A:97:GLU:OE2   | 1:A:294:GLY:HA3  | 2.14                     | 0.48              |
| 1:A:184:GLU:OE1  | 1:A:186:THR:N    | 2.47                     | 0.48              |
| 1:A:334:ARG:O    | 1:A:434:PRO:HG3  | 2.14                     | 0.48              |
| 1:A:385:GLU:O    | 1:A:388:GLU:HB3  | 2.13                     | 0.48              |
| 3:C:33:PHE:HE2   | 3:C:111:THR:HG21 | 1.79                     | 0.48              |
| 3:C:409:LEU:HD12 | 3:C:535:MET:CE   | 2.42                     | 0.48              |
| 3:C:488:GLU:O    | 3:C:491:ALA:HB3  | 2.14                     | 0.48              |
| 4:D:148:TYR:HB3  | 4:D:200:ARG:HH12 | 1.77                     | 0.48              |
| 4:D:161:GLU:OE2  | 6:F:143:ARG:NH1  | 2.47                     | 0.48              |
| 4:D:236:GLY:C    | 4:D:238:SER:N    | 2.71                     | 0.48              |
| 8:H:63:LEU:HD13  | 8:H:129:ALA:HB3  | 1.96                     | 0.48              |
| 1:J:29:LEU:HD22  | 1:J:33:LEU:CD1   | 2.44                     | 0.48              |
| 3:L:237:ASP:OD1  | 3:L:239:THR:HG22 | 2.14                     | 0.48              |
| 6:O:140:CYS:SG   | 7:P:99:ILE:HG13  | 2.54                     | 0.48              |
| 1:S:290:ILE:HG22 | 1:S:330:LEU:HD22 | 1.96                     | 0.48              |
| 3:U:470:PRO:O    | 3:U:471:GLY:C    | 2.57                     | 0.48              |
| 3:3:19:VAL:HG23  | 3:3:85:THR:O     | 2.14                     | 0.47              |
| 3:3:55:PRO:CG    | 3:3:74:GLN:N     | 2.73                     | 0.47              |
| 3:3:184:CYS:O    | 9:3:785:SF4:S4   | 2.71                     | 0.47              |
| 4:4:85:MET:HE3   | 4:4:409:ARG:CB   | 2.44                     | 0.47              |
| 6:6:138:PRO:HG3  | 7:9:121:MET:HG3  | 1.96                     | 0.47              |
| 2:B:27:ILE:HG13  | 2:B:53:VAL:HG21  | 1.96                     | 0.47              |
| 3:C:185:LYS:HG2  | 3:C:188:VAL:CG2  | 2.44                     | 0.47              |
| 3:L:168:HIS:HA   | 3:L:169:PRO:HD2  | 1.74                     | 0.47              |
| 3:L:382:PHE:CD1  | 3:L:382:PHE:N    | 2.81                     | 0.47              |
| 4:M:252:TYR:CE2  | 5:N:87:ARG:NH2   | 2.82                     | 0.47              |
| 6:O:121:TYR:HD1  | 6:O:121:TYR:H    | 1.62                     | 0.47              |
| 7:P:39:GLY:O     | 7:P:40:ARG:C     | 2.55                     | 0.47              |
| 1:S:341:MET:CE   | 1:S:409:PRO:HB2  | 2.43                     | 0.47              |
| 1:S:360:ARG:O    | 3:U:207:VAL:HG13 | 2.14                     | 0.47              |
| 4:V:203:GLU:O    | 4:V:207:LEU:HG   | 2.14                     | 0.47              |
| 1:1:195:LEU:HA   | 2:2:24:ARG:HH21  | 1.79                     | 0.47              |
| 6:6:128:ASP:HA   | 6:6:131:VAL:O    | 2.14                     | 0.47              |
| 1:A:424:LEU:HD21 | 1:A:431:VAL:HG12 | 1.97                     | 0.47              |
| 4:D:168:PHE:HA   | 4:D:170:HIS:CD2  | 2.49                     | 0.47              |
| 4:D:197:LEU:HA   | 4:D:200:ARG:HB3  | 1.96                     | 0.47              |
| 4:D:393:MET:C    | 4:D:396:ILE:HG22 | 2.39                     | 0.47              |
| 6:F:130:VAL:HG23 | 6:F:131:VAL:HG13 | 1.96                     | 0.47              |
| 1:J:92:ASN:HD21  | 10:J:440:FMN:C2  | 2.27                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:84:ARG:CD    | 6:O:117:MET:HE1  | 2.44                     | 0.47              |
| 4:M:148:TYR:HB3  | 4:M:200:ARG:HH12 | 1.77                     | 0.47              |
| 5:N:98:ASP:C     | 5:N:100:ARG:H    | 2.23                     | 0.47              |
| 3:U:269:THR:HG22 | 3:U:274:LEU:HA   | 1.95                     | 0.47              |
| 3:U:591:HIS:ND1  | 3:U:592:PRO:CD   | 2.76                     | 0.47              |
| 1:1:183:GLY:O    | 10:1:440:FMN:H2' | 2.14                     | 0.47              |
| 3:3:583:VAL:HG21 | 3:3:597:TYR:O    | 2.14                     | 0.47              |
| 4:4:133:LEU:HD21 | 4:4:204:TYR:CE2  | 2.49                     | 0.47              |
| 4:4:263:ASP:HB2  | 4:4:285:GLU:OE1  | 2.14                     | 0.47              |
| 4:4:381:LEU:H    | 4:4:382:PRO:CD   | 2.27                     | 0.47              |
| 5:5:16:PRO:HB2   | 5:5:28:VAL:CG1   | 2.44                     | 0.47              |
| 6:6:84:LEU:HD11  | 6:6:89:ALA:HA    | 1.96                     | 0.47              |
| 2:B:87:SER:OG    | 2:B:128:CYS:HB3  | 2.13                     | 0.47              |
| 3:C:550:LEU:HD23 | 3:C:684:ARG:NH2  | 2.29                     | 0.47              |
| 4:D:254:TYR:CE2  | 4:D:346:THR:CA   | 2.94                     | 0.47              |
| 1:J:360:ARG:O    | 1:J:364:ALA:HB3  | 2.13                     | 0.47              |
| 3:L:337:ARG:HD2  | 3:L:337:ARG:N    | 2.29                     | 0.47              |
| 3:L:368:HIS:CD2  | 3:L:556:ALA:HB3  | 2.48                     | 0.47              |
| 4:M:213:ILE:HG22 | 4:M:217:ARG:HG3  | 1.95                     | 0.47              |
| 5:N:104:VAL:CG1  | 5:N:108:TRP:HE3  | 2.27                     | 0.47              |
| 8:Q:117:ALA:O    | 8:Q:121:ARG:HG2  | 2.14                     | 0.47              |
| 1:S:104:ARG:HH21 | 2:T:127:SER:HB2  | 1.79                     | 0.47              |
| 3:U:337:ARG:HD2  | 3:U:337:ARG:N    | 2.27                     | 0.47              |
| 3:U:612:GLY:O    | 3:U:624:LEU:HB2  | 2.14                     | 0.47              |
| 4:V:393:MET:HA   | 4:V:396:ILE:CG2  | 2.43                     | 0.47              |
| 6:X:165:GLU:HG3  | 7:Y:144:LYS:HE2  | 1.97                     | 0.47              |
| 1:1:272:PHE:CE1  | 1:1:311:MET:HG2  | 2.49                     | 0.47              |
| 4:4:115:THR:HG22 | 4:4:297:LEU:HD23 | 1.97                     | 0.47              |
| 4:4:263:ASP:O    | 4:4:285:GLU:HG3  | 2.14                     | 0.47              |
| 6:6:96:TRP:HA    | 6:6:99:MET:CE    | 2.41                     | 0.47              |
| 3:C:2:VAL:CG1    | 3:C:89:ASP:HA    | 2.44                     | 0.47              |
| 3:C:470:PRO:O    | 3:C:471:GLY:C    | 2.58                     | 0.47              |
| 6:F:48:ILE:O     | 6:F:48:ILE:HG22  | 2.13                     | 0.47              |
| 1:J:205:PHE:HD1  | 1:J:206:PRO:HD2  | 1.80                     | 0.47              |
| 2:K:3:PHE:C      | 2:K:3:PHE:CD1    | 2.92                     | 0.47              |
| 2:K:88:CYS:HB3   | 2:K:93:ALA:HB2   | 1.97                     | 0.47              |
| 2:K:102:GLU:HA   | 8:Q:108:ILE:HD11 | 1.96                     | 0.47              |
| 3:L:20:MET:HE2   | 3:L:433:ALA:HB2  | 1.96                     | 0.47              |
| 4:M:197:LEU:N    | 4:M:198:PRO:CD   | 2.78                     | 0.47              |
| 4:M:211:SER:HB2  | 4:M:215:TYR:N    | 2.29                     | 0.47              |
| 4:M:226:PRO:HG3  | 4:M:242:SER:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:263:ASP:O    | 4:M:285:GLU:HG3  | 2.14                     | 0.47              |
| 6:O:110:ALA:HB1  | 6:O:116:GLY:HA2  | 1.96                     | 0.47              |
| 2:T:109:GLY:HA2  | 8:Z:91:ILE:HD13  | 1.97                     | 0.47              |
| 4:V:316:LEU:C    | 4:V:318:GLU:H    | 2.21                     | 0.47              |
| 1:1:332:PRO:HD2  | 2:2:90:LEU:CD2   | 2.42                     | 0.47              |
| 1:1:420:GLN:O    | 1:1:424:LEU:HD13 | 2.14                     | 0.47              |
| 3:3:732:ALA:H    | 3:3:747:VAL:CG1  | 2.28                     | 0.47              |
| 6:6:105:VAL:HG11 | 6:6:131:VAL:CG2  | 2.44                     | 0.47              |
| 6:6:121:TYR:HD1  | 6:6:121:TYR:H    | 1.63                     | 0.47              |
| 8:7:108:ILE:HD12 | 8:7:108:ILE:N    | 2.29                     | 0.47              |
| 1:A:260:ARG:HA   | 2:B:177:HIS:O    | 2.15                     | 0.47              |
| 1:A:341:MET:HE2  | 1:A:409:PRO:O    | 2.14                     | 0.47              |
| 3:C:186:ARG:HD2  | 3:C:231:PRO:HD3  | 1.95                     | 0.47              |
| 4:D:376:VAL:O    | 4:D:379:GLN:HG3  | 2.15                     | 0.47              |
| 6:F:43:LEU:HD11  | 6:F:84:LEU:HD23  | 1.96                     | 0.47              |
| 1:J:184:GLU:HG2  | 10:J:440:FMN:C8M | 2.45                     | 0.47              |
| 3:L:506:ILE:HG21 | 3:L:535:MET:HE3  | 1.95                     | 0.47              |
| 1:S:40:THR:O     | 1:S:44:VAL:HG23  | 2.15                     | 0.47              |
| 1:S:267:PRO:O    | 1:S:268:MET:C    | 2.56                     | 0.47              |
| 3:U:378:PRO:O    | 3:U:381:LEU:HB2  | 2.15                     | 0.47              |
| 3:U:498:GLU:C    | 3:U:500:ALA:H    | 2.21                     | 0.47              |
| 4:V:350:ARG:HD3  | 4:V:374:SER:OG   | 2.15                     | 0.47              |
| 2:2:3:PHE:CD1    | 2:2:3:PHE:C      | 2.92                     | 0.47              |
| 4:4:116:ILE:HD11 | 4:4:182:LEU:CD2  | 2.44                     | 0.47              |
| 6:6:130:VAL:HG23 | 6:6:131:VAL:HG13 | 1.97                     | 0.47              |
| 8:7:37:PHE:HE2   | 8:7:74:PRO:HA    | 1.80                     | 0.47              |
| 3:C:55:PRO:HG3   | 3:C:73:ILE:C     | 2.39                     | 0.47              |
| 4:D:343:TYR:C    | 4:D:343:TYR:CD1  | 2.92                     | 0.47              |
| 8:H:37:PHE:CE2   | 8:H:74:PRO:HA    | 2.49                     | 0.47              |
| 1:J:161:ASN:OD1  | 1:J:166:ASP:HA   | 2.14                     | 0.47              |
| 3:L:241:ARG:HH11 | 7:P:74:GLU:CD    | 2.22                     | 0.47              |
| 3:L:385:ALA:HB3  | 3:L:533:LEU:HD23 | 1.96                     | 0.47              |
| 3:L:732:ALA:H    | 3:L:747:VAL:CG1  | 2.28                     | 0.47              |
| 5:N:141:LEU:HD21 | 5:N:145:PRO:HD3  | 1.96                     | 0.47              |
| 2:T:3:PHE:CD1    | 2:T:3:PHE:C      | 2.92                     | 0.47              |
| 3:U:693:TYR:HB3  | 3:U:759:TYR:HD2  | 1.78                     | 0.47              |
| 3:U:724:ARG:O    | 3:U:724:ARG:HG2  | 2.14                     | 0.47              |
| 1:1:102:LYS:HG3  | 1:1:103:ASP:N    | 2.30                     | 0.47              |
| 1:1:205:PHE:HD1  | 1:1:206:PRO:HD2  | 1.80                     | 0.47              |
| 2:2:116:LEU:HD23 | 2:2:116:LEU:N    | 2.30                     | 0.47              |
| 3:3:197:ASP:OD2  | 3:3:220:SER:HB2  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:688:ARG:HD3  | 3:3:688:ARG:HA   | 1.52                     | 0.47              |
| 4:4:106:GLY:O    | 5:5:194:SER:HB3  | 2.15                     | 0.47              |
| 4:4:226:PRO:HG3  | 4:4:242:SER:O    | 2.15                     | 0.47              |
| 4:4:256:GLY:C    | 4:4:258:GLU:N    | 2.71                     | 0.47              |
| 4:4:376:VAL:O    | 4:4:379:GLN:HG3  | 2.15                     | 0.47              |
| 6:6:37:TRP:CE3   | 6:6:37:TRP:HA    | 2.48                     | 0.47              |
| 6:6:110:ALA:HB1  | 6:6:116:GLY:HA2  | 1.97                     | 0.47              |
| 1:A:399:PHE:HB3  | 9:A:439:SF4:S2   | 2.55                     | 0.47              |
| 4:D:106:GLY:O    | 5:E:194:SER:HB3  | 2.14                     | 0.47              |
| 4:D:188:PRO:O    | 4:D:191:LYS:HB2  | 2.14                     | 0.47              |
| 4:D:314:ARG:NH1  | 4:D:314:ARG:CG   | 2.75                     | 0.47              |
| 4:D:346:THR:HG22 | 4:D:353:LEU:O    | 2.14                     | 0.47              |
| 6:F:16:ARG:HA    | 6:F:21:PHE:CD2   | 2.50                     | 0.47              |
| 6:F:108:MET:HA   | 6:F:137:VAL:CG1  | 2.44                     | 0.47              |
| 8:H:8:GLU:HG2    | 8:H:97:TYR:OH    | 2.14                     | 0.47              |
| 8:H:88:ARG:HE    | 8:H:126:LEU:CD2  | 2.28                     | 0.47              |
| 1:J:272:PHE:CE2  | 1:J:311:MET:HE3  | 2.50                     | 0.47              |
| 2:K:11:LEU:O     | 2:K:12:GLU:C     | 2.57                     | 0.47              |
| 2:K:42:ARG:HB2   | 2:K:45:ARG:HG2   | 1.96                     | 0.47              |
| 3:L:224:GLY:HA3  | 3:L:295:ARG:HD2  | 1.97                     | 0.47              |
| 3:L:508:GLY:HA2  | 3:L:535:MET:HB2  | 1.97                     | 0.47              |
| 3:L:689:LYS:HB2  | 3:L:772:GLU:HG2  | 1.96                     | 0.47              |
| 6:O:149:TYR:CZ   | 6:O:153:GLN:NE2  | 2.82                     | 0.47              |
| 8:Q:63:LEU:HD13  | 8:Q:129:ALA:HB3  | 1.97                     | 0.47              |
| 8:Q:121:ARG:NH1  | 8:Q:121:ARG:CG   | 2.78                     | 0.47              |
| 1:S:162:LEU:HB3  | 1:S:163:PHE:CD1  | 2.49                     | 0.47              |
| 1:S:163:PHE:C    | 1:S:165:THR:H    | 2.23                     | 0.47              |
| 2:T:106:ILE:CG2  | 2:T:110:GLU:HB2  | 2.44                     | 0.47              |
| 3:U:381:LEU:HD12 | 3:U:522:ARG:HD3  | 1.96                     | 0.47              |
| 3:U:505:LEU:HD21 | 3:U:507:LEU:HD23 | 1.97                     | 0.47              |
| 3:U:506:ILE:CG2  | 3:U:535:MET:HE3  | 2.45                     | 0.47              |
| 4:V:79:ILE:HG22  | 4:V:79:ILE:O     | 2.14                     | 0.47              |
| 6:X:108:MET:HA   | 6:X:137:VAL:CG1  | 2.45                     | 0.47              |
| 3:3:385:ALA:HB2  | 3:3:531:LYS:CB   | 2.45                     | 0.47              |
| 4:4:138:LEU:HD11 | 4:4:146:PHE:CD2  | 2.50                     | 0.47              |
| 4:4:311:PRO:HD3  | 4:4:330:HIS:CE1  | 2.49                     | 0.47              |
| 5:5:174:LEU:CD2  | 5:5:180:GLY:HA2  | 2.44                     | 0.47              |
| 7:9:53:CYS:HB2   | 7:9:112:ALA:HB1  | 1.95                     | 0.47              |
| 3:C:19:VAL:HG12  | 3:C:82:SER:HB2   | 1.97                     | 0.47              |
| 3:C:381:LEU:HD12 | 3:C:522:ARG:HD3  | 1.97                     | 0.47              |
| 4:D:99:LEU:HD13  | 4:D:99:LEU:HA    | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:211:SER:CB   | 4:D:214:PHE:HB3  | 2.45                     | 0.47              |
| 4:D:358:VAL:O    | 4:D:366:TYR:HB3  | 2.15                     | 0.47              |
| 5:E:168:ALA:HA   | 5:E:171:ARG:HH12 | 1.80                     | 0.47              |
| 8:H:20:MET:HE3   | 8:H:59:LEU:HG    | 1.97                     | 0.47              |
| 1:J:41:ALA:HA    | 1:J:120:LEU:HD21 | 1.97                     | 0.47              |
| 3:L:478:LEU:HD21 | 3:L:483:ASP:HB2  | 1.96                     | 0.47              |
| 3:L:671:GLU:HG3  | 3:L:672:ALA:H    | 1.80                     | 0.47              |
| 4:M:85:MET:HE3   | 4:M:409:ARG:CB   | 2.45                     | 0.47              |
| 4:V:211:SER:HB2  | 4:V:215:TYR:H    | 1.79                     | 0.47              |
| 5:W:25:LEU:CD2   | 5:W:25:LEU:H     | 2.28                     | 0.47              |
| 5:5:34:PHE:HE1   | 5:5:38:MET:SD    | 2.37                     | 0.47              |
| 5:5:77:LEU:HA    | 5:5:78:PRO:HD3   | 1.59                     | 0.47              |
| 6:6:17:GLU:O     | 1:J:273:ARG:HD3  | 2.15                     | 0.47              |
| 8:7:86:LEU:HD11  | 8:7:118:LEU:HD11 | 1.97                     | 0.47              |
| 4:D:198:PRO:HG3  | 4:D:291:LYS:NZ   | 2.30                     | 0.47              |
| 4:D:287:VAL:O    | 4:D:291:LYS:HG3  | 2.15                     | 0.47              |
| 4:D:342:VAL:HG22 | 4:D:343:TYR:N    | 2.29                     | 0.47              |
| 1:J:195:LEU:HA   | 2:K:24:ARG:HH21  | 1.80                     | 0.47              |
| 1:J:267:PRO:O    | 1:J:268:MET:C    | 2.57                     | 0.47              |
| 1:J:293:GLY:HA3  | 1:J:324:GLY:N    | 2.10                     | 0.47              |
| 4:M:73:ARG:HG3   | 4:M:77:GLN:OE1   | 2.14                     | 0.47              |
| 3:U:361:ALA:HB1  | 3:U:366:THR:CG2  | 2.44                     | 0.47              |
| 3:U:655:ARG:HH12 | 3:U:659:GLU:CB   | 2.27                     | 0.47              |
| 3:U:664:LEU:O    | 3:U:669:VAL:HG12 | 2.15                     | 0.47              |
| 5:W:25:LEU:H     | 5:W:25:LEU:HD23  | 1.80                     | 0.47              |
| 6:X:33:SER:HA    | 6:X:158:VAL:HG21 | 1.96                     | 0.47              |
| 7:Y:40:ARG:CB    | 7:Y:121:MET:HE1  | 2.35                     | 0.47              |
| 1:1:38:TYR:OH    | 1:1:112:HIS:ND1  | 2.40                     | 0.47              |
| 3:3:254:THR:HG23 | 3:3:255:THR:N    | 2.28                     | 0.47              |
| 6:6:146:ALA:HB2  | 7:9:119:PHE:HD1  | 1.79                     | 0.47              |
| 8:7:13:TRP:CZ2   | 8:7:17:LEU:HD11  | 2.49                     | 0.47              |
| 4:D:261:THR:HB   | 4:D:292:GLN:OE1  | 2.15                     | 0.47              |
| 5:E:141:LEU:HD21 | 5:E:145:PRO:HD3  | 1.97                     | 0.47              |
| 1:J:89:LEU:HD23  | 1:J:118:MET:HE3  | 1.97                     | 0.47              |
| 1:J:264:TYR:CD2  | 1:J:279:TRP:HB3  | 2.50                     | 0.47              |
| 3:L:513:GLN:HG2  | 3:L:769:LEU:CD2  | 2.45                     | 0.47              |
| 4:M:188:PRO:O    | 4:M:191:LYS:HB2  | 2.15                     | 0.47              |
| 5:N:168:ALA:HA   | 5:N:171:ARG:HH12 | 1.79                     | 0.47              |
| 6:O:117:MET:HE3  | 6:O:118:PHE:CZ   | 2.50                     | 0.47              |
| 1:S:291:ILE:HD11 | 1:S:331:ILE:HD11 | 1.97                     | 0.47              |
| 2:T:58:THR:HG21  | 3:U:200:LEU:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:100:VAL:O    | 3:U:104:GLN:HG3  | 2.14                     | 0.47              |
| 3:U:440:ARG:CG   | 3:U:440:ARG:NH1  | 2.76                     | 0.47              |
| 3:U:591:HIS:ND1  | 3:U:592:PRO:N    | 2.63                     | 0.47              |
| 8:Z:29:VAL:HG22  | 8:Z:60:SER:O     | 2.15                     | 0.47              |
| 1:1:162:LEU:HB3  | 1:1:163:PHE:CD1  | 2.51                     | 0.46              |
| 1:A:98:PRO:HB3   | 2:B:85:THR:HG21  | 1.97                     | 0.46              |
| 3:C:409:LEU:HD23 | 3:C:409:LEU:HA   | 1.76                     | 0.46              |
| 3:C:483:ASP:O    | 3:C:484:LYS:HG2  | 2.15                     | 0.46              |
| 3:C:670:PRO:CD   | 3:C:676:LEU:HD23 | 2.44                     | 0.46              |
| 4:D:76:LEU:HD12  | 4:D:76:LEU:O     | 2.15                     | 0.46              |
| 1:J:81:LYS:CE    | 1:J:81:LYS:HA    | 2.46                     | 0.46              |
| 2:K:142:VAL:HG11 | 2:K:153:LEU:HG   | 1.96                     | 0.46              |
| 4:M:122:GLU:OE2  | 4:M:249:ARG:NH1  | 2.47                     | 0.46              |
| 1:S:6:LEU:HD21   | 1:S:12:ARG:CG    | 2.44                     | 0.46              |
| 1:S:29:LEU:HD22  | 1:S:33:LEU:CD1   | 2.46                     | 0.46              |
| 2:T:85:THR:HG22  | 2:T:86:LEU:N     | 2.30                     | 0.46              |
| 3:U:45:CYS:O     | 3:U:46:ARG:HB2   | 2.15                     | 0.46              |
| 4:V:173:ILE:HG23 | 4:V:173:ILE:O    | 2.14                     | 0.46              |
| 2:2:33:ARG:HH21  | 2:2:37:GLU:HG3   | 1.79                     | 0.46              |
| 2:2:89:LYS:HE3   | 2:2:94:GLU:OE1   | 2.15                     | 0.46              |
| 5:5:13:LYS:HG2   | 5:5:13:LYS:O     | 2.15                     | 0.46              |
| 5:5:195:LEU:HD22 | 5:5:195:LEU:N    | 2.31                     | 0.46              |
| 1:A:211:LEU:HG   | 1:A:212:TRP:CE3  | 2.49                     | 0.46              |
| 1:A:211:LEU:HG   | 1:A:212:TRP:CZ3  | 2.49                     | 0.46              |
| 3:C:225:ASN:O    | 3:C:229:ILE:HG13 | 2.15                     | 0.46              |
| 3:C:285:VAL:HG22 | 3:C:286:ASN:H    | 1.80                     | 0.46              |
| 4:D:133:LEU:HD21 | 4:D:204:TYR:CE2  | 2.50                     | 0.46              |
| 4:D:369:LYS:HD3  | 4:D:370:VAL:N    | 2.30                     | 0.46              |
| 6:F:128:ASP:HA   | 6:F:131:VAL:O    | 2.15                     | 0.46              |
| 8:H:13:TRP:CZ2   | 8:H:17:LEU:HD11  | 2.51                     | 0.46              |
| 8:H:117:ALA:O    | 8:H:121:ARG:HG2  | 2.15                     | 0.46              |
| 1:J:202:LYS:N    | 1:J:203:PRO:HD2  | 2.31                     | 0.46              |
| 3:L:45:CYS:O     | 3:L:46:ARG:HB2   | 2.15                     | 0.46              |
| 3:L:378:PRO:O    | 3:L:381:LEU:HB2  | 2.14                     | 0.46              |
| 4:M:197:LEU:N    | 4:M:198:PRO:HD2  | 2.30                     | 0.46              |
| 4:M:256:GLY:C    | 4:M:258:GLU:N    | 2.71                     | 0.46              |
| 1:S:92:ASN:ND2   | 10:S:440:FMN:N1  | 2.63                     | 0.46              |
| 3:U:326:PHE:CZ   | 3:U:330:LYS:HE3  | 2.50                     | 0.46              |
| 3:U:497:TRP:NE1  | 3:U:524:LEU:CD1  | 2.75                     | 0.46              |
| 3:U:583:VAL:HG23 | 3:U:598:ALA:HA   | 1.96                     | 0.46              |
| 4:V:393:MET:C    | 4:V:396:ILE:HG22 | 2.40                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:Z:37:PHE:HE2   | 8:Z:74:PRO:HA    | 1.79                     | 0.46              |
| 3:3:116:PRO:O    | 3:3:117:LEU:HB2  | 2.14                     | 0.46              |
| 4:4:212:PRO:HG2  | 4:4:213:ILE:H    | 1.80                     | 0.46              |
| 4:4:283:MET:O    | 4:4:287:VAL:HG23 | 2.15                     | 0.46              |
| 2:B:142:VAL:HG11 | 2:B:153:LEU:HG   | 1.98                     | 0.46              |
| 3:C:385:ALA:HB3  | 3:C:533:LEU:CD2  | 2.45                     | 0.46              |
| 5:E:1:MET:SD     | 8:Z:113:GLU:OE1  | 2.73                     | 0.46              |
| 6:F:121:TYR:HD1  | 6:F:121:TYR:H    | 1.63                     | 0.46              |
| 1:J:356:CYS:HB3  | 1:J:358:PRO:HD2  | 1.98                     | 0.46              |
| 3:L:33:PHE:HB2   | 3:L:45:CYS:SG    | 2.55                     | 0.46              |
| 3:L:732:ALA:O    | 3:L:747:VAL:HG12 | 2.15                     | 0.46              |
| 4:M:125:ARG:HD2  | 4:M:286:SER:OG   | 2.16                     | 0.46              |
| 1:S:420:GLN:O    | 1:S:424:LEU:HD13 | 2.15                     | 0.46              |
| 3:U:160:THR:OG1  | 8:Z:73:SER:HB3   | 2.15                     | 0.46              |
| 3:U:237:ASP:OD1  | 3:U:239:THR:HG22 | 2.15                     | 0.46              |
| 4:V:115:THR:HG22 | 4:V:297:LEU:HD23 | 1.96                     | 0.46              |
| 4:V:338:PRO:HG3  | 5:W:193:ARG:HB2  | 1.96                     | 0.46              |
| 5:W:13:LYS:O     | 5:W:13:LYS:HG2   | 2.15                     | 0.46              |
| 7:Y:29:ALA:HA    | 7:Y:30:PRO:HD2   | 1.79                     | 0.46              |
| 2:2:11:LEU:O     | 2:2:12:GLU:C     | 2.57                     | 0.46              |
| 3:3:506:ILE:CG2  | 3:3:535:MET:HE3  | 2.45                     | 0.46              |
| 4:4:254:TYR:CE2  | 4:4:346:THR:CA   | 2.93                     | 0.46              |
| 8:7:63:LEU:HD13  | 8:7:129:ALA:HB3  | 1.97                     | 0.46              |
| 8:7:70:ALA:HA    | 8:7:83:GLY:O     | 2.16                     | 0.46              |
| 1:A:154:ALA:O    | 1:A:156:GLY:N    | 2.48                     | 0.46              |
| 3:C:583:VAL:HG21 | 3:C:597:TYR:O    | 2.16                     | 0.46              |
| 5:E:195:LEU:HD22 | 5:E:195:LEU:N    | 2.31                     | 0.46              |
| 3:L:290:ILE:HG22 | 3:L:291:CYS:O    | 2.16                     | 0.46              |
| 3:L:497:TRP:CD1  | 3:L:524:LEU:HD11 | 2.49                     | 0.46              |
| 3:L:591:HIS:ND1  | 3:L:592:PRO:CD   | 2.78                     | 0.46              |
| 3:L:664:LEU:O    | 3:L:669:VAL:HG12 | 2.16                     | 0.46              |
| 5:N:13:LYS:O     | 5:N:13:LYS:HG2   | 2.15                     | 0.46              |
| 5:N:37:GLU:O     | 5:N:40:HIS:HB3   | 2.16                     | 0.46              |
| 8:Q:86:LEU:HD11  | 8:Q:118:LEU:HD11 | 1.98                     | 0.46              |
| 1:S:107:LEU:HD23 | 1:S:114:LEU:HD12 | 1.97                     | 0.46              |
| 2:T:24:ARG:O     | 2:T:27:ILE:HD12  | 2.15                     | 0.46              |
| 4:V:197:LEU:N    | 4:V:198:PRO:HD2  | 2.31                     | 0.46              |
| 6:X:96:TRP:HA    | 6:X:99:MET:CE    | 2.41                     | 0.46              |
| 1:1:334:ARG:O    | 1:1:434:PRO:HG3  | 2.16                     | 0.46              |
| 3:3:700:LYS:HA   | 3:3:763:LEU:O    | 2.16                     | 0.46              |
| 1:A:116:GLU:HG2  | 1:A:228:VAL:HG22 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:397:ARG:NE   | 3:C:79:LEU:HD12  | 2.31                     | 0.46              |
| 2:B:112:THR:HG22 | 2:B:116:LEU:H    | 1.81                     | 0.46              |
| 3:C:243:ARG:HB3  | 3:C:275:LEU:HD12 | 1.98                     | 0.46              |
| 3:C:478:LEU:HD12 | 3:C:520:ARG:NH1  | 2.30                     | 0.46              |
| 4:D:211:SER:HB2  | 4:D:215:TYR:H    | 1.80                     | 0.46              |
| 4:D:230:ILE:HD11 | 4:D:244:VAL:CG2  | 2.46                     | 0.46              |
| 5:E:104:VAL:CG1  | 5:E:108:TRP:HE3  | 2.29                     | 0.46              |
| 1:J:249:MET:HE2  | 1:J:249:MET:H    | 1.80                     | 0.46              |
| 3:L:689:LYS:HD2  | 3:L:772:GLU:H    | 1.81                     | 0.46              |
| 4:M:379:GLN:HG2  | 5:N:113:PHE:CD1  | 2.50                     | 0.46              |
| 8:Q:49:ASP:N     | 8:Q:49:ASP:OD1   | 2.49                     | 0.46              |
| 1:S:49:THR:OG1   | 1:S:52:GLU:HG3   | 2.15                     | 0.46              |
| 1:S:72:THR:HG21  | 1:S:223:THR:HG21 | 1.96                     | 0.46              |
| 3:U:268:ASP:OD2  | 3:U:278:ARG:NH1  | 2.48                     | 0.46              |
| 4:V:211:SER:OG   | 4:V:215:TYR:HB2  | 2.16                     | 0.46              |
| 4:V:381:LEU:H    | 4:V:382:PRO:CD   | 2.28                     | 0.46              |
| 6:X:40:THR:HB    | 6:X:50:MET:SD    | 2.55                     | 0.46              |
| 1:1:211:LEU:HG   | 1:1:212:TRP:CE3  | 2.50                     | 0.46              |
| 3:3:732:ALA:O    | 3:3:747:VAL:HG12 | 2.15                     | 0.46              |
| 4:4:159:LEU:O    | 4:4:163:VAL:HG12 | 2.15                     | 0.46              |
| 4:4:294:LEU:O    | 4:4:294:LEU:HD23 | 2.16                     | 0.46              |
| 5:5:54:GLY:C     | 5:5:55:LEU:HD12  | 2.41                     | 0.46              |
| 6:6:30:TRP:O     | 6:6:33:SER:HB3   | 2.15                     | 0.46              |
| 1:A:162:LEU:HB3  | 1:A:163:PHE:CD1  | 2.50                     | 0.46              |
| 1:A:366:PHE:O    | 1:A:370:LEU:HD23 | 2.14                     | 0.46              |
| 3:C:700:LYS:HA   | 3:C:763:LEU:O    | 2.15                     | 0.46              |
| 6:F:149:TYR:CZ   | 6:F:153:GLN:NE2  | 2.83                     | 0.46              |
| 2:K:85:THR:HG22  | 2:K:86:LEU:H     | 1.81                     | 0.46              |
| 4:M:254:TYR:C    | 4:M:256:GLY:H    | 2.19                     | 0.46              |
| 6:O:117:MET:CE   | 7:P:99:ILE:HG12  | 2.45                     | 0.46              |
| 4:V:240:ARG:NH2  | 4:V:347:GLU:OE2  | 2.45                     | 0.46              |
| 4:V:369:LYS:HD3  | 4:V:370:VAL:N    | 2.31                     | 0.46              |
| 1:1:298:PRO:HD2  | 1:1:321:SER:OG   | 2.16                     | 0.46              |
| 3:3:18:SER:HB3   | 3:3:21:ASP:OD1   | 2.15                     | 0.46              |
| 3:3:290:ILE:HG22 | 3:3:291:CYS:O    | 2.16                     | 0.46              |
| 4:4:236:GLY:C    | 4:4:238:SER:N    | 2.73                     | 0.46              |
| 4:4:393:MET:HA   | 4:4:396:ILE:CG2  | 2.46                     | 0.46              |
| 7:9:33:LEU:HD22  | 7:9:37:PHE:CD2   | 2.50                     | 0.46              |
| 7:9:44:THR:OG1   | 7:9:52:LYS:HD2   | 2.15                     | 0.46              |
| 1:A:163:PHE:C    | 1:A:165:THR:H    | 2.23                     | 0.46              |
| 2:B:3:PHE:CD1    | 2:B:3:PHE:C      | 2.94                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:732:ALA:H    | 3:C:747:VAL:HG12 | 1.80                     | 0.46              |
| 4:D:173:ILE:HG23 | 4:D:173:ILE:O    | 2.16                     | 0.46              |
| 6:F:78:MET:HE2   | 6:F:99:MET:HE1   | 1.98                     | 0.46              |
| 8:H:38:PRO:C     | 8:H:40:PHE:H     | 2.24                     | 0.46              |
| 8:H:88:ARG:HE    | 8:H:126:LEU:HD22 | 1.81                     | 0.46              |
| 3:L:31:PRO:HD2   | 3:L:104:GLN:NE2  | 2.30                     | 0.46              |
| 5:N:194:SER:O    | 5:N:195:LEU:HD13 | 2.15                     | 0.46              |
| 7:P:134:GLU:CD   | 7:P:134:GLU:N    | 2.73                     | 0.46              |
| 3:U:19:VAL:HG23  | 3:U:85:THR:O     | 2.16                     | 0.46              |
| 3:U:732:ALA:H    | 3:U:747:VAL:CG1  | 2.29                     | 0.46              |
| 4:V:104:LEU:HD22 | 4:V:338:PRO:HD2  | 1.97                     | 0.46              |
| 1:1:264:TYR:CD2  | 1:1:279:TRP:HB3  | 2.51                     | 0.46              |
| 3:3:641:LEU:HD23 | 3:3:641:LEU:HA   | 1.77                     | 0.46              |
| 1:A:211:LEU:HB2  | 1:A:216:THR:HG21 | 1.96                     | 0.46              |
| 3:C:337:ARG:HD2  | 3:C:337:ARG:N    | 2.27                     | 0.46              |
| 3:C:646:GLU:C    | 3:C:648:LEU:H    | 2.24                     | 0.46              |
| 4:D:62:LEU:HD21  | 6:F:43:LEU:HB3   | 1.97                     | 0.46              |
| 4:D:256:GLY:C    | 4:D:258:GLU:N    | 2.70                     | 0.46              |
| 6:F:141:PRO:HB3  | 9:F:182:SF4:S1   | 2.56                     | 0.46              |
| 1:J:87:HIS:HB2   | 1:J:126:ARG:O    | 2.16                     | 0.46              |
| 1:J:107:LEU:CD2  | 1:J:114:LEU:HD12 | 2.46                     | 0.46              |
| 1:J:323:LEU:HD23 | 1:J:323:LEU:C    | 2.40                     | 0.46              |
| 1:J:397:ARG:HD2  | 1:J:397:ARG:N    | 2.29                     | 0.46              |
| 3:L:161:ARG:HG2  | 3:L:161:ARG:HH11 | 1.81                     | 0.46              |
| 4:M:385:CYS:HB3  | 4:M:396:ILE:HG12 | 1.96                     | 0.46              |
| 1:S:201:LEU:O    | 1:S:204:PRO:HD2  | 2.16                     | 0.46              |
| 1:S:264:TYR:CD2  | 1:S:279:TRP:HB3  | 2.50                     | 0.46              |
| 4:V:138:LEU:HD11 | 4:V:146:PHE:CD2  | 2.51                     | 0.46              |
| 4:V:263:ASP:O    | 4:V:285:GLU:HG3  | 2.15                     | 0.46              |
| 4:V:276:MET:O    | 4:V:280:ILE:HG13 | 2.15                     | 0.46              |
| 1:1:341:MET:HE2  | 1:1:409:PRO:C    | 2.41                     | 0.46              |
| 2:2:59:GLU:O     | 2:2:63:VAL:HG23  | 2.16                     | 0.46              |
| 3:3:385:ALA:HB3  | 3:3:533:LEU:HD23 | 1.97                     | 0.46              |
| 5:5:98:ASP:C     | 5:5:100:ARG:H    | 2.24                     | 0.46              |
| 6:6:34:ASN:C     | 6:6:36:LEU:H     | 2.24                     | 0.46              |
| 2:B:11:LEU:O     | 2:B:12:GLU:C     | 2.58                     | 0.46              |
| 2:B:85:THR:HG22  | 2:B:86:LEU:H     | 1.80                     | 0.46              |
| 2:B:88:CYS:HB3   | 2:B:93:ALA:HB2   | 1.98                     | 0.46              |
| 3:C:197:ASP:CB   | 3:C:220:SER:HB3  | 2.46                     | 0.46              |
| 3:C:559:ASP:HB2  | 3:C:573:PRO:HG3  | 1.96                     | 0.46              |
| 1:J:272:PHE:CE1  | 1:J:311:MET:HG2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:2:VAL:CG1    | 3:L:89:ASP:HA    | 2.46                     | 0.46              |
| 3:L:132:ASP:O    | 3:L:136:GLU:HG3  | 2.15                     | 0.46              |
| 3:L:250:GLU:CD   | 3:L:628:PRO:HG2  | 2.40                     | 0.46              |
| 3:L:559:ASP:HB2  | 3:L:573:PRO:HG3  | 1.97                     | 0.46              |
| 4:M:249:ARG:HB2  | 4:M:262:PHE:HE2  | 1.81                     | 0.46              |
| 5:N:123:GLY:HA2  | 5:N:144:HIS:CD2  | 2.50                     | 0.46              |
| 7:P:26:TYR:N     | 7:P:27:PRO:CD    | 2.76                     | 0.46              |
| 3:U:690:GLY:HA3  | 3:U:770:ARG:HH21 | 1.81                     | 0.46              |
| 5:W:132:LEU:HD23 | 5:W:132:LEU:HA   | 1.68                     | 0.46              |
| 6:X:16:ARG:HA    | 6:X:21:PHE:CD2   | 2.50                     | 0.46              |
| 6:X:106:ILE:CD1  | 6:X:151:VAL:HG12 | 2.46                     | 0.46              |
| 4:4:125:ARG:HD2  | 4:4:286:SER:OG   | 2.16                     | 0.46              |
| 4:4:173:ILE:O    | 4:4:173:ILE:HG23 | 2.15                     | 0.46              |
| 4:4:223:VAL:O    | 4:4:383:TYR:HE1  | 1.99                     | 0.46              |
| 6:6:19:ILE:HD11  | 1:J:271:THR:HG23 | 1.96                     | 0.46              |
| 1:A:29:LEU:HD22  | 1:A:33:LEU:CD1   | 2.45                     | 0.46              |
| 1:A:290:ILE:HG22 | 1:A:330:LEU:HD22 | 1.98                     | 0.46              |
| 3:C:216:PHE:CZ   | 8:H:128:PHE:CD2  | 3.00                     | 0.46              |
| 3:C:420:LEU:HD22 | 3:C:436:GLN:HG2  | 1.98                     | 0.46              |
| 3:C:689:LYS:HD2  | 3:C:772:GLU:H    | 1.81                     | 0.46              |
| 5:E:52:ILE:CG2   | 5:E:114:LEU:HB3  | 2.42                     | 0.46              |
| 5:E:132:LEU:HD23 | 5:E:132:LEU:HA   | 1.65                     | 0.46              |
| 8:H:16:LEU:O     | 8:H:16:LEU:HD13  | 2.16                     | 0.46              |
| 2:K:24:ARG:O     | 2:K:27:ILE:HD12  | 2.15                     | 0.46              |
| 3:L:218:LEU:N    | 3:L:219:PRO:HD3  | 2.31                     | 0.46              |
| 3:L:225:ASN:O    | 3:L:229:ILE:HG13 | 2.16                     | 0.46              |
| 3:L:367:PRO:CB   | 3:L:554:LYS:HB2  | 2.46                     | 0.46              |
| 3:L:641:LEU:HD23 | 3:L:641:LEU:HA   | 1.79                     | 0.46              |
| 4:M:276:MET:O    | 4:M:280:ILE:HG13 | 2.16                     | 0.46              |
| 6:O:106:ILE:CD1  | 6:O:151:VAL:HG12 | 2.46                     | 0.46              |
| 8:Q:37:PHE:CE1   | 8:Q:55:MET:HB2   | 2.50                     | 0.46              |
| 1:S:315:HIS:O    | 1:S:319:LYS:HB2  | 2.17                     | 0.46              |
| 4:V:168:PHE:CE1  | 6:X:141:PRO:HG3  | 2.51                     | 0.46              |
| 6:X:149:TYR:CZ   | 6:X:153:GLN:NE2  | 2.84                     | 0.46              |
| 7:Y:123:ASP:CB   | 7:Y:129:LEU:HD21 | 2.46                     | 0.46              |
| 1:1:107:LEU:CD2  | 1:1:114:LEU:HD12 | 2.47                     | 0.45              |
| 1:1:254:ILE:HB   | 1:1:275:LEU:HD21 | 1.98                     | 0.45              |
| 4:4:241:ALA:CB   | 4:4:278:VAL:HG21 | 2.46                     | 0.45              |
| 4:4:374:SER:HB2  | 4:4:406:ASP:HB3  | 1.97                     | 0.45              |
| 1:A:104:ARG:HH21 | 2:B:127:SER:CB   | 2.28                     | 0.45              |
| 1:A:202:LYS:N    | 1:A:203:PRO:HD2  | 2.30                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:233:ARG:H    | 1:A:233:ARG:HG2  | 1.57                     | 0.45              |
| 1:A:249:MET:H    | 1:A:249:MET:HE2  | 1.82                     | 0.45              |
| 1:A:420:GLN:O    | 1:A:424:LEU:HD13 | 2.16                     | 0.45              |
| 3:C:30:VAL:CG2   | 3:C:31:PRO:HD2   | 2.46                     | 0.45              |
| 3:C:397:LEU:HD21 | 3:C:480:LEU:HD13 | 1.98                     | 0.45              |
| 4:D:263:ASP:HB2  | 4:D:285:GLU:OE1  | 2.15                     | 0.45              |
| 4:D:371:ARG:NH2  | 4:D:376:VAL:CG2  | 2.79                     | 0.45              |
| 4:D:381:LEU:H    | 4:D:382:PRO:HD2  | 1.80                     | 0.45              |
| 6:F:37:TRP:CE3   | 6:F:37:TRP:HA    | 2.51                     | 0.45              |
| 3:L:116:PRO:O    | 3:L:117:LEU:HB2  | 2.16                     | 0.45              |
| 3:L:583:VAL:HG21 | 3:L:597:TYR:O    | 2.15                     | 0.45              |
| 4:M:241:ALA:O    | 4:M:267:GLY:HA3  | 2.15                     | 0.45              |
| 3:U:118:ASP:O    | 3:U:121:THR:N    | 2.49                     | 0.45              |
| 3:U:583:VAL:HG21 | 3:U:597:TYR:O    | 2.16                     | 0.45              |
| 4:V:221:VAL:O    | 4:V:272:VAL:HG12 | 2.16                     | 0.45              |
| 4:V:241:ALA:O    | 4:V:267:GLY:HA3  | 2.16                     | 0.45              |
| 6:X:48:ILE:O     | 6:X:48:ILE:HG22  | 2.15                     | 0.45              |
| 6:X:114:SER:CB   | 7:Y:97:ARG:HD2   | 2.43                     | 0.45              |
| 8:Z:8:GLU:HG2    | 8:Z:97:TYR:OH    | 2.15                     | 0.45              |
| 1:1:385:GLU:O    | 1:1:388:GLU:HB3  | 2.16                     | 0.45              |
| 3:3:655:ARG:HH12 | 3:3:659:GLU:CB   | 2.29                     | 0.45              |
| 3:3:689:LYS:HB2  | 3:3:772:GLU:HG2  | 1.97                     | 0.45              |
| 4:4:224:ILE:HA   | 4:4:225:PRO:HD2  | 1.76                     | 0.45              |
| 5:5:194:SER:C    | 5:5:195:LEU:HD22 | 2.42                     | 0.45              |
| 6:6:46:CYS:HB3   | 6:6:81:ALA:HB1   | 1.98                     | 0.45              |
| 1:A:267:PRO:O    | 1:A:270:THR:HG23 | 2.16                     | 0.45              |
| 2:B:40:TRP:CH2   | 2:B:42:ARG:HG2   | 2.51                     | 0.45              |
| 3:C:513:GLN:HG2  | 3:C:769:LEU:CD2  | 2.46                     | 0.45              |
| 1:J:39:GLU:O     | 1:J:43:ARG:HG3   | 2.16                     | 0.45              |
| 1:J:64:GLY:HA3   | 10:J:440:FMN:O1P | 2.16                     | 0.45              |
| 3:L:180:ARG:O    | 3:L:181:CYS:C    | 2.60                     | 0.45              |
| 3:L:455:ARG:HG3  | 3:L:455:ARG:O    | 2.17                     | 0.45              |
| 5:N:34:PHE:O     | 5:N:35:LYS:C     | 2.60                     | 0.45              |
| 6:O:37:TRP:HA    | 6:O:37:TRP:CE3   | 2.50                     | 0.45              |
| 3:U:19:VAL:O     | 3:U:22:ALA:HB3   | 2.16                     | 0.45              |
| 3:U:83:CYS:SG    | 3:U:84:VAL:HG13  | 2.57                     | 0.45              |
| 3:U:515:THR:HG23 | 3:U:683:LEU:CD1  | 2.43                     | 0.45              |
| 4:V:197:LEU:N    | 4:V:198:PRO:CD   | 2.79                     | 0.45              |
| 5:W:157:THR:C    | 5:W:158:LEU:HD23 | 2.41                     | 0.45              |
| 6:X:110:ALA:HB1  | 6:X:116:GLY:HA2  | 1.98                     | 0.45              |
| 1:1:145:LEU:O    | 1:1:149:ILE:HG13 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:211:LEU:HG   | 1:1:212:TRP:CZ3  | 2.50                     | 0.45              |
| 3:3:45:CYS:O     | 3:3:46:ARG:HB2   | 2.16                     | 0.45              |
| 3:3:55:PRO:HG3   | 3:3:73:ILE:C     | 2.40                     | 0.45              |
| 3:3:508:GLY:HA2  | 3:3:535:MET:HB2  | 1.99                     | 0.45              |
| 3:3:513:GLN:HG2  | 3:3:769:LEU:CD2  | 2.45                     | 0.45              |
| 4:4:254:TYR:C    | 4:4:256:GLY:H    | 2.20                     | 0.45              |
| 5:5:1:MET:C      | 5:5:3:LEU:N      | 2.75                     | 0.45              |
| 6:6:43:LEU:HD11  | 6:6:84:LEU:HD23  | 1.97                     | 0.45              |
| 6:6:152:MET:HE2  | 6:6:152:MET:HB3  | 1.50                     | 0.45              |
| 7:9:39:GLY:O     | 7:9:40:ARG:C     | 2.59                     | 0.45              |
| 8:7:49:ASP:N     | 8:7:49:ASP:OD1   | 2.50                     | 0.45              |
| 1:A:145:LEU:HA   | 1:A:145:LEU:HD23 | 1.70                     | 0.45              |
| 1:A:359:CYS:O    | 1:A:363:VAL:HG22 | 2.16                     | 0.45              |
| 3:C:118:ASP:O    | 3:C:119:CYS:C    | 2.59                     | 0.45              |
| 4:D:249:ARG:HB2  | 4:D:262:PHE:HE2  | 1.81                     | 0.45              |
| 4:D:367:ARG:HH12 | 4:D:369:LYS:CA   | 2.30                     | 0.45              |
| 5:E:194:SER:O    | 5:E:195:LEU:HD13 | 2.16                     | 0.45              |
| 7:G:45:ARG:NH2   | 7:G:137:LEU:CD2  | 2.77                     | 0.45              |
| 3:L:232:VAL:HB   | 9:L:784:SF4:S2   | 2.56                     | 0.45              |
| 4:M:82:THR:N     | 4:M:83:PRO:HD2   | 2.31                     | 0.45              |
| 4:M:328:PHE:CD2  | 4:M:328:PHE:C    | 2.95                     | 0.45              |
| 5:N:1:MET:C      | 5:N:3:LEU:N      | 2.75                     | 0.45              |
| 1:S:184:GLU:OE1  | 1:S:186:THR:N    | 2.49                     | 0.45              |
| 3:U:184:CYS:O    | 9:U:785:SF4:S4   | 2.75                     | 0.45              |
| 3:U:243:ARG:HB3  | 3:U:275:LEU:HD12 | 1.98                     | 0.45              |
| 3:U:397:LEU:HD21 | 3:U:480:LEU:HD13 | 1.98                     | 0.45              |
| 3:U:513:GLN:HG2  | 3:U:769:LEU:CD2  | 2.45                     | 0.45              |
| 4:V:122:GLU:HB2  | 4:V:290:ILE:CD1  | 2.44                     | 0.45              |
| 6:X:155:GLN:C    | 6:X:157:LYS:H    | 2.23                     | 0.45              |
| 7:Y:93:ILE:HG13  | 7:Y:136:MET:HE1  | 1.98                     | 0.45              |
| 7:Y:129:LEU:HD23 | 7:Y:129:LEU:HA   | 1.72                     | 0.45              |
| 1:1:149:ILE:O    | 1:1:153:ARG:HB2  | 2.17                     | 0.45              |
| 3:3:197:ASP:CB   | 3:3:220:SER:HB3  | 2.46                     | 0.45              |
| 3:3:470:PRO:O    | 3:3:471:GLY:C    | 2.59                     | 0.45              |
| 4:4:197:LEU:HA   | 4:4:200:ARG:HB3  | 1.98                     | 0.45              |
| 6:6:123:ILE:HG22 | 6:6:124:VAL:N    | 2.32                     | 0.45              |
| 7:9:134:GLU:CD   | 7:9:134:GLU:N    | 2.74                     | 0.45              |
| 3:C:184:CYS:SG   | 3:C:186:ARG:HB2  | 2.57                     | 0.45              |
| 3:C:487:SER:OG   | 3:C:490:VAL:HG23 | 2.16                     | 0.45              |
| 3:C:737:GLU:HB2  | 3:C:776:LEU:HD21 | 1.97                     | 0.45              |
| 5:E:54:GLY:C     | 5:E:55:LEU:HD12  | 2.41                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:181:LEU:HD12 | 5:E:181:LEU:HA   | 1.80                     | 0.45              |
| 1:J:264:TYR:CE2  | 1:J:279:TRP:HB3  | 2.51                     | 0.45              |
| 3:L:131:GLN:O    | 3:L:134:THR:HB   | 2.17                     | 0.45              |
| 3:L:269:THR:HG23 | 3:L:274:LEU:HD13 | 1.98                     | 0.45              |
| 3:L:646:GLU:C    | 3:L:648:LEU:H    | 2.25                     | 0.45              |
| 4:M:122:GLU:HB2  | 4:M:290:ILE:CD1  | 2.47                     | 0.45              |
| 4:M:376:VAL:O    | 4:M:379:GLN:HG3  | 2.16                     | 0.45              |
| 5:N:48:PHE:CE2   | 5:N:50:ALA:HB2   | 2.51                     | 0.45              |
| 1:S:202:LYS:N    | 1:S:203:PRO:HD2  | 2.31                     | 0.45              |
| 3:U:250:GLU:CD   | 3:U:628:PRO:HG2  | 2.40                     | 0.45              |
| 3:U:732:ALA:O    | 3:U:747:VAL:HG12 | 2.16                     | 0.45              |
| 7:Y:99:ILE:HG22  | 7:Y:101:CYS:SG   | 2.56                     | 0.45              |
| 1:1:238:PHE:HE1  | 1:1:249:MET:HE1  | 1.81                     | 0.45              |
| 1:1:297:THR:HG22 | 1:1:322:MET:HG3  | 1.99                     | 0.45              |
| 3:3:351:LEU:HD12 | 3:3:351:LEU:HA   | 1.79                     | 0.45              |
| 3:3:594:ALA:C    | 3:3:596:ARG:H    | 2.24                     | 0.45              |
| 4:4:84:ARG:CD    | 6:6:117:MET:HE1  | 2.45                     | 0.45              |
| 4:4:197:LEU:N    | 4:4:198:PRO:CD   | 2.80                     | 0.45              |
| 5:5:37:GLU:O     | 5:5:40:HIS:HB3   | 2.17                     | 0.45              |
| 3:C:83:CYS:SG    | 3:C:84:VAL:HG13  | 2.56                     | 0.45              |
| 3:C:117:LEU:H    | 4:D:321:MET:CE   | 2.16                     | 0.45              |
| 3:C:216:PHE:CZ   | 8:H:128:PHE:HD2  | 2.31                     | 0.45              |
| 3:C:459:MET:HG3  | 3:C:465:HIS:HB2  | 1.99                     | 0.45              |
| 3:C:505:LEU:HB3  | 3:C:532:VAL:HG22 | 1.98                     | 0.45              |
| 3:C:583:VAL:HG23 | 3:C:598:ALA:HA   | 1.98                     | 0.45              |
| 1:J:118:MET:O    | 1:J:122:GLY:N    | 2.47                     | 0.45              |
| 4:M:222:GLY:HA2  | 4:M:384:ALA:O    | 2.16                     | 0.45              |
| 5:N:195:LEU:HD22 | 5:N:195:LEU:N    | 2.32                     | 0.45              |
| 6:O:16:ARG:NH1   | 6:O:17:GLU:OE2   | 2.50                     | 0.45              |
| 1:S:211:LEU:HG   | 1:S:212:TRP:CE3  | 2.52                     | 0.45              |
| 2:T:88:CYS:HB3   | 2:T:93:ALA:HB2   | 1.99                     | 0.45              |
| 3:U:6:VAL:HG21   | 3:U:26:ALA:CB    | 2.47                     | 0.45              |
| 3:U:197:ASP:CB   | 3:U:220:SER:HB3  | 2.46                     | 0.45              |
| 3:U:245:ARG:HA   | 3:U:245:ARG:HD2  | 1.74                     | 0.45              |
| 4:V:263:ASP:HB2  | 4:V:285:GLU:OE1  | 2.17                     | 0.45              |
| 5:W:104:VAL:CG1  | 5:W:108:TRP:HE3  | 2.29                     | 0.45              |
| 8:Z:108:ILE:HD12 | 8:Z:108:ILE:N    | 2.31                     | 0.45              |
| 1:1:202:LYS:N    | 1:1:203:PRO:HD2  | 2.32                     | 0.45              |
| 3:3:368:HIS:CD2  | 3:3:556:ALA:HB3  | 2.51                     | 0.45              |
| 8:H:16:LEU:HG    | 8:H:82:ILE:HD11  | 1.97                     | 0.45              |
| 1:J:107:LEU:HD23 | 1:J:114:LEU:HD12 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:110:VAL:N    | 1:J:111:PRO:CD   | 2.79                     | 0.45              |
| 1:J:317:GLN:C    | 1:J:319:LYS:H    | 2.25                     | 0.45              |
| 1:J:332:PRO:HD2  | 2:K:90:LEU:CD2   | 2.44                     | 0.45              |
| 3:L:109:GLU:OE1  | 3:L:156:ARG:NH1  | 2.50                     | 0.45              |
| 3:L:343:LEU:O    | 3:L:369:LEU:HA   | 2.16                     | 0.45              |
| 1:S:334:ARG:O    | 1:S:434:PRO:HG3  | 2.17                     | 0.45              |
| 4:V:360:ASP:OD2  | 5:W:176:GLY:HA3  | 2.17                     | 0.45              |
| 1:1:272:PHE:CD1  | 1:1:311:MET:HG2  | 2.52                     | 0.45              |
| 1:1:356:CYS:HB3  | 1:1:358:PRO:HD2  | 1.99                     | 0.45              |
| 3:3:305:ARG:NH2  | 3:3:609:GLU:OE1  | 2.47                     | 0.45              |
| 3:3:403:THR:O    | 3:3:403:THR:HG22 | 2.16                     | 0.45              |
| 4:4:316:LEU:C    | 4:4:318:GLU:N    | 2.74                     | 0.45              |
| 5:5:129:HIS:CD2  | 5:5:130:PRO:HD2  | 2.51                     | 0.45              |
| 6:6:48:ILE:HG22  | 6:6:48:ILE:O     | 2.15                     | 0.45              |
| 1:A:18:TYR:OH    | 1:A:105:TYR:HB2  | 2.17                     | 0.45              |
| 1:A:366:PHE:HD1  | 1:A:370:LEU:CD2  | 2.29                     | 0.45              |
| 2:B:89:LYS:HE3   | 2:B:94:GLU:OE1   | 2.16                     | 0.45              |
| 3:C:132:ASP:O    | 3:C:136:GLU:HG3  | 2.17                     | 0.45              |
| 7:G:177:THR:O    | 7:G:179:GLY:N    | 2.49                     | 0.45              |
| 3:L:286:ASN:ND2  | 3:L:286:ASN:C    | 2.74                     | 0.45              |
| 3:L:724:ARG:HG2  | 3:L:724:ARG:O    | 2.16                     | 0.45              |
| 4:M:237:GLY:HA2  | 4:M:240:ARG:NH2  | 2.31                     | 0.45              |
| 4:M:350:ARG:HG3  | 4:M:350:ARG:NH1  | 2.32                     | 0.45              |
| 7:P:108:CYS:HA   | 9:P:184:SF4:S3   | 2.56                     | 0.45              |
| 1:S:104:ARG:HH21 | 2:T:127:SER:CB   | 2.29                     | 0.45              |
| 1:S:205:PHE:HD1  | 1:S:206:PRO:HD2  | 1.80                     | 0.45              |
| 2:T:142:VAL:HG11 | 2:T:153:LEU:HG   | 1.99                     | 0.45              |
| 3:U:55:PRO:CG    | 3:U:74:GLN:N     | 2.72                     | 0.45              |
| 3:U:113:LEU:HD12 | 3:U:157:PHE:CG   | 2.51                     | 0.45              |
| 3:U:119:CYS:O    | 3:U:120:PRO:C    | 2.60                     | 0.45              |
| 3:U:132:ASP:O    | 3:U:136:GLU:HG3  | 2.16                     | 0.45              |
| 2:2:78:TYR:CE1   | 2:2:157:LEU:HD22 | 2.52                     | 0.45              |
| 2:2:85:THR:HG22  | 2:2:86:LEU:H     | 1.82                     | 0.45              |
| 3:3:218:LEU:N    | 3:3:219:PRO:HD3  | 2.31                     | 0.45              |
| 3:3:559:ASP:HB2  | 3:3:573:PRO:HG3  | 1.98                     | 0.45              |
| 1:A:88:TYR:HB2   | 1:A:216:THR:CG2  | 2.46                     | 0.45              |
| 2:B:59:GLU:O     | 2:B:63:VAL:HG23  | 2.16                     | 0.45              |
| 3:C:689:LYS:HB2  | 3:C:772:GLU:HG2  | 1.98                     | 0.45              |
| 4:D:26:MET:N     | 4:D:48:SER:HG    | 2.15                     | 0.45              |
| 4:D:138:LEU:HD11 | 4:D:146:PHE:CD2  | 2.51                     | 0.45              |
| 4:D:188:PRO:CB   | 3:U:724:ARG:CD   | 2.59                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:254:TYR:C    | 4:D:256:GLY:H    | 2.20                     | 0.45              |
| 4:D:306:ASN:HA   | 4:D:307:PRO:HD3  | 1.77                     | 0.45              |
| 4:D:321:MET:HE2  | 4:D:321:MET:HB2  | 1.65                     | 0.45              |
| 4:D:375:PHE:HD1  | 4:D:407:VAL:HG23 | 1.82                     | 0.45              |
| 5:E:37:GLU:O     | 5:E:40:HIS:HB3   | 2.17                     | 0.45              |
| 5:E:111:ALA:HB1  | 5:E:115:GLU:HG3  | 1.98                     | 0.45              |
| 1:J:315:HIS:O    | 1:J:319:LYS:HB2  | 2.17                     | 0.45              |
| 2:K:131:ALA:HB1  | 2:K:132:PRO:HA   | 1.99                     | 0.45              |
| 3:L:594:ALA:C    | 3:L:596:ARG:H    | 2.25                     | 0.45              |
| 5:N:54:GLY:C     | 5:N:55:LEU:HD12  | 2.42                     | 0.45              |
| 1:S:92:ASN:ND2   | 10:S:440:FMN:C2  | 2.80                     | 0.45              |
| 1:S:197:ALA:HB3  | 2:T:66:PHE:CE1   | 2.52                     | 0.45              |
| 3:U:218:LEU:N    | 3:U:219:PRO:HD3  | 2.32                     | 0.45              |
| 4:V:178:VAL:CG2  | 4:V:302:VAL:HB   | 2.47                     | 0.45              |
| 4:V:321:MET:HE2  | 4:V:321:MET:HB2  | 1.74                     | 0.45              |
| 5:W:1:MET:C      | 5:W:3:LEU:N      | 2.75                     | 0.45              |
| 5:W:35:LYS:HD3   | 5:W:102:PRO:CB   | 2.47                     | 0.45              |
| 1:1:203:PRO:HB2  | 1:1:204:PRO:HD3  | 1.98                     | 0.45              |
| 2:2:88:CYS:HB3   | 2:2:93:ALA:HB2   | 1.99                     | 0.45              |
| 2:2:112:THR:HG22 | 2:2:116:LEU:H    | 1.82                     | 0.45              |
| 3:3:19:VAL:HG12  | 3:3:82:SER:HB2   | 1.98                     | 0.45              |
| 3:3:168:HIS:HA   | 3:3:169:PRO:HD2  | 1.73                     | 0.45              |
| 4:4:211:SER:HB2  | 4:4:215:TYR:H    | 1.82                     | 0.45              |
| 5:5:54:GLY:O     | 5:5:55:LEU:HD12  | 2.17                     | 0.45              |
| 5:5:141:LEU:HD21 | 5:5:145:PRO:HD3  | 1.98                     | 0.45              |
| 6:6:16:ARG:NH1   | 6:6:17:GLU:OE2   | 2.50                     | 0.45              |
| 8:7:60:SER:HB3   | 8:7:64:GLY:O     | 2.16                     | 0.45              |
| 1:A:205:PHE:HD1  | 1:A:206:PRO:HD2  | 1.82                     | 0.45              |
| 1:A:291:ILE:O    | 1:A:328:VAL:HA   | 2.17                     | 0.45              |
| 1:A:424:LEU:CD2  | 1:A:431:VAL:HG12 | 2.47                     | 0.45              |
| 3:C:19:VAL:O     | 3:C:22:ALA:HB3   | 2.17                     | 0.45              |
| 3:C:351:LEU:HD12 | 3:C:351:LEU:HA   | 1.78                     | 0.45              |
| 3:C:732:ALA:O    | 3:C:747:VAL:HG12 | 2.16                     | 0.45              |
| 4:D:242:SER:HB2  | 4:D:270:GLY:HA3  | 1.99                     | 0.45              |
| 4:D:350:ARG:NE   | 4:D:403:VAL:CG2  | 2.75                     | 0.45              |
| 8:H:37:PHE:CE1   | 8:H:55:MET:HB2   | 2.52                     | 0.45              |
| 1:J:163:PHE:C    | 1:J:165:THR:H    | 2.24                     | 0.45              |
| 2:K:11:LEU:HD22  | 2:K:30:LEU:HD21  | 1.98                     | 0.45              |
| 3:L:498:GLU:C    | 3:L:500:ALA:H    | 2.24                     | 0.45              |
| 4:M:63:HIS:O     | 6:O:122:ALA:HB1  | 2.17                     | 0.45              |
| 4:M:211:SER:HB2  | 4:M:215:TYR:H    | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:264:TYR:CE2  | 1:S:279:TRP:HB3  | 2.52                     | 0.45              |
| 4:V:241:ALA:CB   | 4:V:278:VAL:HG21 | 2.46                     | 0.45              |
| 8:Z:38:PRO:C     | 8:Z:40:PHE:H     | 2.24                     | 0.45              |
| 3:3:38:HIS:CE1   | 3:3:430:THR:HG21 | 2.52                     | 0.45              |
| 3:3:612:GLY:O    | 3:3:624:LEU:HB2  | 2.17                     | 0.45              |
| 4:4:249:ARG:HB2  | 4:4:262:PHE:HE2  | 1.82                     | 0.45              |
| 1:A:264:TYR:CE2  | 1:A:279:TRP:HB3  | 2.52                     | 0.45              |
| 1:A:267:PRO:O    | 1:A:268:MET:C    | 2.60                     | 0.45              |
| 2:B:86:LEU:CD1   | 2:B:90:LEU:HD11  | 2.47                     | 0.45              |
| 4:D:306:ASN:C    | 4:D:306:ASN:OD1  | 2.60                     | 0.45              |
| 5:E:1:MET:C      | 5:E:3:LEU:N      | 2.74                     | 0.45              |
| 5:E:192:TYR:CG   | 5:E:193:ARG:N    | 2.85                     | 0.45              |
| 1:J:93:ALA:O     | 1:J:134:VAL:HA   | 2.17                     | 0.45              |
| 1:J:417:PHE:O    | 1:J:418:LYS:C    | 2.60                     | 0.45              |
| 4:M:218:ALA:HB1  | 4:M:272:VAL:HG22 | 1.99                     | 0.45              |
| 5:N:77:LEU:HA    | 5:N:78:PRO:HD3   | 1.57                     | 0.45              |
| 6:O:96:TRP:HA    | 6:O:99:MET:CE    | 2.44                     | 0.45              |
| 1:S:211:LEU:HG   | 1:S:212:TRP:CZ3  | 2.52                     | 0.45              |
| 4:V:122:GLU:OE2  | 4:V:249:ARG:NH1  | 2.49                     | 0.45              |
| 4:V:212:PRO:HG2  | 4:V:213:ILE:H    | 1.81                     | 0.45              |
| 8:Z:68:LEU:HD13  | 8:Z:69:LEU:N     | 2.32                     | 0.45              |
| 1:1:154:ALA:O    | 1:1:156:GLY:N    | 2.50                     | 0.44              |
| 1:1:211:LEU:HD12 | 1:1:211:LEU:HA   | 1.80                     | 0.44              |
| 1:1:316:LEU:HD23 | 1:1:316:LEU:HA   | 1.83                     | 0.44              |
| 1:1:397:ARG:HG2  | 3:3:49:LEU:HD13  | 1.97                     | 0.44              |
| 3:3:33:PHE:HE2   | 3:3:111:THR:HG21 | 1.81                     | 0.44              |
| 3:3:378:PRO:O    | 3:3:381:LEU:HB2  | 2.16                     | 0.44              |
| 4:4:104:LEU:HD22 | 4:4:338:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:81:LYS:HA    | 1:A:81:LYS:HE3   | 1.99                     | 0.44              |
| 2:B:144:CYS:O    | 2:B:149:ARG:HD3  | 2.16                     | 0.44              |
| 3:C:168:HIS:HA   | 3:C:169:PRO:HD2  | 1.72                     | 0.44              |
| 3:C:326:PHE:CZ   | 3:C:330:LYS:HE3  | 2.52                     | 0.44              |
| 3:C:655:ARG:HH12 | 3:C:659:GLU:CB   | 2.29                     | 0.44              |
| 4:D:109:VAL:HG12 | 4:D:113:ALA:HB3  | 1.98                     | 0.44              |
| 5:E:194:SER:C    | 5:E:195:LEU:HD22 | 2.42                     | 0.44              |
| 7:G:134:GLU:CD   | 7:G:134:GLU:N    | 2.74                     | 0.44              |
| 8:H:37:PHE:HE2   | 8:H:74:PRO:HA    | 1.82                     | 0.44              |
| 1:J:233:ARG:H    | 1:J:233:ARG:HG2  | 1.57                     | 0.44              |
| 1:J:420:GLN:O    | 1:J:424:LEU:HD13 | 2.16                     | 0.44              |
| 2:K:106:ILE:CG2  | 2:K:110:GLU:HB2  | 2.47                     | 0.44              |
| 3:L:281:GLU:HG3  | 3:L:288:ILE:HG22 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:487:SER:OG   | 3:L:490:VAL:HG23 | 2.17                     | 0.44              |
| 4:M:235:THR:O    | 4:M:235:THR:HG22 | 2.17                     | 0.44              |
| 1:S:38:TYR:OH    | 1:S:112:HIS:ND1  | 2.42                     | 0.44              |
| 2:T:27:ILE:HG13  | 2:T:53:VAL:HG21  | 1.99                     | 0.44              |
| 3:U:30:VAL:CG2   | 3:U:31:PRO:HD2   | 2.47                     | 0.44              |
| 3:U:290:ILE:HD13 | 3:U:290:ILE:HA   | 1.76                     | 0.44              |
| 3:U:470:PRO:HG3  | 3:U:759:TYR:HE2  | 1.82                     | 0.44              |
| 4:V:85:MET:HE3   | 4:V:409:ARG:CB   | 2.47                     | 0.44              |
| 4:V:115:THR:HG21 | 4:V:297:LEU:HD23 | 1.97                     | 0.44              |
| 4:V:224:ILE:HA   | 4:V:225:PRO:HD2  | 1.77                     | 0.44              |
| 4:V:236:GLY:C    | 4:V:238:SER:N    | 2.72                     | 0.44              |
| 4:V:278:VAL:O    | 4:V:282:GLU:HG3  | 2.17                     | 0.44              |
| 4:V:375:PHE:HD1  | 4:V:407:VAL:HG23 | 1.81                     | 0.44              |
| 6:X:105:VAL:HG11 | 6:X:131:VAL:HG21 | 1.98                     | 0.44              |
| 7:Y:100:PHE:N    | 7:Y:100:PHE:CD1  | 2.85                     | 0.44              |
| 1:1:197:ALA:HB3  | 2:2:66:PHE:CE1   | 2.52                     | 0.44              |
| 2:2:27:ILE:HG13  | 2:2:53:VAL:HG21  | 1.98                     | 0.44              |
| 3:3:478:LEU:HD21 | 3:3:483:ASP:HB2  | 1.98                     | 0.44              |
| 3:3:664:LEU:O    | 3:3:669:VAL:HG12 | 2.18                     | 0.44              |
| 3:3:689:LYS:HD2  | 3:3:772:GLU:H    | 1.83                     | 0.44              |
| 4:4:95:LEU:HA    | 4:4:173:ILE:CD1  | 2.47                     | 0.44              |
| 1:A:355:LYS:HD3  | 1:A:399:PHE:CD2  | 2.52                     | 0.44              |
| 3:C:31:PRO:HD2   | 3:C:104:GLN:NE2  | 2.33                     | 0.44              |
| 3:C:594:ALA:C    | 3:C:596:ARG:H    | 2.24                     | 0.44              |
| 3:C:724:ARG:O    | 3:C:724:ARG:HG2  | 2.17                     | 0.44              |
| 6:F:110:ALA:HB1  | 6:F:116:GLY:HA2  | 1.99                     | 0.44              |
| 1:J:162:LEU:HB3  | 1:J:163:PHE:CD1  | 2.52                     | 0.44              |
| 2:K:86:LEU:CD1   | 2:K:90:LEU:HD11  | 2.47                     | 0.44              |
| 2:K:90:LEU:HD12  | 2:K:90:LEU:H     | 1.82                     | 0.44              |
| 3:L:33:PHE:HE2   | 3:L:111:THR:HG21 | 1.82                     | 0.44              |
| 3:L:203:ILE:HD13 | 3:L:203:ILE:N    | 2.32                     | 0.44              |
| 3:L:505:LEU:HB3  | 3:L:532:VAL:HG22 | 1.99                     | 0.44              |
| 3:L:583:VAL:HG21 | 3:L:598:ALA:HA   | 1.99                     | 0.44              |
| 4:M:63:HIS:HA    | 4:M:409:ARG:OXT  | 2.16                     | 0.44              |
| 4:M:224:ILE:HA   | 4:M:225:PRO:HD2  | 1.79                     | 0.44              |
| 8:Q:88:ARG:HE    | 8:Q:126:LEU:HD22 | 1.82                     | 0.44              |
| 1:S:139:ARG:CG   | 2:T:140:PRO:HD3  | 2.45                     | 0.44              |
| 1:S:162:LEU:HB3  | 1:S:163:PHE:HD1  | 1.83                     | 0.44              |
| 3:U:118:ASP:O    | 3:U:119:CYS:C    | 2.60                     | 0.44              |
| 3:U:202:PHE:HA   | 3:U:210:PHE:O    | 2.17                     | 0.44              |
| 3:U:700:LYS:HA   | 3:U:763:LEU:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:758:LEU:HD12 | 3:U:758:LEU:N    | 2.32                     | 0.44              |
| 4:V:358:VAL:O    | 4:V:366:TYR:HB3  | 2.17                     | 0.44              |
| 6:X:108:MET:CE   | 6:X:147:LEU:HG   | 2.35                     | 0.44              |
| 2:2:45:ARG:HG2   | 2:2:45:ARG:H     | 1.66                     | 0.44              |
| 4:4:241:ALA:O    | 4:4:267:GLY:HA3  | 2.16                     | 0.44              |
| 5:5:157:THR:C    | 5:5:158:LEU:HD23 | 2.42                     | 0.44              |
| 3:C:38:HIS:CE1   | 3:C:430:THR:HG21 | 2.52                     | 0.44              |
| 4:D:237:GLY:HA2  | 4:D:240:ARG:NE   | 2.31                     | 0.44              |
| 4:D:241:ALA:CA   | 4:D:278:VAL:HG21 | 2.45                     | 0.44              |
| 4:D:283:MET:O    | 4:D:287:VAL:HG23 | 2.17                     | 0.44              |
| 8:H:70:ALA:HA    | 8:H:83:GLY:O     | 2.17                     | 0.44              |
| 8:H:86:LEU:HD12  | 8:H:91:ILE:HD12  | 1.98                     | 0.44              |
| 3:L:483:ASP:O    | 3:L:484:LYS:HG2  | 2.17                     | 0.44              |
| 3:L:694:LEU:C    | 3:L:762:ALA:HB2  | 2.42                     | 0.44              |
| 4:M:369:LYS:HD3  | 4:M:370:VAL:N    | 2.32                     | 0.44              |
| 7:P:99:ILE:HG22  | 7:P:101:CYS:SG   | 2.57                     | 0.44              |
| 3:U:31:PRO:HD2   | 3:U:104:GLN:NE2  | 2.31                     | 0.44              |
| 3:U:367:PRO:CB   | 3:U:554:LYS:HB2  | 2.47                     | 0.44              |
| 3:U:408:ILE:HD12 | 3:U:408:ILE:HA   | 1.77                     | 0.44              |
| 3:U:508:GLY:HA2  | 3:U:535:MET:HB2  | 1.99                     | 0.44              |
| 4:V:211:SER:CB   | 4:V:214:PHE:HB3  | 2.47                     | 0.44              |
| 4:V:342:VAL:HG22 | 4:V:343:TYR:N    | 2.31                     | 0.44              |
| 1:1:192:LEU:HD23 | 1:1:192:LEU:C    | 2.42                     | 0.44              |
| 2:2:109:GLY:HA2  | 8:7:91:ILE:HD13  | 1.99                     | 0.44              |
| 2:2:168:LEU:HA   | 2:2:169:PRO:HD2  | 1.81                     | 0.44              |
| 4:4:168:PHE:HA   | 4:4:170:HIS:CD2  | 2.53                     | 0.44              |
| 3:C:202:PHE:HA   | 3:C:210:PHE:O    | 2.18                     | 0.44              |
| 3:C:422:PRO:HA   | 3:C:423:PRO:HD2  | 1.81                     | 0.44              |
| 2:K:27:ILE:HG13  | 2:K:53:VAL:HG21  | 1.97                     | 0.44              |
| 3:L:208:HIS:HB3  | 8:Q:85:ARG:NH2   | 2.32                     | 0.44              |
| 4:M:195:GLU:C    | 4:M:198:PRO:HD2  | 2.42                     | 0.44              |
| 2:T:59:GLU:O     | 2:T:63:VAL:HG23  | 2.16                     | 0.44              |
| 3:U:33:PHE:HB2   | 3:U:45:CYS:SG    | 2.57                     | 0.44              |
| 3:U:478:LEU:HD12 | 3:U:520:ARG:NH1  | 2.32                     | 0.44              |
| 3:U:559:ASP:HB2  | 3:U:573:PRO:HG3  | 1.99                     | 0.44              |
| 4:V:159:LEU:O    | 4:V:163:VAL:HG12 | 2.17                     | 0.44              |
| 4:V:249:ARG:HB2  | 4:V:262:PHE:HE2  | 1.82                     | 0.44              |
| 4:V:343:TYR:CD1  | 4:V:343:TYR:C    | 2.94                     | 0.44              |
| 1:1:267:PRO:O    | 1:1:268:MET:C    | 2.60                     | 0.44              |
| 1:1:315:HIS:O    | 1:1:319:LYS:HB2  | 2.18                     | 0.44              |
| 1:1:363:VAL:CG2  | 1:1:364:ALA:N    | 2.80                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:30:VAL:CG2   | 3:3:31:PRO:HD2   | 2.47                     | 0.44              |
| 3:3:30:VAL:CG2   | 3:3:48:CYS:HA    | 2.45                     | 0.44              |
| 3:3:356:LEU:HD13 | 3:3:654:PHE:HD1  | 1.83                     | 0.44              |
| 4:4:82:THR:N     | 4:4:83:PRO:HD2   | 2.32                     | 0.44              |
| 4:4:350:ARG:HG3  | 4:4:350:ARG:HH11 | 1.82                     | 0.44              |
| 1:A:6:LEU:HD21   | 1:A:12:ARG:CG    | 2.47                     | 0.44              |
| 2:B:153:LEU:C    | 2:B:153:LEU:HD13 | 2.43                     | 0.44              |
| 4:D:236:GLY:O    | 4:D:238:SER:N    | 2.51                     | 0.44              |
| 4:D:350:ARG:HG3  | 4:D:350:ARG:NH1  | 2.33                     | 0.44              |
| 4:D:380:SER:O    | 4:D:384:ALA:HB2  | 2.18                     | 0.44              |
| 7:G:123:ASP:CB   | 7:G:129:LEU:HD21 | 2.48                     | 0.44              |
| 2:K:78:TYR:CE1   | 2:K:157:LEU:HD22 | 2.53                     | 0.44              |
| 3:L:55:PRO:HG3   | 3:L:73:ILE:C     | 2.40                     | 0.44              |
| 3:L:469:ARG:HB2  | 3:L:470:PRO:CD   | 2.46                     | 0.44              |
| 6:O:40:THR:HB    | 6:O:50:MET:SD    | 2.58                     | 0.44              |
| 7:P:40:ARG:CB    | 7:P:121:MET:HE1  | 2.34                     | 0.44              |
| 3:U:225:ASN:O    | 3:U:229:ILE:HG13 | 2.17                     | 0.44              |
| 4:V:379:GLN:CD   | 5:W:113:PHE:HB2  | 2.43                     | 0.44              |
| 5:W:104:VAL:HG12 | 5:W:108:TRP:CE3  | 2.49                     | 0.44              |
| 6:X:16:ARG:NH1   | 6:X:17:GLU:OE2   | 2.51                     | 0.44              |
| 6:X:157:LYS:O    | 6:X:157:LYS:HG2  | 2.17                     | 0.44              |
| 8:Z:84:LEU:HB2   | 8:Z:93:LEU:HB2   | 2.00                     | 0.44              |
| 1:1:28:THR:HB    | 1:1:31:TYR:H     | 1.83                     | 0.44              |
| 3:3:125:GLY:HA3  | 3:3:246:ASN:ND2  | 2.31                     | 0.44              |
| 3:3:224:GLY:HA3  | 3:3:295:ARG:HD2  | 1.99                     | 0.44              |
| 3:3:582:PHE:HA   | 3:3:599:HIS:ND1  | 2.32                     | 0.44              |
| 3:3:591:HIS:ND1  | 3:3:592:PRO:CD   | 2.81                     | 0.44              |
| 4:4:306:ASN:HA   | 4:4:307:PRO:HD3  | 1.78                     | 0.44              |
| 4:4:390:VAL:N    | 4:4:391:PRO:CD   | 2.80                     | 0.44              |
| 7:9:40:ARG:CB    | 7:9:121:MET:HE1  | 2.35                     | 0.44              |
| 4:D:211:SER:OG   | 4:D:215:TYR:HB2  | 2.18                     | 0.44              |
| 4:D:226:PRO:HG3  | 4:D:242:SER:O    | 2.17                     | 0.44              |
| 4:D:240:ARG:NH2  | 4:D:347:GLU:OE2  | 2.46                     | 0.44              |
| 4:D:250:LYS:CE   | 4:D:262:PHE:HB3  | 2.44                     | 0.44              |
| 4:D:379:GLN:HG2  | 5:E:113:PHE:CD1  | 2.52                     | 0.44              |
| 5:E:107:LEU:HA   | 5:E:107:LEU:HD23 | 1.72                     | 0.44              |
| 2:K:59:GLU:O     | 2:K:63:VAL:HG23  | 2.17                     | 0.44              |
| 3:L:738:THR:HG22 | 3:L:739:PRO:CD   | 2.38                     | 0.44              |
| 4:M:108:VAL:HG23 | 4:M:108:VAL:O    | 2.17                     | 0.44              |
| 6:O:105:VAL:HG11 | 6:O:131:VAL:HG21 | 2.00                     | 0.44              |
| 7:P:100:PHE:HA   | 9:P:183:SF4:S4   | 2.57                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:Q:20:MET:HE3   | 8:Q:59:LEU:HG    | 1.98                     | 0.44              |
| 1:S:81:LYS:HA    | 1:S:81:LYS:CE    | 2.47                     | 0.44              |
| 4:V:198:PRO:HG3  | 4:V:291:LYS:HZ3  | 1.81                     | 0.44              |
| 4:V:285:GLU:O    | 4:V:289:ILE:HG12 | 2.17                     | 0.44              |
| 1:1:272:PHE:O    | 1:1:276:ILE:HG13 | 2.17                     | 0.44              |
| 3:3:422:PRO:HA   | 3:3:423:PRO:HD2  | 1.79                     | 0.44              |
| 3:3:469:ARG:HB2  | 3:3:470:PRO:CD   | 2.47                     | 0.44              |
| 4:4:230:ILE:HD11 | 4:4:244:VAL:CG2  | 2.48                     | 0.44              |
| 4:4:235:THR:O    | 4:4:235:THR:HG22 | 2.17                     | 0.44              |
| 1:A:53:VAL:HG23  | 1:A:231:MET:CE   | 2.46                     | 0.44              |
| 1:A:408:TRP:N    | 1:A:409:PRO:HD2  | 2.32                     | 0.44              |
| 3:C:185:LYS:HB3  | 3:C:189:ARG:HH11 | 1.83                     | 0.44              |
| 3:C:575:GLU:OE1  | 3:C:575:GLU:HA   | 2.17                     | 0.44              |
| 5:E:16:PRO:HB2   | 5:E:28:VAL:CG1   | 2.48                     | 0.44              |
| 6:F:33:SER:HA    | 6:F:158:VAL:HG21 | 1.98                     | 0.44              |
| 6:F:117:MET:HE3  | 6:F:118:PHE:CZ   | 2.52                     | 0.44              |
| 8:H:73:SER:HA    | 8:H:74:PRO:HD2   | 1.81                     | 0.44              |
| 1:J:145:LEU:HA   | 1:J:145:LEU:HD23 | 1.75                     | 0.44              |
| 1:J:201:LEU:HG   | 1:J:203:PRO:HD2  | 1.98                     | 0.44              |
| 3:L:30:VAL:CG2   | 3:L:31:PRO:HD2   | 2.48                     | 0.44              |
| 3:L:243:ARG:HB3  | 3:L:275:LEU:HD12 | 1.99                     | 0.44              |
| 3:L:690:GLY:HA3  | 3:L:770:ARG:HH21 | 1.82                     | 0.44              |
| 4:M:138:LEU:HD11 | 4:M:146:PHE:CD2  | 2.52                     | 0.44              |
| 7:P:53:CYS:HB2   | 7:P:112:ALA:HB1  | 1.99                     | 0.44              |
| 2:T:89:LYS:HE3   | 2:T:94:GLU:OE1   | 2.16                     | 0.44              |
| 3:U:30:VAL:CG2   | 3:U:48:CYS:HA    | 2.46                     | 0.44              |
| 3:U:115:HIS:C    | 4:V:321:MET:HE3  | 2.43                     | 0.44              |
| 3:U:417:VAL:O    | 3:U:417:VAL:HG12 | 2.18                     | 0.44              |
| 4:V:222:GLY:HA2  | 4:V:384:ALA:O    | 2.18                     | 0.44              |
| 4:V:304:ASP:HA   | 4:V:305:PRO:HD2  | 1.85                     | 0.44              |
| 6:X:34:ASN:C     | 6:X:36:LEU:H     | 2.25                     | 0.44              |
| 1:1:161:ASN:OD1  | 1:1:166:ASP:HA   | 2.17                     | 0.44              |
| 2:2:24:ARG:O     | 2:2:27:ILE:HD12  | 2.17                     | 0.44              |
| 3:3:194:VAL:HB   | 3:3:195:PRO:CD   | 2.48                     | 0.44              |
| 3:3:690:GLY:HA3  | 3:3:770:ARG:HH21 | 1.82                     | 0.44              |
| 4:4:63:HIS:O     | 6:6:122:ALA:HB1  | 2.18                     | 0.44              |
| 3:C:230:CYS:HA   | 3:C:231:PRO:HD2  | 1.72                     | 0.44              |
| 3:C:368:HIS:CG   | 3:C:556:ALA:HB3  | 2.53                     | 0.44              |
| 4:D:116:ILE:O    | 4:D:120:LEU:HB2  | 2.18                     | 0.44              |
| 5:E:25:LEU:CD2   | 5:E:25:LEU:H     | 2.31                     | 0.44              |
| 7:G:53:CYS:HB2   | 7:G:112:ALA:HB1  | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:38:TYR:HA    | 1:J:116:GLU:OE1  | 2.18                     | 0.44              |
| 4:M:106:GLY:O    | 5:N:194:SER:HB3  | 2.18                     | 0.44              |
| 5:N:157:THR:C    | 5:N:158:LEU:HD23 | 2.42                     | 0.44              |
| 6:O:34:ASN:C     | 6:O:36:LEU:H     | 2.26                     | 0.44              |
| 6:O:146:ALA:HB2  | 7:P:119:PHE:HD1  | 1.82                     | 0.44              |
| 3:U:333:LEU:HD13 | 3:U:648:LEU:HD21 | 1.99                     | 0.44              |
| 4:V:76:LEU:HD12  | 4:V:76:LEU:O     | 2.18                     | 0.44              |
| 4:V:235:THR:HG22 | 4:V:235:THR:O    | 2.18                     | 0.44              |
| 5:W:48:PHE:CE2   | 5:W:50:ALA:HB2   | 2.53                     | 0.44              |
| 5:W:48:PHE:CD2   | 5:W:77:LEU:HD21  | 2.52                     | 0.44              |
| 6:X:146:ALA:HB2  | 7:Y:119:PHE:CD1  | 2.52                     | 0.44              |
| 1:1:162:LEU:HB3  | 1:1:163:PHE:HD1  | 1.83                     | 0.44              |
| 1:1:211:LEU:HB2  | 1:1:216:THR:HG21 | 1.99                     | 0.44              |
| 1:1:264:TYR:CE2  | 1:1:279:TRP:HB3  | 2.52                     | 0.44              |
| 3:3:243:ARG:HB3  | 3:3:275:LEU:HD12 | 1.99                     | 0.44              |
| 3:3:555:GLY:O    | 3:3:556:ALA:C    | 2.61                     | 0.44              |
| 3:3:694:LEU:C    | 3:3:762:ALA:HB2  | 2.43                     | 0.44              |
| 7:9:100:PHE:HA   | 9:9:183:SF4:S4   | 2.58                     | 0.44              |
| 1:A:195:LEU:HA   | 2:B:24:ARG:HH21  | 1.83                     | 0.44              |
| 1:A:291:ILE:HD11 | 1:A:331:ILE:HD11 | 1.99                     | 0.44              |
| 3:C:164:VAL:HB   | 3:C:165:ASP:H    | 1.56                     | 0.44              |
| 4:D:82:THR:N     | 4:D:83:PRO:HD2   | 2.32                     | 0.44              |
| 4:D:116:ILE:HD11 | 4:D:182:LEU:CD2  | 2.47                     | 0.44              |
| 4:D:223:VAL:O    | 4:D:383:TYR:HE1  | 2.00                     | 0.44              |
| 4:D:278:VAL:O    | 4:D:282:GLU:HG3  | 2.18                     | 0.44              |
| 6:F:157:LYS:O    | 6:F:157:LYS:HG2  | 2.16                     | 0.44              |
| 7:G:115:LEU:HD23 | 7:G:115:LEU:HA   | 1.66                     | 0.44              |
| 3:L:49:LEU:HA    | 3:L:80:ALA:O     | 2.18                     | 0.44              |
| 3:L:372:GLN:O    | 3:L:558:TRP:CD2  | 2.71                     | 0.44              |
| 5:N:104:VAL:CG1  | 5:N:108:TRP:CE3  | 3.01                     | 0.44              |
| 8:Q:38:PRO:C     | 8:Q:40:PHE:H     | 2.26                     | 0.44              |
| 2:T:144:CYS:O    | 2:T:149:ARG:HD3  | 2.18                     | 0.44              |
| 3:U:560:GLU:HA   | 3:U:561:PRO:HD2  | 1.93                     | 0.44              |
| 4:V:82:THR:N     | 4:V:83:PRO:HD2   | 2.33                     | 0.44              |
| 5:W:121:LEU:HB3  | 5:W:146:LEU:CB   | 2.26                     | 0.44              |
| 6:X:140:CYS:HA   | 6:X:141:PRO:HA   | 1.69                     | 0.44              |
| 1:1:107:LEU:HD23 | 1:1:114:LEU:HD12 | 1.99                     | 0.43              |
| 1:1:323:LEU:HD23 | 1:1:323:LEU:C    | 2.43                     | 0.43              |
| 3:3:229:ILE:HD11 | 3:3:289:TRP:CH2  | 2.53                     | 0.43              |
| 3:3:614:LEU:O    | 3:3:621:VAL:HA   | 2.18                     | 0.43              |
| 3:3:734:VAL:HG13 | 3:3:775:VAL:HG13 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:168:PHE:CE1  | 6:6:141:PRO:HG3  | 2.53                     | 0.43              |
| 7:9:123:ASP:CG   | 7:9:148:ARG:HH22 | 2.24                     | 0.43              |
| 1:A:107:LEU:HD23 | 1:A:114:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:323:LEU:HD23 | 1:A:323:LEU:C    | 2.42                     | 0.43              |
| 1:A:356:CYS:HB3  | 1:A:358:PRO:CG   | 2.48                     | 0.43              |
| 1:A:356:CYS:HB3  | 1:A:358:PRO:HD2  | 2.00                     | 0.43              |
| 3:C:6:VAL:HG21   | 3:C:26:ALA:CB    | 2.47                     | 0.43              |
| 3:C:245:ARG:NH1  | 7:G:56:CYS:O     | 2.50                     | 0.43              |
| 7:G:44:THR:OG1   | 7:G:52:LYS:HD2   | 2.17                     | 0.43              |
| 8:H:72:VAL:HG22  | 8:H:73:SER:N     | 2.33                     | 0.43              |
| 1:J:272:PHE:CD1  | 1:J:311:MET:HG2  | 2.53                     | 0.43              |
| 1:J:341:MET:HE2  | 1:J:409:PRO:C    | 2.43                     | 0.43              |
| 3:L:403:THR:O    | 3:L:403:THR:HG22 | 2.18                     | 0.43              |
| 3:L:612:GLY:O    | 3:L:624:LEU:HB2  | 2.17                     | 0.43              |
| 4:M:316:LEU:C    | 4:M:316:LEU:HD12 | 2.42                     | 0.43              |
| 4:M:321:MET:HE2  | 4:M:321:MET:HB2  | 1.70                     | 0.43              |
| 5:N:167:PRO:HB3  | 7:P:66:TYR:CD2   | 2.53                     | 0.43              |
| 6:O:117:MET:HB3  | 7:P:99:ILE:CD1   | 2.47                     | 0.43              |
| 3:U:168:HIS:HA   | 3:U:169:PRO:HD2  | 1.71                     | 0.43              |
| 3:U:290:ILE:HG22 | 3:U:291:CYS:O    | 2.17                     | 0.43              |
| 3:U:641:LEU:HD23 | 3:U:641:LEU:HA   | 1.77                     | 0.43              |
| 4:V:108:VAL:O    | 4:V:108:VAL:HG23 | 2.18                     | 0.43              |
| 4:V:129:HIS:HE1  | 4:V:349:ALA:HB1  | 1.76                     | 0.43              |
| 4:V:354:GLY:H    | 4:V:371:ARG:HB3  | 1.83                     | 0.43              |
| 5:W:161:GLU:HG2  | 5:W:163:ARG:NH2  | 2.33                     | 0.43              |
| 6:X:137:VAL:HA   | 6:X:138:PRO:HD2  | 1.79                     | 0.43              |
| 7:Y:39:GLY:O     | 7:Y:40:ARG:C     | 2.61                     | 0.43              |
| 1:1:81:LYS:HA    | 1:1:81:LYS:CE    | 2.46                     | 0.43              |
| 1:1:267:PRO:O    | 1:1:270:THR:HG23 | 2.18                     | 0.43              |
| 2:2:131:ALA:HB1  | 2:2:132:PRO:HA   | 2.00                     | 0.43              |
| 3:3:2:VAL:CG1    | 3:3:89:ASP:HA    | 2.48                     | 0.43              |
| 3:3:241:ARG:HH11 | 7:9:74:GLU:CD    | 2.26                     | 0.43              |
| 3:3:269:THR:HG23 | 3:3:274:LEU:HD13 | 1.99                     | 0.43              |
| 3:3:333:LEU:HD13 | 3:3:648:LEU:HD21 | 1.99                     | 0.43              |
| 3:3:497:TRP:NE1  | 3:3:524:LEU:CD1  | 2.80                     | 0.43              |
| 3:3:724:ARG:O    | 3:3:724:ARG:HG2  | 2.18                     | 0.43              |
| 4:4:63:HIS:HA    | 4:4:409:ARG:OXT  | 2.18                     | 0.43              |
| 4:4:122:GLU:OE2  | 4:4:249:ARG:NH1  | 2.50                     | 0.43              |
| 4:4:369:LYS:HD3  | 4:4:370:VAL:N    | 2.33                     | 0.43              |
| 5:5:41:TYR:HA    | 5:5:44:MET:HE3   | 2.01                     | 0.43              |
| 6:6:141:PRO:HB3  | 9:6:182:SF4:S1   | 2.58                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:45:LEU:HD23  | 1:A:123:TYR:CG   | 2.53                     | 0.43              |
| 3:C:119:CYS:O    | 3:C:120:PRO:C    | 2.58                     | 0.43              |
| 3:C:290:ILE:HG22 | 3:C:291:CYS:O    | 2.18                     | 0.43              |
| 4:D:143:LEU:HD23 | 4:D:143:LEU:O    | 2.18                     | 0.43              |
| 4:D:393:MET:HA   | 4:D:396:ILE:CG2  | 2.47                     | 0.43              |
| 1:J:102:LYS:HG3  | 1:J:103:ASP:N    | 2.33                     | 0.43              |
| 1:J:149:ILE:O    | 1:J:153:ARG:HB2  | 2.18                     | 0.43              |
| 1:J:254:ILE:HB   | 1:J:275:LEU:HD21 | 2.00                     | 0.43              |
| 3:L:343:LEU:HD12 | 3:L:361:ALA:HB2  | 1.99                     | 0.43              |
| 3:L:722:THR:HG23 | 3:L:755:LYS:HD2  | 2.00                     | 0.43              |
| 4:M:159:LEU:O    | 4:M:163:VAL:HG12 | 2.18                     | 0.43              |
| 6:O:140:CYS:HA   | 6:O:141:PRO:HA   | 1.70                     | 0.43              |
| 1:S:102:LYS:HG3  | 1:S:103:ASP:N    | 2.33                     | 0.43              |
| 1:S:243:THR:HG22 | 1:S:244:GLU:N    | 2.27                     | 0.43              |
| 3:U:505:LEU:HB3  | 3:U:532:VAL:HG22 | 2.00                     | 0.43              |
| 3:U:737:GLU:HB2  | 3:U:776:LEU:HD21 | 2.00                     | 0.43              |
| 5:W:38:MET:O     | 5:W:41:TYR:HB2   | 2.18                     | 0.43              |
| 1:1:45:LEU:HD23  | 1:1:123:TYR:CG   | 2.53                     | 0.43              |
| 1:1:65:ARG:NH2   | 1:1:268:MET:CE   | 2.80                     | 0.43              |
| 1:1:366:PHE:O    | 1:1:370:LEU:HD23 | 2.17                     | 0.43              |
| 3:3:161:ARG:HG2  | 3:3:161:ARG:NH1  | 2.32                     | 0.43              |
| 3:3:225:ASN:O    | 3:3:229:ILE:HG13 | 2.18                     | 0.43              |
| 3:3:372:GLN:O    | 3:3:558:TRP:CD2  | 2.72                     | 0.43              |
| 3:3:532:VAL:HG12 | 3:3:533:LEU:N    | 2.34                     | 0.43              |
| 4:4:84:ARG:HD3   | 6:6:117:MET:HE1  | 2.00                     | 0.43              |
| 4:4:130:LEU:HD23 | 4:4:283:MET:HE1  | 2.00                     | 0.43              |
| 6:6:149:TYR:CZ   | 6:6:153:GLN:NE2  | 2.86                     | 0.43              |
| 6:6:158:VAL:HA   | 6:6:172:PRO:HB3  | 2.01                     | 0.43              |
| 8:7:17:LEU:HD13  | 8:7:54:ILE:HD13  | 1.99                     | 0.43              |
| 1:A:416:HIS:HB2  | 1:A:417:PHE:CE1  | 2.52                     | 0.43              |
| 3:C:596:ARG:C    | 3:C:597:TYR:HD1  | 2.27                     | 0.43              |
| 3:C:739:PRO:HD2  | 3:C:771:VAL:HG11 | 2.00                     | 0.43              |
| 4:D:275:ARG:HD2  | 4:D:399:SER:O    | 2.18                     | 0.43              |
| 1:J:290:ILE:HG22 | 1:J:330:LEU:HD22 | 2.00                     | 0.43              |
| 1:J:356:CYS:HB3  | 1:J:358:PRO:CG   | 2.47                     | 0.43              |
| 1:J:366:PHE:O    | 1:J:370:LEU:HD23 | 2.18                     | 0.43              |
| 4:M:346:THR:HG22 | 4:M:353:LEU:O    | 2.18                     | 0.43              |
| 5:N:103:THR:HB   | 5:N:115:GLU:OE1  | 2.18                     | 0.43              |
| 5:N:161:GLU:HG2  | 5:N:163:ARG:NH2  | 2.32                     | 0.43              |
| 6:O:48:ILE:HG22  | 6:O:48:ILE:O     | 2.17                     | 0.43              |
| 6:O:163:TYR:CD1  | 7:P:152:ARG:HD2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:P:177:THR:O    | 7:P:179:GLY:N    | 2.51                     | 0.43              |
| 1:S:366:PHE:O    | 1:S:370:LEU:HD23 | 2.18                     | 0.43              |
| 1:S:427:GLU:HB2  | 1:S:429:ARG:HD3  | 2.00                     | 0.43              |
| 3:U:23:VAL:HG13  | 3:U:28:TYR:HB2   | 2.00                     | 0.43              |
| 3:U:356:LEU:HD13 | 3:U:654:PHE:HD1  | 1.83                     | 0.43              |
| 4:V:109:VAL:HG12 | 4:V:113:ALA:HB3  | 2.00                     | 0.43              |
| 4:V:234:LEU:O    | 4:V:239:LEU:CG   | 2.64                     | 0.43              |
| 4:V:291:LYS:O    | 4:V:295:GLU:HG3  | 2.18                     | 0.43              |
| 5:W:77:LEU:HA    | 5:W:78:PRO:HD3   | 1.60                     | 0.43              |
| 5:W:129:HIS:CD2  | 5:W:130:PRO:HD2  | 2.53                     | 0.43              |
| 6:X:117:MET:HB3  | 7:Y:99:ILE:CD1   | 2.48                     | 0.43              |
| 6:X:158:VAL:HA   | 6:X:172:PRO:HB3  | 2.00                     | 0.43              |
| 7:Y:125:GLU:O    | 7:Y:126:TYR:C    | 2.61                     | 0.43              |
| 8:Z:108:ILE:HA   | 8:Z:109:PRO:HD3  | 1.90                     | 0.43              |
| 1:1:145:LEU:HD23 | 1:1:145:LEU:HA   | 1.69                     | 0.43              |
| 3:3:49:LEU:HA    | 3:3:80:ALA:O     | 2.19                     | 0.43              |
| 3:3:185:LYS:HG2  | 3:3:188:VAL:CG2  | 2.47                     | 0.43              |
| 5:5:111:ALA:HB1  | 5:5:115:GLU:HG3  | 2.01                     | 0.43              |
| 7:9:123:ASP:HB2  | 7:9:129:LEU:HD21 | 1.99                     | 0.43              |
| 2:B:116:LEU:HG   | 2:B:117:PHE:CD2  | 2.53                     | 0.43              |
| 3:C:478:LEU:HD12 | 3:C:520:ARG:CZ   | 2.48                     | 0.43              |
| 3:C:555:GLY:O    | 3:C:556:ALA:C    | 2.61                     | 0.43              |
| 4:D:108:VAL:HG23 | 4:D:108:VAL:O    | 2.18                     | 0.43              |
| 6:F:34:ASN:C     | 6:F:36:LEU:H     | 2.26                     | 0.43              |
| 6:F:40:THR:HB    | 6:F:50:MET:SD    | 2.58                     | 0.43              |
| 6:F:43:LEU:HA    | 6:F:43:LEU:HD23  | 1.75                     | 0.43              |
| 8:H:16:LEU:HD21  | 8:H:115:PHE:CE1  | 2.54                     | 0.43              |
| 3:L:203:ILE:HG22 | 3:L:204:GLU:HG3  | 2.00                     | 0.43              |
| 3:L:582:PHE:HA   | 3:L:599:HIS:ND1  | 2.34                     | 0.43              |
| 5:N:42:LYS:HB3   | 5:N:107:LEU:CD1  | 2.33                     | 0.43              |
| 6:O:141:PRO:HB3  | 9:O:182:SF4:S1   | 2.59                     | 0.43              |
| 3:U:286:ASN:ND2  | 3:U:286:ASN:C    | 2.76                     | 0.43              |
| 3:U:688:ARG:HD3  | 3:U:688:ARG:HA   | 1.51                     | 0.43              |
| 4:V:242:SER:HB2  | 4:V:270:GLY:HA3  | 2.00                     | 0.43              |
| 4:V:374:SER:HB2  | 4:V:406:ASP:HB3  | 2.00                     | 0.43              |
| 5:W:195:LEU:HD22 | 5:W:195:LEU:N    | 2.33                     | 0.43              |
| 1:1:38:TYR:HA    | 1:1:116:GLU:OE1  | 2.19                     | 0.43              |
| 2:2:87:SER:OG    | 2:2:128:CYS:HB3  | 2.18                     | 0.43              |
| 2:2:116:LEU:HG   | 2:2:117:PHE:CD2  | 2.53                     | 0.43              |
| 3:3:197:ASP:HB2  | 3:3:220:SER:HB3  | 2.00                     | 0.43              |
| 3:3:286:ASN:ND2  | 3:3:286:ASN:C    | 2.75                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:455:ARG:O    | 3:3:455:ARG:HG3  | 2.19                     | 0.43              |
| 4:4:44:MET:HA    | 4:4:44:MET:HE3   | 2.01                     | 0.43              |
| 4:4:76:LEU:HD12  | 4:4:76:LEU:C     | 2.43                     | 0.43              |
| 4:4:167:ARG:HD3  | 6:6:143:ARG:NH1  | 2.32                     | 0.43              |
| 4:4:350:ARG:NE   | 4:4:403:VAL:CG2  | 2.77                     | 0.43              |
| 5:5:194:SER:O    | 5:5:195:LEU:HD13 | 2.18                     | 0.43              |
| 7:9:177:THR:O    | 7:9:179:GLY:N    | 2.50                     | 0.43              |
| 1:A:118:MET:O    | 1:A:122:GLY:N    | 2.44                     | 0.43              |
| 3:C:366:THR:OG1  | 3:C:367:PRO:HD2  | 2.17                     | 0.43              |
| 3:C:497:TRP:NE1  | 3:C:524:LEU:CD1  | 2.79                     | 0.43              |
| 4:D:159:LEU:O    | 4:D:163:VAL:HG12 | 2.18                     | 0.43              |
| 4:D:235:THR:O    | 4:D:235:THR:HG22 | 2.18                     | 0.43              |
| 4:D:319:THR:HG22 | 4:D:320:SER:N    | 2.32                     | 0.43              |
| 5:E:38:MET:O     | 5:E:41:TYR:HB2   | 2.18                     | 0.43              |
| 8:H:121:ARG:NH1  | 8:H:121:ARG:CG   | 2.76                     | 0.43              |
| 1:J:272:PHE:O    | 1:J:276:ILE:HG13 | 2.17                     | 0.43              |
| 1:J:297:THR:HG22 | 1:J:322:MET:HG3  | 2.01                     | 0.43              |
| 4:M:173:ILE:O    | 4:M:173:ILE:HG23 | 2.18                     | 0.43              |
| 5:N:104:VAL:HG12 | 5:N:108:TRP:CE3  | 2.48                     | 0.43              |
| 5:N:111:ALA:HB1  | 5:N:115:GLU:HG3  | 2.01                     | 0.43              |
| 3:U:197:ASP:OD2  | 3:U:220:SER:CB   | 2.67                     | 0.43              |
| 3:3:180:ARG:O    | 3:3:181:CYS:C    | 2.61                     | 0.43              |
| 3:3:367:PRO:CB   | 3:3:554:LYS:HB2  | 2.49                     | 0.43              |
| 3:3:397:LEU:HD21 | 3:3:480:LEU:HD13 | 2.00                     | 0.43              |
| 3:3:408:ILE:HD12 | 3:3:408:ILE:HA   | 1.78                     | 0.43              |
| 3:3:469:ARG:O    | 3:3:472:GLU:HB3  | 2.19                     | 0.43              |
| 4:4:122:GLU:HB2  | 4:4:290:ILE:CD1  | 2.49                     | 0.43              |
| 4:4:276:MET:O    | 4:4:280:ILE:HG13 | 2.18                     | 0.43              |
| 4:4:343:TYR:C    | 4:4:343:TYR:CD1  | 2.97                     | 0.43              |
| 6:6:117:MET:HB3  | 7:9:99:ILE:CD1   | 2.48                     | 0.43              |
| 7:9:105:GLU:HG3  | 7:9:114:VAL:HA   | 1.99                     | 0.43              |
| 3:C:398:VAL:CB   | 3:C:450:LEU:HD22 | 2.48                     | 0.43              |
| 3:C:591:HIS:ND1  | 3:C:592:PRO:CD   | 2.80                     | 0.43              |
| 5:E:152:LEU:O    | 5:E:152:LEU:HG   | 2.19                     | 0.43              |
| 6:F:108:MET:CE   | 6:F:147:LEU:HG   | 2.40                     | 0.43              |
| 6:F:137:VAL:HA   | 6:F:138:PRO:HD2  | 1.79                     | 0.43              |
| 1:J:211:LEU:HG   | 1:J:212:TRP:CE3  | 2.53                     | 0.43              |
| 1:J:267:PRO:O    | 1:J:270:THR:HG23 | 2.19                     | 0.43              |
| 1:J:343:ASN:O    | 1:J:346:ARG:HG2  | 2.18                     | 0.43              |
| 3:L:469:ARG:O    | 3:L:472:GLU:HB3  | 2.18                     | 0.43              |
| 3:L:695:ARG:NH1  | 3:L:717:TRP:CZ2  | 2.86                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:168:PHE:HA   | 4:M:170:HIS:CD2  | 2.53                     | 0.43              |
| 4:M:390:VAL:N    | 4:M:391:PRO:CD   | 2.81                     | 0.43              |
| 5:N:129:HIS:CD2  | 5:N:130:PRO:HD2  | 2.53                     | 0.43              |
| 6:O:36:LEU:O     | 6:O:38:PRO:HD3   | 2.18                     | 0.43              |
| 8:Q:16:LEU:HD21  | 8:Q:115:PHE:CE1  | 2.53                     | 0.43              |
| 1:S:65:ARG:NH2   | 1:S:268:MET:CE   | 2.79                     | 0.43              |
| 1:S:161:ASN:OD1  | 1:S:166:ASP:HA   | 2.17                     | 0.43              |
| 2:T:116:LEU:HG   | 2:T:117:PHE:CD2  | 2.53                     | 0.43              |
| 3:U:184:CYS:SG   | 3:U:186:ARG:HB2  | 2.58                     | 0.43              |
| 3:U:203:ILE:HD13 | 3:U:203:ILE:N    | 2.34                     | 0.43              |
| 3:U:398:VAL:CB   | 3:U:450:LEU:HD22 | 2.45                     | 0.43              |
| 3:U:509:ALA:O    | 3:U:510:GLY:C    | 2.62                     | 0.43              |
| 4:V:109:VAL:HG12 | 4:V:113:ALA:CB   | 2.49                     | 0.43              |
| 6:X:46:CYS:HB3   | 6:X:81:ALA:HB1   | 2.00                     | 0.43              |
| 1:1:139:ARG:CG   | 2:2:140:PRO:HD3  | 2.45                     | 0.43              |
| 1:1:184:GLU:OE1  | 1:1:186:THR:N    | 2.52                     | 0.43              |
| 6:6:33:SER:HA    | 6:6:158:VAL:HG21 | 2.01                     | 0.43              |
| 1:A:58:LYS:HA    | 1:A:73:GLY:HA3   | 2.01                     | 0.43              |
| 1:A:102:LYS:HG3  | 1:A:103:ASP:N    | 2.33                     | 0.43              |
| 1:A:434:PRO:HG2  | 1:A:436:LEU:CD1  | 2.49                     | 0.43              |
| 2:B:112:THR:OG1  | 2:B:113:PRO:HD2  | 2.19                     | 0.43              |
| 3:C:317:LEU:N    | 3:C:317:LEU:CD2  | 2.82                     | 0.43              |
| 3:C:505:LEU:HD21 | 3:C:507:LEU:HD23 | 2.00                     | 0.43              |
| 4:D:224:ILE:HA   | 4:D:225:PRO:HD2  | 1.79                     | 0.43              |
| 4:D:276:MET:O    | 4:D:280:ILE:HG13 | 2.19                     | 0.43              |
| 6:F:117:MET:HE2  | 7:G:99:ILE:HG12  | 1.99                     | 0.43              |
| 1:J:276:ILE:HG23 | 1:J:330:LEU:HD11 | 2.01                     | 0.43              |
| 1:J:363:VAL:CG2  | 1:J:364:ALA:N    | 2.81                     | 0.43              |
| 4:M:197:LEU:HA   | 4:M:200:ARG:HB3  | 2.00                     | 0.43              |
| 4:M:211:SER:CB   | 4:M:214:PHE:HB3  | 2.47                     | 0.43              |
| 4:M:311:PRO:HD3  | 4:M:330:HIS:CE1  | 2.53                     | 0.43              |
| 6:O:108:MET:CE   | 6:O:147:LEU:HG   | 2.40                     | 0.43              |
| 6:O:123:ILE:HG22 | 6:O:124:VAL:N    | 2.34                     | 0.43              |
| 1:S:107:LEU:CD2  | 1:S:114:LEU:HD12 | 2.48                     | 0.43              |
| 1:S:133:TYR:HB2  | 1:S:188:LEU:HD21 | 2.01                     | 0.43              |
| 1:S:249:MET:H    | 1:S:249:MET:HE2  | 1.83                     | 0.43              |
| 1:S:343:ASN:O    | 1:S:346:ARG:HG2  | 2.19                     | 0.43              |
| 3:U:230:CYS:HA   | 3:U:231:PRO:HD2  | 1.69                     | 0.43              |
| 3:U:368:HIS:CG   | 3:U:556:ALA:HB3  | 2.53                     | 0.43              |
| 4:V:254:TYR:C    | 4:V:256:GLY:H    | 2.23                     | 0.43              |
| 4:V:306:ASN:HA   | 4:V:307:PRO:HD3  | 1.79                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:W:49:LEU:HD13  | 5:W:74:LEU:HD23  | 2.00                     | 0.43              |
| 5:W:116:ARG:HG3  | 5:W:129:HIS:HE1  | 1.83                     | 0.43              |
| 7:Y:110:THR:HG22 | 8:Z:41:ILE:O     | 2.19                     | 0.43              |
| 3:3:160:THR:CG2  | 8:7:73:SER:HB3   | 2.48                     | 0.43              |
| 5:5:75:VAL:HG12  | 5:5:76:SER:N     | 2.34                     | 0.43              |
| 7:9:113:ILE:HG23 | 7:9:113:ILE:O    | 2.18                     | 0.43              |
| 3:C:469:ARG:O    | 3:C:472:GLU:HB3  | 2.19                     | 0.43              |
| 3:C:509:ALA:O    | 3:C:510:GLY:C    | 2.61                     | 0.43              |
| 5:E:48:PHE:CD2   | 5:E:77:LEU:HD21  | 2.54                     | 0.43              |
| 1:J:184:GLU:OE1  | 1:J:186:THR:N    | 2.52                     | 0.43              |
| 2:K:31:LEU:HD13  | 2:K:31:LEU:HA    | 1.90                     | 0.43              |
| 3:L:474:ARG:CZ   | 3:L:516:VAL:HG21 | 2.42                     | 0.43              |
| 3:L:583:VAL:HG23 | 3:L:583:VAL:O    | 2.19                     | 0.43              |
| 5:N:41:TYR:HA    | 5:N:44:MET:HE3   | 2.01                     | 0.43              |
| 8:Q:16:LEU:HD13  | 8:Q:16:LEU:C     | 2.44                     | 0.43              |
| 1:S:93:ALA:O     | 1:S:134:VAL:HA   | 2.19                     | 0.43              |
| 1:S:95:GLU:HA    | 10:S:440:FMN:HN3 | 1.84                     | 0.43              |
| 1:S:323:LEU:C    | 1:S:323:LEU:HD23 | 2.43                     | 0.43              |
| 3:U:385:ALA:HB3  | 3:U:533:LEU:HD23 | 2.01                     | 0.43              |
| 3:U:398:VAL:CG2  | 3:U:448:MET:HE2  | 2.48                     | 0.43              |
| 3:U:403:THR:OG1  | 3:U:458:LEU:HD11 | 2.19                     | 0.43              |
| 3:U:469:ARG:O    | 3:U:472:GLU:HB3  | 2.19                     | 0.43              |
| 3:U:575:GLU:HA   | 3:U:575:GLU:OE1  | 2.18                     | 0.43              |
| 4:V:366:TYR:CE1  | 5:W:148:LYS:HE3  | 2.54                     | 0.43              |
| 5:W:3:LEU:HB2    | 5:W:86:SER:HB2   | 2.00                     | 0.43              |
| 5:W:54:GLY:C     | 5:W:55:LEU:HD12  | 2.44                     | 0.43              |
| 6:X:30:TRP:CD1   | 6:X:30:TRP:C     | 2.97                     | 0.43              |
| 6:X:121:TYR:H    | 6:X:121:TYR:HD1  | 1.67                     | 0.43              |
| 8:Z:88:ARG:HE    | 8:Z:126:LEU:CD2  | 2.32                     | 0.43              |
| 1:1:317:GLN:C    | 1:1:319:LYS:H    | 2.27                     | 0.43              |
| 3:3:474:ARG:H    | 3:3:474:ARG:HG2  | 1.65                     | 0.43              |
| 3:3:505:LEU:HD21 | 3:3:507:LEU:HD23 | 2.01                     | 0.43              |
| 4:4:338:PRO:HG3  | 5:5:193:ARG:HB2  | 2.00                     | 0.43              |
| 1:A:38:TYR:HA    | 1:A:116:GLU:OE1  | 2.18                     | 0.43              |
| 1:A:161:ASN:OD1  | 1:A:166:ASP:HA   | 2.19                     | 0.43              |
| 1:A:162:LEU:HB3  | 1:A:163:PHE:HD1  | 1.84                     | 0.43              |
| 1:A:203:PRO:HB2  | 1:A:204:PRO:HD3  | 2.00                     | 0.43              |
| 3:C:614:LEU:O    | 3:C:621:VAL:HA   | 2.18                     | 0.43              |
| 4:D:74:THR:HG22  | 4:D:75:TYR:N     | 2.34                     | 0.43              |
| 4:D:109:VAL:HG12 | 4:D:113:ALA:CB   | 2.48                     | 0.43              |
| 4:D:112:ARG:HH21 | 4:D:297:LEU:CD1  | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:30:TRP:O     | 6:F:33:SER:HB3   | 2.18                     | 0.43              |
| 3:L:546:ALA:O    | 3:L:547:MET:HE2  | 2.18                     | 0.43              |
| 3:L:575:GLU:OE1  | 3:L:575:GLU:HA   | 2.18                     | 0.43              |
| 3:L:652:PRO:HA   | 3:L:653:PRO:HD3  | 1.87                     | 0.43              |
| 4:M:167:ARG:HD3  | 6:O:143:ARG:HH12 | 1.84                     | 0.43              |
| 4:M:306:ASN:HA   | 4:M:307:PRO:HD3  | 1.80                     | 0.43              |
| 5:N:160:ARG:HD2  | 7:P:92:GLU:OE2   | 2.19                     | 0.43              |
| 1:S:154:ALA:O    | 1:S:156:GLY:N    | 2.52                     | 0.43              |
| 1:S:211:LEU:H    | 1:S:216:THR:HG21 | 1.83                     | 0.43              |
| 1:S:276:ILE:HG23 | 1:S:330:LEU:HD11 | 2.00                     | 0.43              |
| 2:T:11:LEU:HD22  | 2:T:30:LEU:HD21  | 2.00                     | 0.43              |
| 3:U:343:LEU:O    | 3:U:369:LEU:HA   | 2.19                     | 0.43              |
| 3:U:695:ARG:NH1  | 3:U:717:TRP:CZ2  | 2.87                     | 0.43              |
| 4:V:40:VAL:HG23  | 6:X:88:MET:CE    | 2.49                     | 0.43              |
| 4:V:329:LYS:HD2  | 4:V:329:LYS:HA   | 1.94                     | 0.43              |
| 5:W:107:LEU:HA   | 5:W:107:LEU:HD23 | 1.74                     | 0.43              |
| 5:W:174:LEU:CD2  | 5:W:180:GLY:HA2  | 2.48                     | 0.43              |
| 5:W:187:GLY:C    | 5:W:189:ARG:H    | 2.27                     | 0.43              |
| 6:X:171:PRO:HA   | 6:X:172:PRO:HD3  | 1.89                     | 0.43              |
| 1:1:219:ASN:ND2  | 1:1:223:THR:HG21 | 2.31                     | 0.43              |
| 1:1:253:GLN:HG2  | 1:1:327:GLY:CA   | 2.46                     | 0.43              |
| 3:3:290:ILE:HD13 | 3:3:290:ILE:HA   | 1.78                     | 0.43              |
| 3:3:591:HIS:CE1  | 3:3:593:LEU:HB2  | 2.54                     | 0.43              |
| 3:3:652:PRO:HA   | 3:3:653:PRO:HD3  | 1.86                     | 0.43              |
| 4:4:197:LEU:N    | 4:4:198:PRO:HD2  | 2.34                     | 0.43              |
| 4:4:358:VAL:O    | 4:4:366:TYR:HB3  | 2.18                     | 0.43              |
| 1:A:45:LEU:HB3   | 1:A:165:THR:HG21 | 2.01                     | 0.43              |
| 3:C:258:LEU:HD12 | 3:C:294:GLY:HA2  | 2.01                     | 0.43              |
| 3:C:417:VAL:O    | 3:C:417:VAL:HG12 | 2.18                     | 0.43              |
| 3:C:564:LEU:HD12 | 3:C:564:LEU:HA   | 1.82                     | 0.43              |
| 3:C:591:HIS:ND1  | 3:C:592:PRO:N    | 2.66                     | 0.43              |
| 4:D:63:HIS:O     | 6:F:122:ALA:HB1  | 2.18                     | 0.43              |
| 4:D:98:ALA:O     | 4:D:102:GLU:HG3  | 2.18                     | 0.43              |
| 4:D:197:LEU:O    | 4:D:198:PRO:C    | 2.60                     | 0.43              |
| 5:E:126:PHE:H    | 5:E:132:LEU:HD11 | 1.84                     | 0.43              |
| 6:F:123:ILE:HG22 | 6:F:124:VAL:N    | 2.34                     | 0.43              |
| 7:G:40:ARG:CB    | 7:G:121:MET:HE1  | 2.38                     | 0.43              |
| 1:J:6:LEU:HD21   | 1:J:12:ARG:CG    | 2.47                     | 0.43              |
| 1:J:70:PHE:HA    | 1:J:71:PRO:HD3   | 1.92                     | 0.43              |
| 3:L:397:LEU:HD21 | 3:L:480:LEU:HD13 | 2.00                     | 0.43              |
| 3:L:420:LEU:HD22 | 3:L:436:GLN:HG2  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:591:HIS:ND1  | 3:L:592:PRO:N    | 2.67                     | 0.43              |
| 5:N:103:THR:HG23 | 5:N:127:GLU:O    | 2.19                     | 0.43              |
| 6:O:161:GLN:HG2  | 6:O:161:GLN:O    | 2.19                     | 0.43              |
| 1:S:98:PRO:HB3   | 2:T:85:THR:HG21  | 1.99                     | 0.43              |
| 3:U:239:THR:HG21 | 3:U:298:HIS:NE2  | 2.34                     | 0.43              |
| 5:W:160:ARG:HH21 | 7:Y:144:LYS:NZ   | 2.16                     | 0.43              |
| 1:1:29:LEU:HD22  | 1:1:33:LEU:CD1   | 2.48                     | 0.42              |
| 3:3:118:ASP:O    | 3:3:121:THR:N    | 2.51                     | 0.42              |
| 3:3:298:HIS:ND1  | 3:3:298:HIS:C    | 2.77                     | 0.42              |
| 3:3:317:LEU:N    | 3:3:317:LEU:CD2  | 2.80                     | 0.42              |
| 3:3:575:GLU:OE1  | 3:3:575:GLU:HA   | 2.18                     | 0.42              |
| 4:4:114:GLU:O    | 4:4:118:VAL:HG13 | 2.19                     | 0.42              |
| 4:4:203:GLU:O    | 4:4:207:LEU:HG   | 2.19                     | 0.42              |
| 5:5:187:GLY:C    | 5:5:189:ARG:H    | 2.27                     | 0.42              |
| 8:7:88:ARG:HE    | 8:7:126:LEU:HD22 | 1.83                     | 0.42              |
| 1:A:295:SER:C    | 1:A:297:THR:H    | 2.26                     | 0.42              |
| 3:C:117:LEU:HD23 | 4:D:321:MET:HA   | 2.01                     | 0.42              |
| 3:C:582:PHE:HA   | 3:C:599:HIS:ND1  | 2.33                     | 0.42              |
| 6:F:117:MET:CE   | 7:G:99:ILE:HG12  | 2.49                     | 0.42              |
| 1:J:95:GLU:HA    | 10:J:440:FMN:HN3 | 1.83                     | 0.42              |
| 1:J:180:TYR:CE2  | 10:J:440:FMN:H6  | 2.54                     | 0.42              |
| 2:K:40:TRP:CH2   | 2:K:42:ARG:HG2   | 2.54                     | 0.42              |
| 3:L:329:LEU:CD1  | 3:L:584:VAL:HG11 | 2.49                     | 0.42              |
| 3:L:351:LEU:HD12 | 3:L:351:LEU:HA   | 1.77                     | 0.42              |
| 3:L:700:LYS:HA   | 3:L:763:LEU:O    | 2.18                     | 0.42              |
| 4:M:109:VAL:HG12 | 4:M:113:ALA:HB3  | 2.01                     | 0.42              |
| 4:M:115:THR:HG21 | 4:M:297:LEU:HD23 | 2.01                     | 0.42              |
| 1:S:291:ILE:HA   | 1:S:292:PRO:HD2  | 1.86                     | 0.42              |
| 3:U:317:LEU:N    | 3:U:317:LEU:CD2  | 2.81                     | 0.42              |
| 3:U:372:GLN:O    | 3:U:558:TRP:CD2  | 2.72                     | 0.42              |
| 4:V:312:PRO:HA   | 4:V:313:PRO:HD2  | 1.90                     | 0.42              |
| 4:V:404:MET:O    | 4:V:408:ASP:HB2  | 2.19                     | 0.42              |
| 5:W:52:ILE:HG23  | 5:W:114:LEU:CB   | 2.42                     | 0.42              |
| 6:X:30:TRP:O     | 6:X:33:SER:HB3   | 2.19                     | 0.42              |
| 2:2:142:VAL:HG11 | 2:2:153:LEU:HG   | 2.00                     | 0.42              |
| 3:3:19:VAL:O     | 3:3:22:ALA:HB3   | 2.18                     | 0.42              |
| 3:3:208:HIS:HB3  | 8:7:85:ARG:NH2   | 2.34                     | 0.42              |
| 3:3:669:VAL:HA   | 3:3:670:PRO:HD2  | 1.83                     | 0.42              |
| 6:6:105:VAL:HG11 | 6:6:131:VAL:HG21 | 2.02                     | 0.42              |
| 6:6:140:CYS:HA   | 6:6:141:PRO:HA   | 1.71                     | 0.42              |
| 1:A:192:LEU:HD23 | 1:A:192:LEU:C    | 2.43                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:254:ILE:HB   | 1:A:275:LEU:HD21 | 2.01                     | 0.42              |
| 3:C:298:HIS:ND1  | 3:C:298:HIS:C    | 2.77                     | 0.42              |
| 3:C:378:PRO:O    | 3:C:381:LEU:HB2  | 2.19                     | 0.42              |
| 4:D:222:GLY:HA2  | 4:D:384:ALA:O    | 2.18                     | 0.42              |
| 4:D:381:LEU:H    | 4:D:382:PRO:CD   | 2.32                     | 0.42              |
| 5:E:160:ARG:HG3  | 7:G:130:VAL:HG11 | 2.01                     | 0.42              |
| 5:E:175:THR:O    | 5:E:175:THR:OG1  | 2.28                     | 0.42              |
| 3:L:347:HIS:N    | 3:L:372:GLN:HB3  | 2.35                     | 0.42              |
| 5:N:35:LYS:HD3   | 5:N:102:PRO:CB   | 2.49                     | 0.42              |
| 5:N:75:VAL:HG12  | 5:N:76:SER:N     | 2.34                     | 0.42              |
| 6:O:43:LEU:HD23  | 6:O:43:LEU:HA    | 1.80                     | 0.42              |
| 6:O:130:VAL:HG23 | 6:O:131:VAL:HG13 | 2.01                     | 0.42              |
| 7:P:45:ARG:NH2   | 7:P:137:LEU:CD2  | 2.82                     | 0.42              |
| 1:S:26:SER:HA    | 1:S:31:TYR:CD2   | 2.54                     | 0.42              |
| 1:S:98:PRO:HA    | 2:T:124:CYS:SG   | 2.59                     | 0.42              |
| 4:V:236:GLY:O    | 4:V:238:SER:N    | 2.52                     | 0.42              |
| 6:X:83:ARG:H     | 6:X:83:ARG:HG2   | 1.60                     | 0.42              |
| 8:Z:88:ARG:HE    | 8:Z:126:LEU:HD22 | 1.84                     | 0.42              |
| 2:2:86:LEU:CD1   | 2:2:90:LEU:HD11  | 2.49                     | 0.42              |
| 3:3:684:ARG:HA   | 3:3:685:PRO:HD2  | 1.85                     | 0.42              |
| 6:6:36:LEU:O     | 6:6:38:PRO:HD3   | 2.18                     | 0.42              |
| 8:7:8:GLU:HG2    | 8:7:97:TYR:OH    | 2.19                     | 0.42              |
| 8:7:20:MET:HE3   | 8:7:59:LEU:HG    | 2.00                     | 0.42              |
| 1:A:417:PHE:O    | 1:A:418:LYS:C    | 2.61                     | 0.42              |
| 2:B:109:GLY:HA2  | 8:H:91:ILE:HD13  | 2.01                     | 0.42              |
| 3:C:136:GLU:CG   | 5:E:189:ARG:HG2  | 2.39                     | 0.42              |
| 3:C:208:HIS:HB3  | 8:H:85:ARG:NH2   | 2.34                     | 0.42              |
| 3:C:517:ALA:O    | 3:C:518:ALA:C    | 2.62                     | 0.42              |
| 3:C:591:HIS:CE1  | 3:C:593:LEU:HB2  | 2.54                     | 0.42              |
| 4:D:285:GLU:O    | 4:D:289:ILE:HG12 | 2.19                     | 0.42              |
| 5:E:35:LYS:HD3   | 5:E:102:PRO:CB   | 2.47                     | 0.42              |
| 5:E:64:ARG:HA    | 5:E:64:ARG:HD3   | 1.75                     | 0.42              |
| 1:J:97:GLU:OE2   | 1:J:294:GLY:HA3  | 2.20                     | 0.42              |
| 1:J:203:PRO:HB2  | 1:J:204:PRO:HD3  | 2.00                     | 0.42              |
| 1:J:359:CYS:O    | 1:J:363:VAL:HG22 | 2.19                     | 0.42              |
| 2:K:87:SER:OG    | 2:K:128:CYS:HB3  | 2.18                     | 0.42              |
| 3:L:356:LEU:HA   | 3:L:654:PHE:CE1  | 2.55                     | 0.42              |
| 3:L:356:LEU:HD13 | 3:L:654:PHE:HD1  | 1.84                     | 0.42              |
| 4:M:236:GLY:C    | 4:M:238:SER:N    | 2.72                     | 0.42              |
| 4:M:343:TYR:CD1  | 4:M:343:TYR:C    | 2.98                     | 0.42              |
| 4:M:358:VAL:O    | 4:M:366:TYR:HB3  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:O:46:CYS:HB3   | 6:O:81:ALA:HB1   | 2.00                     | 0.42              |
| 7:P:129:LEU:HD23 | 7:P:129:LEU:HA   | 1.62                     | 0.42              |
| 2:T:153:LEU:HD13 | 2:T:153:LEU:C    | 2.43                     | 0.42              |
| 3:U:449:ALA:HA   | 3:U:464:ILE:O    | 2.19                     | 0.42              |
| 4:V:143:LEU:HD23 | 4:V:143:LEU:O    | 2.19                     | 0.42              |
| 1:1:64:GLY:HA3   | 10:1:440:FMN:O1P | 2.18                     | 0.42              |
| 1:1:243:THR:HG22 | 1:1:244:GLU:N    | 2.26                     | 0.42              |
| 1:1:271:THR:H    | 1:1:271:THR:HG23 | 1.51                     | 0.42              |
| 3:3:133:ARG:HA   | 3:3:136:GLU:HB2  | 2.00                     | 0.42              |
| 3:3:571:VAL:HG23 | 3:3:587:LEU:HD11 | 2.01                     | 0.42              |
| 3:3:758:LEU:HD12 | 3:3:758:LEU:N    | 2.34                     | 0.42              |
| 4:4:304:ASP:HA   | 4:4:305:PRO:HD2  | 1.86                     | 0.42              |
| 5:5:48:PHE:CE2   | 5:5:50:ALA:HB2   | 2.54                     | 0.42              |
| 5:5:104:VAL:HG12 | 5:5:108:TRP:CE3  | 2.49                     | 0.42              |
| 8:7:38:PRO:C     | 8:7:40:PHE:H     | 2.28                     | 0.42              |
| 1:A:202:LYS:N    | 1:A:203:PRO:CD   | 2.83                     | 0.42              |
| 1:A:391:LEU:HA   | 1:A:391:LEU:HD23 | 1.88                     | 0.42              |
| 3:C:408:ILE:HD12 | 3:C:408:ILE:HA   | 1.77                     | 0.42              |
| 4:D:120:LEU:HD13 | 4:D:160:PHE:CE1  | 2.45                     | 0.42              |
| 4:D:224:ILE:HD11 | 4:D:275:ARG:CZ   | 2.48                     | 0.42              |
| 4:D:366:TYR:CE1  | 5:E:148:LYS:HE3  | 2.54                     | 0.42              |
| 6:F:148:ILE:O    | 6:F:151:VAL:HG22 | 2.19                     | 0.42              |
| 7:G:96:LEU:HD23  | 7:G:96:LEU:HA    | 1.69                     | 0.42              |
| 8:H:60:SER:HB3   | 8:H:64:GLY:O     | 2.19                     | 0.42              |
| 1:J:253:GLN:HG2  | 1:J:327:GLY:CA   | 2.46                     | 0.42              |
| 3:L:509:ALA:O    | 3:L:510:GLY:C    | 2.63                     | 0.42              |
| 5:N:66:GLU:HG2   | 5:N:95:PRO:CA    | 2.48                     | 0.42              |
| 5:N:194:SER:C    | 5:N:195:LEU:HD22 | 2.45                     | 0.42              |
| 6:O:33:SER:HA    | 6:O:158:VAL:HG21 | 2.01                     | 0.42              |
| 6:O:114:SER:CB   | 7:P:97:ARG:HD2   | 2.50                     | 0.42              |
| 8:Q:17:LEU:HD13  | 8:Q:54:ILE:HD13  | 2.00                     | 0.42              |
| 2:T:7:LYS:H      | 2:T:7:LYS:CD     | 2.27                     | 0.42              |
| 3:U:37:LYS:O     | 3:U:38:HIS:HB2   | 2.19                     | 0.42              |
| 3:U:139:LEU:HD12 | 4:V:326:TYR:CE2  | 2.54                     | 0.42              |
| 3:U:351:LEU:HD12 | 3:U:351:LEU:HA   | 1.82                     | 0.42              |
| 3:U:403:THR:O    | 3:U:403:THR:HG22 | 2.18                     | 0.42              |
| 4:V:316:LEU:C    | 4:V:316:LEU:HD12 | 2.44                     | 0.42              |
| 5:W:98:ASP:C     | 5:W:100:ARG:H    | 2.26                     | 0.42              |
| 5:W:111:ALA:HB1  | 5:W:115:GLU:HG3  | 2.02                     | 0.42              |
| 8:Z:63:LEU:HD13  | 8:Z:129:ALA:HB3  | 2.01                     | 0.42              |
| 1:1:6:LEU:HD21   | 1:1:12:ARG:CG    | 2.47                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:117:LEU:HD23 | 4:4:321:MET:HA   | 2.02                     | 0.42              |
| 3:3:197:ASP:OD2  | 3:3:220:SER:CB   | 2.68                     | 0.42              |
| 3:3:732:ALA:H    | 3:3:747:VAL:HG12 | 1.83                     | 0.42              |
| 4:4:69:THR:HG21  | 6:6:120:ASN:ND2  | 2.35                     | 0.42              |
| 4:4:140:LEU:HD11 | 4:4:214:PHE:HB2  | 2.01                     | 0.42              |
| 1:A:100:SER:HB2  | 1:A:325:THR:OG1  | 2.19                     | 0.42              |
| 1:A:107:LEU:CD2  | 1:A:114:LEU:HD12 | 2.49                     | 0.42              |
| 1:A:110:VAL:N    | 1:A:111:PRO:CD   | 2.81                     | 0.42              |
| 3:C:508:GLY:HA2  | 3:C:535:MET:HB2  | 2.02                     | 0.42              |
| 4:D:195:GLU:C    | 4:D:198:PRO:HD2  | 2.45                     | 0.42              |
| 7:G:100:PHE:N    | 7:G:100:PHE:CD1  | 2.87                     | 0.42              |
| 1:J:211:LEU:HD12 | 1:J:211:LEU:HA   | 1.85                     | 0.42              |
| 3:L:37:LYS:O     | 3:L:38:HIS:HB2   | 2.18                     | 0.42              |
| 3:L:584:VAL:HG21 | 3:L:644:LEU:CD1  | 2.49                     | 0.42              |
| 3:L:695:ARG:CZ   | 3:L:717:TRP:CH2  | 3.02                     | 0.42              |
| 4:M:44:MET:HA    | 4:M:44:MET:HE3   | 2.02                     | 0.42              |
| 4:M:95:LEU:HA    | 4:M:173:ILE:CD1  | 2.50                     | 0.42              |
| 4:M:130:LEU:HD11 | 4:M:152:GLU:HB3  | 2.01                     | 0.42              |
| 4:M:195:GLU:O    | 4:M:198:PRO:HD2  | 2.19                     | 0.42              |
| 4:M:212:PRO:HG2  | 4:M:213:ILE:H    | 1.84                     | 0.42              |
| 5:N:129:HIS:O    | 5:N:130:PRO:C    | 2.63                     | 0.42              |
| 7:P:96:LEU:HA    | 7:P:96:LEU:HD23  | 1.74                     | 0.42              |
| 3:U:366:THR:OG1  | 3:U:367:PRO:HD2  | 2.19                     | 0.42              |
| 3:U:582:PHE:HA   | 3:U:599:HIS:ND1  | 2.35                     | 0.42              |
| 4:V:328:PHE:CD2  | 4:V:328:PHE:C    | 2.96                     | 0.42              |
| 7:Y:113:ILE:HG23 | 7:Y:113:ILE:O    | 2.19                     | 0.42              |
| 3:3:366:THR:OG1  | 3:3:367:PRO:HD2  | 2.20                     | 0.42              |
| 3:3:478:LEU:HD12 | 3:3:520:ARG:NH1  | 2.35                     | 0.42              |
| 4:4:350:ARG:HD3  | 4:4:374:SER:OG   | 2.19                     | 0.42              |
| 6:6:174:ALA:O    | 6:6:175:ALA:HB2  | 2.20                     | 0.42              |
| 8:7:16:LEU:HD13  | 8:7:16:LEU:C     | 2.45                     | 0.42              |
| 1:A:4:PRO:C      | 1:A:12:ARG:HH22  | 2.28                     | 0.42              |
| 1:A:343:ASN:O    | 1:A:346:ARG:HG2  | 2.18                     | 0.42              |
| 3:C:113:LEU:HD12 | 3:C:157:PHE:CG   | 2.55                     | 0.42              |
| 3:C:694:LEU:C    | 3:C:762:ALA:HB2  | 2.44                     | 0.42              |
| 4:D:168:PHE:HE1  | 6:F:141:PRO:CG   | 2.32                     | 0.42              |
| 4:D:316:LEU:C    | 4:D:318:GLU:H    | 2.27                     | 0.42              |
| 6:F:131:VAL:HA   | 6:F:132:PRO:HD3  | 1.89                     | 0.42              |
| 6:F:163:TYR:HD1  | 7:G:152:ARG:NH1  | 2.17                     | 0.42              |
| 1:J:267:PRO:O    | 1:J:270:THR:CG2  | 2.68                     | 0.42              |
| 2:K:116:LEU:HG   | 2:K:117:PHE:CD2  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:47:LEU:HD11  | 4:M:51:GLU:C     | 2.44                     | 0.42              |
| 4:M:383:TYR:O    | 4:M:384:ALA:C    | 2.62                     | 0.42              |
| 5:N:52:ILE:CG2   | 5:N:114:LEU:HB3  | 2.42                     | 0.42              |
| 6:O:104:TRP:NE1  | 6:O:172:PRO:O    | 2.47                     | 0.42              |
| 1:S:45:LEU:HD23  | 1:S:123:TYR:CG   | 2.54                     | 0.42              |
| 1:S:135:ARG:C    | 1:S:137:GLU:H    | 2.28                     | 0.42              |
| 2:T:24:ARG:HE    | 2:T:24:ARG:HB3   | 1.76                     | 0.42              |
| 2:T:112:THR:HG22 | 2:T:117:PHE:H    | 1.84                     | 0.42              |
| 2:T:114:ASP:HB2  | 2:T:116:LEU:CD2  | 2.50                     | 0.42              |
| 3:U:543:GLY:HA2  | 3:U:615:VAL:HG21 | 2.02                     | 0.42              |
| 3:U:738:THR:HG22 | 3:U:739:PRO:CD   | 2.36                     | 0.42              |
| 3:U:753:VAL:HA   | 3:U:754:PRO:HD2  | 1.93                     | 0.42              |
| 5:W:37:GLU:O     | 5:W:40:HIS:HB3   | 2.19                     | 0.42              |
| 8:Z:37:PHE:CE1   | 8:Z:55:MET:HB2   | 2.54                     | 0.42              |
| 1:1:110:VAL:N    | 1:1:111:PRO:CD   | 2.81                     | 0.42              |
| 3:3:343:LEU:O    | 3:3:369:LEU:HA   | 2.20                     | 0.42              |
| 5:5:52:ILE:CG2   | 5:5:114:LEU:HB3  | 2.41                     | 0.42              |
| 1:A:29:LEU:HB2   | 1:A:151:GLU:OE1  | 2.20                     | 0.42              |
| 1:A:276:ILE:HG23 | 1:A:330:LEU:HD11 | 2.00                     | 0.42              |
| 1:A:351:GLU:HA   | 3:C:205:ARG:NH1  | 2.30                     | 0.42              |
| 2:B:45:ARG:HG2   | 2:B:45:ARG:H     | 1.65                     | 0.42              |
| 3:C:171:SER:CB   | 3:C:172:PRO:HD2  | 2.48                     | 0.42              |
| 3:C:449:ALA:HA   | 3:C:464:ILE:O    | 2.20                     | 0.42              |
| 3:C:690:GLY:HA3  | 3:C:770:ARG:HH21 | 1.84                     | 0.42              |
| 8:H:50:LEU:HD12  | 8:H:50:LEU:HA    | 1.81                     | 0.42              |
| 1:J:155:ARG:H    | 1:J:155:ARG:HG2  | 1.64                     | 0.42              |
| 2:K:114:ASP:HB2  | 2:K:116:LEU:CD2  | 2.50                     | 0.42              |
| 3:L:115:HIS:CG   | 3:L:116:PRO:CD   | 2.97                     | 0.42              |
| 3:L:739:PRO:HG2  | 3:L:771:VAL:HG12 | 2.01                     | 0.42              |
| 8:Q:84:LEU:HB2   | 8:Q:93:LEU:HB2   | 2.01                     | 0.42              |
| 2:T:55:THR:HG23  | 2:T:56:THR:N     | 2.34                     | 0.42              |
| 3:U:564:LEU:HD12 | 3:U:564:LEU:HA   | 1.83                     | 0.42              |
| 5:W:5:ARG:NH1    | 5:W:5:ARG:CG     | 2.67                     | 0.42              |
| 5:W:120:ASP:OD1  | 5:W:134:LYS:HG3  | 2.20                     | 0.42              |
| 6:X:113:SER:HB3  | 7:Y:96:LEU:HD13  | 2.02                     | 0.42              |
| 6:X:132:PRO:HB2  | 6:X:174:ALA:HB1  | 2.01                     | 0.42              |
| 1:1:363:VAL:HG23 | 1:1:364:ALA:N    | 2.35                     | 0.42              |
| 1:1:395:GLU:HB2  | 1:1:407:VAL:HG21 | 2.02                     | 0.42              |
| 3:3:581:ARG:O    | 3:3:599:HIS:HE1  | 2.03                     | 0.42              |
| 4:4:103:LYS:HE2  | 4:4:344:VAL:HG11 | 2.02                     | 0.42              |
| 4:4:108:VAL:HG23 | 4:4:108:VAL:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:130:LEU:HD11 | 4:4:152:GLU:HB3  | 2.02                     | 0.42              |
| 4:4:366:TYR:CE1  | 5:5:148:LYS:HE3  | 2.55                     | 0.42              |
| 7:9:43:LEU:CD2   | 7:9:113:ILE:HD13 | 2.50                     | 0.42              |
| 1:A:65:ARG:HB2   | 1:A:222:GLU:HB3  | 2.02                     | 0.42              |
| 1:A:186:THR:HG21 | 1:A:200:ARG:H    | 1.84                     | 0.42              |
| 7:G:108:CYS:HA   | 9:G:184:SF4:S3   | 2.60                     | 0.42              |
| 7:G:113:ILE:O    | 7:G:113:ILE:HG23 | 2.20                     | 0.42              |
| 8:H:86:LEU:HD11  | 8:H:118:LEU:HD11 | 2.01                     | 0.42              |
| 1:J:45:LEU:HD23  | 1:J:123:TYR:CG   | 2.55                     | 0.42              |
| 1:J:81:LYS:HA    | 1:J:81:LYS:HE3   | 2.02                     | 0.42              |
| 1:J:104:ARG:NH2  | 2:K:127:SER:CB   | 2.82                     | 0.42              |
| 1:J:356:CYS:HB3  | 1:J:358:PRO:CD   | 2.50                     | 0.42              |
| 2:K:168:LEU:HA   | 2:K:169:PRO:HD2  | 1.81                     | 0.42              |
| 3:L:550:LEU:HD12 | 3:L:550:LEU:N    | 2.35                     | 0.42              |
| 3:L:564:LEU:HD12 | 3:L:564:LEU:HA   | 1.81                     | 0.42              |
| 3:L:596:ARG:C    | 3:L:597:TYR:HD1  | 2.28                     | 0.42              |
| 4:M:223:VAL:O    | 4:M:383:TYR:HE1  | 2.02                     | 0.42              |
| 3:U:101:ARG:NH1  | 3:U:140:TYR:CD1  | 2.88                     | 0.42              |
| 3:U:200:LEU:HD12 | 3:U:200:LEU:HA   | 1.93                     | 0.42              |
| 3:U:402:PRO:CA   | 3:U:535:MET:HE1  | 2.49                     | 0.42              |
| 3:U:695:ARG:CZ   | 3:U:717:TRP:CH2  | 3.02                     | 0.42              |
| 4:V:256:GLY:C    | 4:V:258:GLU:N    | 2.75                     | 0.42              |
| 4:V:316:LEU:C    | 4:V:318:GLU:N    | 2.77                     | 0.42              |
| 5:W:104:VAL:CG1  | 5:W:108:TRP:CE3  | 3.03                     | 0.42              |
| 6:X:104:TRP:NE1  | 6:X:172:PRO:O    | 2.50                     | 0.42              |
| 1:1:276:ILE:HG23 | 1:1:330:LEU:HD11 | 2.02                     | 0.42              |
| 1:1:434:PRO:HG2  | 1:1:436:LEU:CD1  | 2.50                     | 0.42              |
| 3:3:100:VAL:O    | 3:3:104:GLN:HG3  | 2.20                     | 0.42              |
| 3:3:517:ALA:O    | 3:3:518:ALA:C    | 2.62                     | 0.42              |
| 3:3:658:LEU:O    | 3:3:658:LEU:HD23 | 2.20                     | 0.42              |
| 4:4:375:PHE:HD1  | 4:4:407:VAL:HG23 | 1.85                     | 0.42              |
| 1:A:87:HIS:HB2   | 1:A:126:ARG:O    | 2.19                     | 0.42              |
| 1:A:125:ILE:O    | 1:A:126:ARG:HB2  | 2.20                     | 0.42              |
| 1:A:267:PRO:O    | 1:A:270:THR:CG2  | 2.68                     | 0.42              |
| 2:B:101:THR:HG22 | 8:H:108:ILE:CD1  | 2.50                     | 0.42              |
| 3:C:224:GLY:HA3  | 3:C:295:ARG:HD2  | 2.02                     | 0.42              |
| 7:G:129:LEU:HD23 | 7:G:129:LEU:HA   | 1.68                     | 0.42              |
| 1:J:192:LEU:HD23 | 1:J:192:LEU:C    | 2.45                     | 0.42              |
| 1:J:202:LYS:N    | 1:J:203:PRO:CD   | 2.83                     | 0.42              |
| 2:K:19:PRO:HB3   | 2:K:20:PRO:HD2   | 2.02                     | 0.42              |
| 3:L:18:SER:OG    | 3:L:433:ALA:HB3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:184:CYS:SG   | 3:L:186:ARG:HB2  | 2.60                     | 0.42              |
| 3:L:555:GLY:O    | 3:L:556:ALA:C    | 2.63                     | 0.42              |
| 6:O:30:TRP:O     | 6:O:33:SER:HB3   | 2.19                     | 0.42              |
| 6:O:137:VAL:HG13 | 6:O:137:VAL:O    | 2.20                     | 0.42              |
| 8:Q:112:LYS:O    | 8:Q:116:PHE:HD1  | 2.02                     | 0.42              |
| 1:S:45:LEU:HB3   | 1:S:165:THR:HG21 | 2.01                     | 0.42              |
| 1:S:63:ARG:CD    | 1:S:313:TYR:HD2  | 2.32                     | 0.42              |
| 1:S:211:LEU:HB2  | 1:S:216:THR:HG21 | 2.02                     | 0.42              |
| 2:T:76:GLY:H     | 2:T:118:SER:HG   | 1.65                     | 0.42              |
| 3:U:417:VAL:HG12 | 3:U:443:ARG:HB3  | 2.01                     | 0.42              |
| 3:U:471:GLY:HA2  | 3:U:473:GLU:OE2  | 2.20                     | 0.42              |
| 8:Z:65:GLU:HA    | 8:Z:66:PRO:HD3   | 1.85                     | 0.42              |
| 1:1:290:ILE:CG2  | 1:1:330:LEU:HD22 | 2.49                     | 0.42              |
| 3:3:113:LEU:HD12 | 3:3:157:PHE:CG   | 2.55                     | 0.42              |
| 3:3:232:VAL:HB   | 3:3:233:GLY:H    | 1.70                     | 0.42              |
| 4:4:47:LEU:HD11  | 4:4:51:GLU:O     | 2.19                     | 0.42              |
| 4:4:109:VAL:HG12 | 4:4:113:ALA:CB   | 2.50                     | 0.42              |
| 4:4:221:VAL:O    | 4:4:272:VAL:HG12 | 2.20                     | 0.42              |
| 4:4:236:GLY:O    | 4:4:238:SER:N    | 2.53                     | 0.42              |
| 5:5:34:PHE:O     | 5:5:35:LYS:C     | 2.63                     | 0.42              |
| 5:5:104:VAL:CG1  | 5:5:108:TRP:CE3  | 3.03                     | 0.42              |
| 7:9:45:ARG:HH21  | 7:9:137:LEU:HD23 | 1.85                     | 0.42              |
| 1:A:155:ARG:H    | 1:A:155:ARG:HG2  | 1.60                     | 0.42              |
| 1:A:397:ARG:HG2  | 3:C:49:LEU:CD1   | 2.50                     | 0.42              |
| 3:C:356:LEU:HD13 | 3:C:654:PHE:HD1  | 1.85                     | 0.42              |
| 5:E:75:VAL:HG12  | 5:E:76:SER:N     | 2.35                     | 0.42              |
| 1:J:92:ASN:ND2   | 10:J:440:FMN:O3' | 2.52                     | 0.42              |
| 3:L:185:LYS:HB3  | 3:L:189:ARG:HH11 | 1.85                     | 0.42              |
| 4:M:69:THR:HG21  | 6:O:120:ASN:ND2  | 2.34                     | 0.42              |
| 4:M:285:GLU:O    | 4:M:289:ILE:HG12 | 2.20                     | 0.42              |
| 1:S:202:LYS:N    | 1:S:203:PRO:CD   | 2.82                     | 0.42              |
| 2:T:26:ALA:O     | 2:T:29:PRO:HG2   | 2.20                     | 0.42              |
| 3:U:506:ILE:HG21 | 3:U:535:MET:HE3  | 2.01                     | 0.42              |
| 3:U:655:ARG:NH1  | 3:U:659:GLU:HG3  | 2.35                     | 0.42              |
| 4:V:84:ARG:HG3   | 4:V:169:HIS:CE1  | 2.54                     | 0.42              |
| 5:W:194:SER:O    | 5:W:195:LEU:HD13 | 2.20                     | 0.42              |
| 3:3:184:CYS:SG   | 3:3:186:ARG:HB2  | 2.60                     | 0.41              |
| 3:3:583:VAL:HG21 | 3:3:598:ALA:HA   | 2.02                     | 0.41              |
| 3:3:627:ALA:HA   | 3:3:628:PRO:HD3  | 1.91                     | 0.41              |
| 3:3:722:THR:HG23 | 3:3:755:LYS:HD2  | 2.02                     | 0.41              |
| 4:4:195:GLU:C    | 4:4:198:PRO:HD2  | 2.44                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:404:MET:SD   | 4:4:407:VAL:HG11 | 2.59                     | 0.41              |
| 1:A:26:SER:HA    | 1:A:31:TYR:CD2   | 2.55                     | 0.41              |
| 1:A:51:ASP:O     | 1:A:54:ILE:HB    | 2.20                     | 0.41              |
| 1:A:317:GLN:C    | 1:A:319:LYS:H    | 2.27                     | 0.41              |
| 2:B:24:ARG:HE    | 2:B:24:ARG:HB3   | 1.76                     | 0.41              |
| 3:C:43:GLY:HA2   | 11:C:787:FES:S1  | 2.60                     | 0.41              |
| 3:C:229:ILE:HD11 | 3:C:289:TRP:CH2  | 2.55                     | 0.41              |
| 3:C:329:LEU:CD1  | 3:C:584:VAL:HG11 | 2.50                     | 0.41              |
| 3:C:372:GLN:O    | 3:C:558:TRP:CD2  | 2.73                     | 0.41              |
| 3:C:652:PRO:HA   | 3:C:653:PRO:HD3  | 1.87                     | 0.41              |
| 4:D:130:LEU:HD11 | 4:D:152:GLU:HB3  | 2.02                     | 0.41              |
| 4:D:338:PRO:HG3  | 5:E:193:ARG:HB2  | 2.01                     | 0.41              |
| 6:F:174:ALA:O    | 6:F:175:ALA:HB2  | 2.20                     | 0.41              |
| 7:G:58:LEU:HA    | 7:G:58:LEU:HD12  | 1.79                     | 0.41              |
| 1:J:434:PRO:HG2  | 1:J:436:LEU:CD1  | 2.50                     | 0.41              |
| 3:L:83:CYS:SG    | 3:L:84:VAL:HG13  | 2.60                     | 0.41              |
| 3:L:197:ASP:CB   | 3:L:220:SER:HB3  | 2.50                     | 0.41              |
| 3:L:368:HIS:CG   | 3:L:556:ALA:HB3  | 2.55                     | 0.41              |
| 3:L:408:ILE:HD12 | 3:L:408:ILE:HA   | 1.78                     | 0.41              |
| 3:L:422:PRO:HA   | 3:L:423:PRO:HD2  | 1.77                     | 0.41              |
| 3:L:627:ALA:HA   | 3:L:628:PRO:HD3  | 1.91                     | 0.41              |
| 3:L:689:LYS:HE3  | 3:L:771:VAL:CG1  | 2.49                     | 0.41              |
| 3:L:739:PRO:HD2  | 3:L:771:VAL:HG11 | 2.02                     | 0.41              |
| 4:M:40:VAL:O     | 4:M:40:VAL:CG2   | 2.67                     | 0.41              |
| 5:N:167:PRO:HB3  | 7:P:66:TYR:CE2   | 2.55                     | 0.41              |
| 6:O:152:MET:O    | 6:O:156:LYS:HG3  | 2.21                     | 0.41              |
| 7:P:123:ASP:CG   | 7:P:148:ARG:HH22 | 2.27                     | 0.41              |
| 1:S:149:ILE:O    | 1:S:153:ARG:HB2  | 2.20                     | 0.41              |
| 3:U:313:LYS:HB3  | 3:U:314:GLU:H    | 1.72                     | 0.41              |
| 3:U:394:ASP:CB   | 3:U:501:LYS:HD3  | 2.50                     | 0.41              |
| 3:U:422:PRO:HA   | 3:U:423:PRO:HD2  | 1.79                     | 0.41              |
| 4:V:343:TYR:HB2  | 4:V:356:TYR:HD1  | 1.85                     | 0.41              |
| 5:W:168:ALA:HA   | 5:W:171:ARG:HH12 | 1.85                     | 0.41              |
| 6:X:174:ALA:O    | 6:X:175:ALA:HB2  | 2.20                     | 0.41              |
| 3:3:509:ALA:O    | 3:3:510:GLY:C    | 2.64                     | 0.41              |
| 4:4:219:ARG:NH1  | 4:4:273:PHE:HD2  | 2.18                     | 0.41              |
| 4:4:242:SER:HB2  | 4:4:270:GLY:HA3  | 2.01                     | 0.41              |
| 4:4:306:ASN:C    | 4:4:306:ASN:OD1  | 2.62                     | 0.41              |
| 4:4:328:PHE:CD2  | 4:4:328:PHE:C    | 2.97                     | 0.41              |
| 5:5:192:TYR:CG   | 5:5:193:ARG:N    | 2.88                     | 0.41              |
| 6:6:145:GLU:CG   | 7:9:31:VAL:HG21  | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:9:108:CYS:HA   | 9:9:184:SF4:S3   | 2.60                     | 0.41              |
| 1:A:316:LEU:HD23 | 1:A:316:LEU:HA   | 1.83                     | 0.41              |
| 3:C:218:LEU:N    | 3:C:219:PRO:HD3  | 2.34                     | 0.41              |
| 3:C:293:ALA:HB2  | 3:C:698:MET:HG2  | 2.02                     | 0.41              |
| 3:C:498:GLU:C    | 3:C:500:ALA:N    | 2.77                     | 0.41              |
| 3:C:501:LYS:HD2  | 3:C:501:LYS:N    | 2.13                     | 0.41              |
| 3:C:695:ARG:NH1  | 3:C:717:TRP:CZ2  | 2.89                     | 0.41              |
| 4:D:95:LEU:HA    | 4:D:173:ILE:CD1  | 2.50                     | 0.41              |
| 7:G:96:LEU:HD21  | 7:G:129:LEU:HD12 | 2.01                     | 0.41              |
| 8:H:65:GLU:HA    | 8:H:66:PRO:HD3   | 1.83                     | 0.41              |
| 2:K:112:THR:OG1  | 2:K:113:PRO:HD2  | 2.20                     | 0.41              |
| 3:L:245:ARG:HA   | 3:L:245:ARG:HD2  | 1.81                     | 0.41              |
| 3:L:473:GLU:O    | 3:L:477:LEU:CD1  | 2.68                     | 0.41              |
| 4:M:143:LEU:O    | 4:M:143:LEU:HD23 | 2.19                     | 0.41              |
| 4:M:404:MET:SD   | 4:M:407:VAL:HG11 | 2.59                     | 0.41              |
| 8:Q:72:VAL:HG22  | 8:Q:73:SER:N     | 2.35                     | 0.41              |
| 1:S:192:LEU:HD23 | 1:S:192:LEU:C    | 2.44                     | 0.41              |
| 3:U:478:LEU:HD12 | 3:U:520:ARG:CZ   | 2.50                     | 0.41              |
| 4:V:161:GLU:OE2  | 6:X:143:ARG:NH1  | 2.52                     | 0.41              |
| 4:V:197:LEU:HA   | 4:V:200:ARG:HB3  | 2.02                     | 0.41              |
| 1:1:408:TRP:N    | 1:1:409:PRO:HD2  | 2.34                     | 0.41              |
| 3:3:115:HIS:CG   | 3:3:116:PRO:CD   | 2.98                     | 0.41              |
| 3:3:591:HIS:ND1  | 3:3:592:PRO:N    | 2.68                     | 0.41              |
| 3:3:615:VAL:HG22 | 3:3:621:VAL:HG12 | 2.02                     | 0.41              |
| 4:4:321:MET:HB2  | 4:4:321:MET:HE2  | 1.82                     | 0.41              |
| 5:5:38:MET:O     | 5:5:41:TYR:HB2   | 2.21                     | 0.41              |
| 5:5:137:THR:O    | 5:5:138:PRO:C    | 2.63                     | 0.41              |
| 7:9:93:ILE:HG13  | 7:9:136:MET:HE1  | 2.00                     | 0.41              |
| 8:7:52:THR:CG2   | 8:7:54:ILE:HG22  | 2.50                     | 0.41              |
| 1:A:341:MET:HE2  | 1:A:409:PRO:C    | 2.45                     | 0.41              |
| 3:C:30:VAL:CG2   | 3:C:48:CYS:HA    | 2.46                     | 0.41              |
| 3:C:100:VAL:O    | 3:C:104:GLN:HG3  | 2.21                     | 0.41              |
| 3:C:118:ASP:O    | 3:C:121:THR:N    | 2.51                     | 0.41              |
| 3:C:203:ILE:HG22 | 3:C:204:GLU:HG3  | 2.02                     | 0.41              |
| 3:C:317:LEU:HD22 | 3:C:317:LEU:H    | 1.84                     | 0.41              |
| 3:C:689:LYS:HE3  | 3:C:771:VAL:CG1  | 2.50                     | 0.41              |
| 4:D:116:ILE:HD11 | 4:D:182:LEU:CG   | 2.49                     | 0.41              |
| 4:D:263:ASP:O    | 4:D:285:GLU:HG3  | 2.20                     | 0.41              |
| 5:E:3:LEU:HB2    | 5:E:86:SER:HB2   | 2.02                     | 0.41              |
| 5:E:104:VAL:CG1  | 5:E:108:TRP:CE3  | 3.03                     | 0.41              |
| 1:J:366:PHE:HD1  | 1:J:370:LEU:CD2  | 2.32                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:395:GLU:HB2  | 1:J:407:VAL:HG21 | 2.02                     | 0.41              |
| 3:L:38:HIS:CE1   | 3:L:430:THR:HG21 | 2.55                     | 0.41              |
| 3:L:571:VAL:HG23 | 3:L:587:LEU:HD11 | 2.01                     | 0.41              |
| 3:L:577:LEU:HD13 | 3:L:577:LEU:HA   | 1.92                     | 0.41              |
| 5:N:38:MET:O     | 5:N:41:TYR:HB2   | 2.21                     | 0.41              |
| 7:P:44:THR:OG1   | 7:P:52:LYS:HD2   | 2.19                     | 0.41              |
| 1:S:434:PRO:HG2  | 1:S:436:LEU:CD1  | 2.51                     | 0.41              |
| 2:T:45:ARG:HG2   | 2:T:45:ARG:H     | 1.64                     | 0.41              |
| 3:U:155:THR:CG2  | 4:V:320:SER:HB2  | 2.50                     | 0.41              |
| 3:U:356:LEU:HA   | 3:U:654:PHE:CE1  | 2.55                     | 0.41              |
| 3:U:517:ALA:O    | 3:U:518:ALA:C    | 2.63                     | 0.41              |
| 4:V:95:LEU:HA    | 4:V:173:ILE:CD1  | 2.49                     | 0.41              |
| 4:V:162:TRP:CE2  | 7:Y:34:LYS:HD2   | 2.55                     | 0.41              |
| 4:V:219:ARG:NH1  | 4:V:273:PHE:HD2  | 2.18                     | 0.41              |
| 5:W:91:ARG:HE    | 5:W:91:ARG:HB2   | 1.57                     | 0.41              |
| 1:1:260:ARG:HA   | 2:2:177:HIS:O    | 2.20                     | 0.41              |
| 3:3:115:HIS:ND1  | 3:3:116:PRO:HD2  | 2.36                     | 0.41              |
| 4:4:109:VAL:HG12 | 4:4:113:ALA:HB3  | 2.02                     | 0.41              |
| 1:A:63:ARG:CD    | 1:A:313:TYR:HD2  | 2.33                     | 0.41              |
| 1:A:70:PHE:HA    | 1:A:71:PRO:HD3   | 1.92                     | 0.41              |
| 3:C:197:ASP:HB2  | 3:C:220:SER:HB3  | 2.02                     | 0.41              |
| 3:C:367:PRO:CB   | 3:C:554:LYS:HB2  | 2.50                     | 0.41              |
| 3:C:506:ILE:CG2  | 3:C:535:MET:HE3  | 2.49                     | 0.41              |
| 4:D:328:PHE:CD2  | 4:D:328:PHE:C    | 2.98                     | 0.41              |
| 5:E:187:GLY:C    | 5:E:189:ARG:H    | 2.28                     | 0.41              |
| 1:J:28:THR:HB    | 1:J:31:TYR:H     | 1.86                     | 0.41              |
| 1:J:45:LEU:HB3   | 1:J:165:THR:HG21 | 2.03                     | 0.41              |
| 3:L:95:THR:C     | 3:L:96:LEU:HD12  | 2.45                     | 0.41              |
| 3:L:229:ILE:HD11 | 3:L:289:TRP:CH2  | 2.56                     | 0.41              |
| 3:L:615:VAL:HG22 | 3:L:621:VAL:HG12 | 2.02                     | 0.41              |
| 3:L:669:VAL:HA   | 3:L:670:PRO:HD2  | 1.82                     | 0.41              |
| 4:M:236:GLY:O    | 4:M:238:SER:N    | 2.54                     | 0.41              |
| 4:M:375:PHE:HD1  | 4:M:407:VAL:HG23 | 1.85                     | 0.41              |
| 8:Q:8:GLU:HG2    | 8:Q:97:TYR:OH    | 2.20                     | 0.41              |
| 8:Q:52:THR:CG2   | 8:Q:54:ILE:HG22  | 2.50                     | 0.41              |
| 1:S:4:PRO:C      | 1:S:5:ILE:HG13   | 2.45                     | 0.41              |
| 1:S:97:GLU:OE2   | 1:S:294:GLY:HA3  | 2.20                     | 0.41              |
| 1:S:233:ARG:H    | 1:S:233:ARG:HG2  | 1.57                     | 0.41              |
| 1:S:414:LEU:HD12 | 1:S:414:LEU:HA   | 1.83                     | 0.41              |
| 3:U:402:PRO:HB3  | 3:U:535:MET:HE1  | 2.02                     | 0.41              |
| 4:V:84:ARG:HD3   | 6:X:117:MET:CE   | 2.47                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:110:PRO:HD2  | 4:V:113:ALA:CB   | 2.51                     | 0.41              |
| 4:V:237:GLY:HA2  | 4:V:240:ARG:NE   | 2.34                     | 0.41              |
| 5:W:38:MET:HA    | 5:W:41:TYR:CD1   | 2.55                     | 0.41              |
| 5:W:40:HIS:CE1   | 5:W:44:MET:HE2   | 2.55                     | 0.41              |
| 5:W:64:ARG:HA    | 5:W:64:ARG:HD3   | 1.74                     | 0.41              |
| 6:X:37:TRP:CD1   | 6:X:75:ALA:HB2   | 2.56                     | 0.41              |
| 7:Y:131:TYR:CZ   | 7:Y:144:LYS:HB2  | 2.56                     | 0.41              |
| 8:Z:17:LEU:HD13  | 8:Z:54:ILE:HD13  | 2.02                     | 0.41              |
| 1:1:93:ALA:O     | 1:1:134:VAL:HA   | 2.20                     | 0.41              |
| 1:1:267:PRO:O    | 1:1:270:THR:CG2  | 2.69                     | 0.41              |
| 3:3:46:ARG:NH1   | 3:3:46:ARG:CG    | 2.59                     | 0.41              |
| 3:3:176:LEU:HD21 | 3:3:178:ARG:HG3  | 2.02                     | 0.41              |
| 3:3:185:LYS:HB3  | 3:3:189:ARG:HH11 | 1.85                     | 0.41              |
| 3:3:203:ILE:HD13 | 3:3:203:ILE:N    | 2.35                     | 0.41              |
| 3:3:347:HIS:N    | 3:3:372:GLN:HB3  | 2.36                     | 0.41              |
| 4:4:101:VAL:HG12 | 4:4:175:ILE:HG23 | 2.02                     | 0.41              |
| 4:4:116:ILE:HD11 | 4:4:182:LEU:CG   | 2.48                     | 0.41              |
| 4:4:404:MET:O    | 4:4:408:ASP:HB2  | 2.20                     | 0.41              |
| 5:5:3:LEU:HB2    | 5:5:86:SER:HB2   | 2.01                     | 0.41              |
| 5:5:40:HIS:CE1   | 5:5:44:MET:HE2   | 2.55                     | 0.41              |
| 7:9:32:ALA:HA    | 7:9:162:VAL:O    | 2.20                     | 0.41              |
| 8:7:72:VAL:HG22  | 8:7:73:SER:N     | 2.36                     | 0.41              |
| 1:A:293:GLY:HA3  | 1:A:324:GLY:N    | 2.11                     | 0.41              |
| 2:B:11:LEU:HD22  | 2:B:30:LEU:HD21  | 2.00                     | 0.41              |
| 7:G:99:ILE:HG22  | 7:G:101:CYS:SG   | 2.60                     | 0.41              |
| 1:J:260:ARG:HA   | 1:J:261:PRO:HD2  | 1.90                     | 0.41              |
| 1:J:344:LEU:HD23 | 1:J:344:LEU:HA   | 1.80                     | 0.41              |
| 1:J:351:GLU:HA   | 3:L:205:ARG:NH1  | 2.35                     | 0.41              |
| 1:J:416:HIS:HB2  | 1:J:417:PHE:CE1  | 2.55                     | 0.41              |
| 2:K:86:LEU:HD11  | 2:K:90:LEU:HD11  | 2.03                     | 0.41              |
| 3:L:133:ARG:HA   | 3:L:136:GLU:HB2  | 2.02                     | 0.41              |
| 3:L:197:ASP:OD2  | 3:L:220:SER:HB2  | 2.21                     | 0.41              |
| 3:L:236:LEU:HD23 | 3:L:236:LEU:HA   | 1.82                     | 0.41              |
| 3:L:614:LEU:O    | 3:L:621:VAL:HA   | 2.20                     | 0.41              |
| 3:L:728:LEU:HB3  | 3:L:747:VAL:HG21 | 2.03                     | 0.41              |
| 3:L:732:ALA:H    | 3:L:747:VAL:HG12 | 1.86                     | 0.41              |
| 4:M:278:VAL:O    | 4:M:282:GLU:HG3  | 2.20                     | 0.41              |
| 6:O:152:MET:HE2  | 6:O:152:MET:HB3  | 1.47                     | 0.41              |
| 1:S:366:PHE:HD1  | 1:S:370:LEU:CD2  | 2.34                     | 0.41              |
| 1:S:424:LEU:CD2  | 1:S:431:VAL:HG12 | 2.51                     | 0.41              |
| 2:T:174:HIS:HB3  | 2:T:175:HIS:H    | 1.68                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:264:GLY:C    | 3:U:280:ARG:HB3  | 2.45                     | 0.41              |
| 3:U:317:LEU:HD22 | 3:U:317:LEU:H    | 1.83                     | 0.41              |
| 4:V:74:THR:HG22  | 4:V:75:TYR:N     | 2.34                     | 0.41              |
| 4:V:130:LEU:HD11 | 4:V:152:GLU:HB3  | 2.03                     | 0.41              |
| 4:V:195:GLU:C    | 4:V:198:PRO:HD2  | 2.45                     | 0.41              |
| 4:V:366:TYR:CZ   | 5:W:148:LYS:HE3  | 2.55                     | 0.41              |
| 5:W:34:PHE:O     | 5:W:35:LYS:C     | 2.63                     | 0.41              |
| 5:W:175:THR:O    | 5:W:175:THR:OG1  | 2.31                     | 0.41              |
| 7:Y:133:LYS:O    | 7:Y:137:LEU:HD13 | 2.21                     | 0.41              |
| 7:Y:177:THR:O    | 7:Y:179:GLY:N    | 2.53                     | 0.41              |
| 1:1:427:GLU:HB2  | 1:1:429:ARG:HD3  | 2.02                     | 0.41              |
| 2:2:114:ASP:HB2  | 2:2:116:LEU:CD2  | 2.51                     | 0.41              |
| 3:3:329:LEU:CD1  | 3:3:584:VAL:HG11 | 2.51                     | 0.41              |
| 3:3:417:VAL:O    | 3:3:417:VAL:HG12 | 2.21                     | 0.41              |
| 4:4:211:SER:CB   | 4:4:214:PHE:HB3  | 2.49                     | 0.41              |
| 4:4:281:ARG:HG3  | 4:4:281:ARG:HH11 | 1.86                     | 0.41              |
| 5:5:66:GLU:HG2   | 5:5:95:PRO:CA    | 2.50                     | 0.41              |
| 5:5:160:ARG:HH21 | 7:9:144:LYS:NZ   | 2.18                     | 0.41              |
| 7:9:56:CYS:SG    | 7:9:58:LEU:HB2   | 2.61                     | 0.41              |
| 3:C:203:ILE:O    | 3:C:204:GLU:O    | 2.38                     | 0.41              |
| 3:C:586:HIS:CE1  | 3:C:604:ALA:HB2  | 2.55                     | 0.41              |
| 4:D:47:LEU:HD11  | 4:D:51:GLU:O     | 2.20                     | 0.41              |
| 4:D:230:ILE:HD13 | 5:E:77:LEU:HD12  | 2.03                     | 0.41              |
| 4:D:390:VAL:H    | 4:D:391:PRO:CD   | 2.34                     | 0.41              |
| 5:E:155:THR:HG22 | 5:E:156:PRO:O    | 2.21                     | 0.41              |
| 7:G:143:THR:HG23 | 7:G:146:GLN:OE1  | 2.21                     | 0.41              |
| 8:H:39:ASP:OD2   | 8:H:75:ARG:HG2   | 2.20                     | 0.41              |
| 1:J:291:ILE:HD11 | 1:J:331:ILE:HD11 | 2.03                     | 0.41              |
| 3:L:100:VAL:O    | 3:L:104:GLN:HG3  | 2.21                     | 0.41              |
| 3:L:160:THR:CG2  | 8:Q:73:SER:HB3   | 2.50                     | 0.41              |
| 3:L:202:PHE:CE1  | 3:L:211:ILE:HD11 | 2.55                     | 0.41              |
| 3:L:364:LEU:O    | 3:L:364:LEU:HG   | 2.19                     | 0.41              |
| 3:L:532:VAL:HG12 | 3:L:533:LEU:N    | 2.35                     | 0.41              |
| 4:M:76:LEU:HD12  | 4:M:76:LEU:C     | 2.46                     | 0.41              |
| 4:M:291:LYS:O    | 4:M:295:GLU:HG3  | 2.21                     | 0.41              |
| 4:M:319:THR:HG22 | 4:M:320:SER:N    | 2.35                     | 0.41              |
| 6:O:151:VAL:O    | 6:O:155:GLN:HB2  | 2.20                     | 0.41              |
| 6:O:157:LYS:O    | 6:O:157:LYS:HG2  | 2.16                     | 0.41              |
| 6:O:158:VAL:HA   | 6:O:172:PRO:HB3  | 2.02                     | 0.41              |
| 8:Q:60:SER:HB3   | 8:Q:64:GLY:O     | 2.19                     | 0.41              |
| 1:S:118:MET:O    | 1:S:122:GLY:N    | 2.49                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:272:PHE:O    | 1:S:276:ILE:HG13 | 2.21                     | 0.41              |
| 2:T:78:TYR:CE1   | 2:T:157:LEU:HD22 | 2.55                     | 0.41              |
| 3:U:49:LEU:HA    | 3:U:80:ALA:O     | 2.21                     | 0.41              |
| 4:V:63:HIS:HA    | 4:V:409:ARG:OXT  | 2.20                     | 0.41              |
| 5:W:25:LEU:N     | 5:W:25:LEU:HD22  | 2.35                     | 0.41              |
| 5:W:126:PHE:H    | 5:W:132:LEU:HD11 | 1.86                     | 0.41              |
| 1:1:40:THR:HB    | 1:1:116:GLU:OE2  | 2.21                     | 0.41              |
| 1:1:63:ARG:CD    | 1:1:313:TYR:HD2  | 2.33                     | 0.41              |
| 1:1:118:MET:O    | 1:1:122:GLY:N    | 2.50                     | 0.41              |
| 1:1:417:PHE:O    | 1:1:418:LYS:C    | 2.63                     | 0.41              |
| 3:3:245:ARG:NH1  | 7:9:56:CYS:O     | 2.53                     | 0.41              |
| 6:6:30:TRP:CD1   | 6:6:30:TRP:C     | 2.99                     | 0.41              |
| 1:A:211:LEU:H    | 1:A:216:THR:CG2  | 2.33                     | 0.41              |
| 1:A:427:GLU:HB2  | 1:A:429:ARG:HD3  | 2.03                     | 0.41              |
| 2:B:6:ASP:OD1    | 2:B:6:ASP:C      | 2.63                     | 0.41              |
| 2:B:78:TYR:CE1   | 2:B:157:LEU:HD22 | 2.56                     | 0.41              |
| 3:C:23:VAL:HG13  | 3:C:28:TYR:HB2   | 2.01                     | 0.41              |
| 3:C:47:MET:HE1   | 3:C:108:VAL:HA   | 2.03                     | 0.41              |
| 3:C:254:THR:HG23 | 3:C:255:THR:N    | 2.35                     | 0.41              |
| 3:C:264:GLY:C    | 3:C:280:ARG:HB3  | 2.46                     | 0.41              |
| 3:C:470:PRO:HG3  | 3:C:759:TYR:HE2  | 1.85                     | 0.41              |
| 3:C:615:VAL:HG22 | 3:C:621:VAL:HG12 | 2.03                     | 0.41              |
| 4:D:87:TYR:CD1   | 6:F:48:ILE:HD12  | 2.56                     | 0.41              |
| 4:D:194:LEU:HD12 | 4:D:194:LEU:HA   | 1.90                     | 0.41              |
| 4:D:360:ASP:OD2  | 5:E:176:GLY:HA3  | 2.21                     | 0.41              |
| 5:E:129:HIS:CD2  | 5:E:130:PRO:HD2  | 2.55                     | 0.41              |
| 5:E:174:LEU:CD2  | 5:E:180:GLY:HA2  | 2.50                     | 0.41              |
| 1:J:98:PRO:HB3   | 2:K:85:THR:HG21  | 2.02                     | 0.41              |
| 3:L:113:LEU:HD12 | 3:L:157:PHE:CG   | 2.56                     | 0.41              |
| 3:L:366:THR:OG1  | 3:L:367:PRO:HD2  | 2.20                     | 0.41              |
| 3:L:734:VAL:HG13 | 3:L:775:VAL:HG13 | 2.03                     | 0.41              |
| 4:M:343:TYR:CE1  | 4:M:345:PRO:HD3  | 2.56                     | 0.41              |
| 7:P:131:TYR:CZ   | 7:P:144:LYS:HB2  | 2.55                     | 0.41              |
| 1:S:107:LEU:HD22 | 1:S:145:LEU:CD1  | 2.50                     | 0.41              |
| 3:U:20:MET:HE3   | 3:U:432:PHE:HB2  | 2.00                     | 0.41              |
| 3:U:197:ASP:OD2  | 3:U:220:SER:HB2  | 2.20                     | 0.41              |
| 4:V:371:ARG:NH2  | 4:V:376:VAL:CG2  | 2.81                     | 0.41              |
| 5:W:44:MET:HE3   | 5:W:44:MET:HB2   | 1.62                     | 0.41              |
| 6:X:43:LEU:HD23  | 6:X:43:LEU:HA    | 1.87                     | 0.41              |
| 2:2:26:ALA:O     | 2:2:29:PRO:HG2   | 2.21                     | 0.41              |
| 4:4:47:LEU:HD11  | 4:4:51:GLU:C     | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:88:LEU:HD21  | 6:6:48:ILE:CD1   | 2.42                     | 0.41              |
| 1:A:28:THR:HB    | 1:A:31:TYR:H     | 1.86                     | 0.41              |
| 1:A:272:PHE:CE2  | 1:A:311:MET:HE3  | 2.55                     | 0.41              |
| 1:A:369:ASN:HB3  | 3:C:159:PHE:CD2  | 2.56                     | 0.41              |
| 2:B:31:LEU:HD13  | 2:B:31:LEU:HA    | 1.92                     | 0.41              |
| 3:C:194:VAL:HB   | 3:C:195:PRO:CD   | 2.51                     | 0.41              |
| 4:D:115:THR:HG21 | 4:D:297:LEU:HD23 | 2.03                     | 0.41              |
| 4:D:178:VAL:CG2  | 4:D:302:VAL:HB   | 2.50                     | 0.41              |
| 4:D:241:ALA:O    | 4:D:267:GLY:HA3  | 2.21                     | 0.41              |
| 5:E:25:LEU:H     | 5:E:25:LEU:HD23  | 1.85                     | 0.41              |
| 6:F:36:LEU:O     | 6:F:38:PRO:HD3   | 2.20                     | 0.41              |
| 6:F:46:CYS:HB3   | 6:F:81:ALA:HB1   | 2.02                     | 0.41              |
| 7:G:105:GLU:HG3  | 7:G:114:VAL:HA   | 2.03                     | 0.41              |
| 3:L:397:LEU:O    | 3:L:505:LEU:HD12 | 2.21                     | 0.41              |
| 4:M:350:ARG:HG3  | 4:M:350:ARG:HH11 | 1.85                     | 0.41              |
| 6:O:137:VAL:HA   | 6:O:138:PRO:HD2  | 1.76                     | 0.41              |
| 1:S:91:CYS:HB3   | 1:S:132:ILE:HG23 | 2.03                     | 0.41              |
| 1:S:158:LEU:CA   | 1:S:162:LEU:HD21 | 2.50                     | 0.41              |
| 3:U:180:ARG:O    | 3:U:181:CYS:C    | 2.63                     | 0.41              |
| 3:U:397:LEU:O    | 3:U:505:LEU:HD12 | 2.21                     | 0.41              |
| 3:U:571:VAL:HG23 | 3:U:587:LEU:HD11 | 2.03                     | 0.41              |
| 3:U:669:VAL:HA   | 3:U:670:PRO:HD2  | 1.83                     | 0.41              |
| 3:U:680:LEU:CD2  | 3:U:682:GLU:HG2  | 2.51                     | 0.41              |
| 4:V:89:HIS:HB2   | 4:V:128:SER:CB   | 2.51                     | 0.41              |
| 4:V:383:TYR:O    | 4:V:384:ALA:C    | 2.64                     | 0.41              |
| 5:W:181:LEU:HA   | 5:W:181:LEU:HD12 | 1.80                     | 0.41              |
| 1:1:97:GLU:OE2   | 1:1:294:GLY:HA3  | 2.21                     | 0.41              |
| 1:1:158:LEU:CA   | 1:1:162:LEU:HD21 | 2.51                     | 0.41              |
| 1:1:184:GLU:HG2  | 10:1:440:FMN:C8M | 2.51                     | 0.41              |
| 1:1:344:LEU:HD23 | 1:1:344:LEU:HA   | 1.82                     | 0.41              |
| 1:1:351:GLU:HA   | 3:3:205:ARG:NH1  | 2.35                     | 0.41              |
| 1:1:424:LEU:CD2  | 1:1:431:VAL:HG12 | 2.50                     | 0.41              |
| 2:2:55:THR:HG23  | 2:2:56:THR:N     | 2.35                     | 0.41              |
| 3:3:420:LEU:HD22 | 3:3:436:GLN:HG2  | 2.03                     | 0.41              |
| 3:3:577:LEU:O    | 3:3:578:LYS:C    | 2.63                     | 0.41              |
| 4:4:40:VAL:HG13  | 4:4:404:MET:HG3  | 2.03                     | 0.41              |
| 4:4:99:LEU:HD13  | 4:4:99:LEU:HA    | 1.80                     | 0.41              |
| 4:4:237:GLY:HA2  | 4:4:240:ARG:NH2  | 2.34                     | 0.41              |
| 5:5:35:LYS:HD3   | 5:5:102:PRO:CB   | 2.51                     | 0.41              |
| 7:9:115:LEU:HA   | 7:9:115:LEU:HD23 | 1.68                     | 0.41              |
| 7:9:130:VAL:O    | 7:9:130:VAL:HG13 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:7:50:LEU:HD12  | 8:7:50:LEU:HA    | 1.83                     | 0.41              |
| 3:C:18:SER:OG    | 3:C:433:ALA:HB3  | 2.21                     | 0.41              |
| 3:C:571:VAL:HG23 | 3:C:587:LEU:HD11 | 2.02                     | 0.41              |
| 3:C:734:VAL:HG13 | 3:C:775:VAL:HG13 | 2.02                     | 0.41              |
| 4:D:62:LEU:HD23  | 4:D:62:LEU:HA    | 1.87                     | 0.41              |
| 4:D:300:GLY:HA3  | 4:D:301:PRO:HD2  | 1.94                     | 0.41              |
| 4:D:350:ARG:HD3  | 4:D:374:SER:OG   | 2.20                     | 0.41              |
| 4:D:390:VAL:HB   | 4:D:391:PRO:HD3  | 2.03                     | 0.41              |
| 5:E:34:PHE:O     | 5:E:35:LYS:C     | 2.63                     | 0.41              |
| 5:E:49:LEU:HD13  | 5:E:74:LEU:HD23  | 2.02                     | 0.41              |
| 5:E:129:HIS:O    | 5:E:130:PRO:C    | 2.63                     | 0.41              |
| 6:F:16:ARG:NH1   | 6:F:17:GLU:OE2   | 2.54                     | 0.41              |
| 8:H:86:LEU:HA    | 8:H:87:PRO:HD2   | 1.83                     | 0.41              |
| 3:L:232:VAL:HB   | 3:L:233:GLY:H    | 1.73                     | 0.41              |
| 3:L:264:GLY:C    | 3:L:280:ARG:HB3  | 2.45                     | 0.41              |
| 3:L:474:ARG:H    | 3:L:474:ARG:HG2  | 1.65                     | 0.41              |
| 3:L:543:GLY:HA2  | 3:L:615:VAL:HG21 | 2.03                     | 0.41              |
| 3:L:590:LEU:HD12 | 3:L:590:LEU:HA   | 1.87                     | 0.41              |
| 3:L:750:ARG:HB2  | 3:L:753:VAL:CG2  | 2.51                     | 0.41              |
| 4:M:109:VAL:HG12 | 4:M:113:ALA:CB   | 2.50                     | 0.41              |
| 4:M:237:GLY:HA2  | 4:M:240:ARG:NE   | 2.36                     | 0.41              |
| 4:M:338:PRO:HG3  | 5:N:193:ARG:HB2  | 2.02                     | 0.41              |
| 5:N:49:LEU:HD13  | 5:N:74:LEU:HD23  | 2.03                     | 0.41              |
| 6:O:20:LEU:O     | 6:O:24:LEU:HD13  | 2.21                     | 0.41              |
| 7:P:56:CYS:SG    | 7:P:58:LEU:HB2   | 2.61                     | 0.41              |
| 7:P:105:GLU:HG3  | 7:P:114:VAL:HA   | 2.01                     | 0.41              |
| 7:P:143:THR:H    | 7:P:146:GLN:HB2  | 1.86                     | 0.41              |
| 8:Q:88:ARG:HE    | 8:Q:126:LEU:CD2  | 2.34                     | 0.41              |
| 1:S:28:THR:HB    | 1:S:31:TYR:H     | 1.86                     | 0.41              |
| 1:S:100:SER:HB2  | 1:S:325:THR:OG1  | 2.21                     | 0.41              |
| 1:S:424:LEU:HD21 | 1:S:431:VAL:HG12 | 2.02                     | 0.41              |
| 3:U:197:ASP:HB2  | 3:U:220:SER:HB3  | 2.02                     | 0.41              |
| 4:V:47:LEU:HD11  | 4:V:51:GLU:O     | 2.21                     | 0.41              |
| 4:V:116:ILE:HD11 | 4:V:182:LEU:CD2  | 2.51                     | 0.41              |
| 4:V:140:LEU:HD11 | 4:V:214:PHE:HB2  | 2.03                     | 0.41              |
| 4:V:249:ARG:HD2  | 4:V:257:TYR:HE1  | 1.84                     | 0.41              |
| 5:W:75:VAL:HG12  | 5:W:76:SER:N     | 2.36                     | 0.41              |
| 3:3:200:LEU:HD12 | 3:3:200:LEU:HA   | 1.93                     | 0.41              |
| 3:3:409:LEU:HD23 | 3:3:409:LEU:HA   | 1.80                     | 0.41              |
| 3:3:459:MET:HG2  | 3:3:465:HIS:CD2  | 2.56                     | 0.41              |
| 3:3:590:LEU:HD12 | 3:3:590:LEU:HA   | 1.91                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:291:LYS:O    | 4:4:295:GLU:HG3  | 2.21                     | 0.41              |
| 3:C:243:ARG:HB3  | 3:C:275:LEU:CD1  | 2.51                     | 0.41              |
| 3:C:343:LEU:O    | 3:C:369:LEU:HA   | 2.20                     | 0.41              |
| 3:C:564:LEU:HG   | 3:C:581:ARG:HG3  | 2.03                     | 0.41              |
| 4:D:140:LEU:HD11 | 4:D:214:PHE:HB2  | 2.03                     | 0.41              |
| 7:G:100:PHE:HA   | 9:G:183:SF4:S4   | 2.61                     | 0.41              |
| 1:J:394:ILE:O    | 1:J:395:GLU:C    | 2.63                     | 0.41              |
| 4:M:219:ARG:NH1  | 4:M:273:PHE:HD2  | 2.17                     | 0.41              |
| 8:Q:108:ILE:HA   | 8:Q:109:PRO:HD3  | 1.93                     | 0.41              |
| 1:S:363:VAL:CG2  | 1:S:364:ALA:N    | 2.84                     | 0.41              |
| 3:U:136:GLU:CG   | 5:W:189:ARG:HG2  | 2.41                     | 0.41              |
| 3:U:432:PHE:N    | 3:U:432:PHE:CD1  | 2.88                     | 0.41              |
| 3:U:701:ALA:N    | 3:U:763:LEU:HB3  | 2.36                     | 0.41              |
| 4:V:396:ILE:HA   | 4:V:396:ILE:HD12 | 1.83                     | 0.41              |
| 5:W:192:TYR:CG   | 5:W:193:ARG:N    | 2.88                     | 0.41              |
| 7:Y:143:THR:H    | 7:Y:146:GLN:HB2  | 1.86                     | 0.41              |
| 1:1:70:PHE:HA    | 1:1:71:PRO:HD3   | 1.96                     | 0.40              |
| 3:3:167:HIS:O    | 3:3:167:HIS:ND1  | 2.53                     | 0.40              |
| 3:3:343:LEU:HD12 | 3:3:361:ALA:HB2  | 2.02                     | 0.40              |
| 4:4:178:VAL:CG2  | 4:4:302:VAL:HB   | 2.51                     | 0.40              |
| 4:4:371:ARG:NH2  | 4:4:376:VAL:CG2  | 2.80                     | 0.40              |
| 6:6:114:SER:CB   | 7:9:97:ARG:HD2   | 2.47                     | 0.40              |
| 7:9:41:HIS:ND1   | 7:9:95:MET:HE1   | 2.36                     | 0.40              |
| 1:A:356:CYS:HB3  | 1:A:358:PRO:CD   | 2.52                     | 0.40              |
| 1:A:367:MET:HE1  | 1:A:410:VAL:HG21 | 2.02                     | 0.40              |
| 3:C:728:LEU:HB3  | 3:C:747:VAL:HG21 | 2.02                     | 0.40              |
| 4:D:311:PRO:HD3  | 4:D:330:HIS:CE1  | 2.56                     | 0.40              |
| 5:E:41:TYR:HA    | 5:E:44:MET:HE3   | 2.03                     | 0.40              |
| 6:F:140:CYS:SG   | 7:G:99:ILE:HG13  | 2.61                     | 0.40              |
| 8:H:52:THR:CG2   | 8:H:54:ILE:HG22  | 2.51                     | 0.40              |
| 1:J:316:LEU:HA   | 1:J:316:LEU:HD23 | 1.85                     | 0.40              |
| 2:K:103:THR:HG22 | 2:K:104:LEU:N    | 2.36                     | 0.40              |
| 3:L:290:ILE:HG23 | 9:L:786:SF4:S4   | 2.61                     | 0.40              |
| 3:L:497:TRP:NE1  | 3:L:524:LEU:CD1  | 2.83                     | 0.40              |
| 4:M:47:LEU:HD11  | 4:M:51:GLU:O     | 2.20                     | 0.40              |
| 4:M:193:LEU:O    | 4:M:193:LEU:HD23 | 2.22                     | 0.40              |
| 4:M:197:LEU:O    | 4:M:198:PRO:C    | 2.63                     | 0.40              |
| 3:U:185:LYS:HB3  | 3:U:189:ARG:HH11 | 1.87                     | 0.40              |
| 3:U:399:LEU:HD22 | 3:U:477:LEU:HD11 | 2.03                     | 0.40              |
| 3:U:555:GLY:O    | 3:U:556:ALA:C    | 2.63                     | 0.40              |
| 3:U:669:VAL:O    | 3:U:669:VAL:HG13 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:47:LEU:HD11  | 4:V:51:GLU:C     | 2.46                     | 0.40              |
| 4:V:116:ILE:O    | 4:V:120:LEU:HB2  | 2.21                     | 0.40              |
| 4:V:168:PHE:HE1  | 6:X:141:PRO:CG   | 2.35                     | 0.40              |
| 5:W:137:THR:HA   | 5:W:138:PRO:HD2  | 1.87                     | 0.40              |
| 6:X:151:VAL:O    | 6:X:155:GLN:HB2  | 2.21                     | 0.40              |
| 7:Y:79:ASN:HA    | 7:Y:80:PRO:HD2   | 1.95                     | 0.40              |
| 1:1:26:SER:HA    | 1:1:31:TYR:CD2   | 2.56                     | 0.40              |
| 1:1:170:ASP:O    | 1:1:171:LEU:HD12 | 2.21                     | 0.40              |
| 3:3:407:PRO:HB2  | 9:3:786:SF4:S1   | 2.61                     | 0.40              |
| 4:4:197:LEU:O    | 4:4:198:PRO:C    | 2.63                     | 0.40              |
| 6:6:151:VAL:O    | 6:6:155:GLN:HB2  | 2.21                     | 0.40              |
| 6:6:152:MET:O    | 6:6:156:LYS:HG3  | 2.22                     | 0.40              |
| 6:6:157:LYS:O    | 6:6:157:LYS:HG2  | 2.18                     | 0.40              |
| 7:9:63:CYS:HA    | 7:9:64:PRO:HD2   | 1.89                     | 0.40              |
| 3:C:133:ARG:HA   | 3:C:136:GLU:HB2  | 2.03                     | 0.40              |
| 3:C:402:PRO:CA   | 3:C:535:MET:HE1  | 2.52                     | 0.40              |
| 3:C:688:ARG:HA   | 3:C:688:ARG:HD3  | 1.50                     | 0.40              |
| 4:D:221:VAL:O    | 4:D:272:VAL:HG12 | 2.22                     | 0.40              |
| 4:D:241:ALA:CB   | 4:D:278:VAL:HG21 | 2.51                     | 0.40              |
| 4:D:249:ARG:CZ   | 4:D:262:PHE:HZ   | 2.34                     | 0.40              |
| 4:D:332:THR:O    | 5:E:172:ALA:HB3  | 2.21                     | 0.40              |
| 6:F:78:MET:HE3   | 6:F:96:TRP:HB2   | 2.04                     | 0.40              |
| 8:H:122:ALA:O    | 8:H:126:LEU:HB2  | 2.21                     | 0.40              |
| 1:J:133:TYR:CB   | 1:J:188:LEU:HD21 | 2.51                     | 0.40              |
| 1:J:158:LEU:CA   | 1:J:162:LEU:HD21 | 2.51                     | 0.40              |
| 1:J:402:LEU:O    | 1:J:405:ALA:HB3  | 2.21                     | 0.40              |
| 3:L:305:ARG:NH2  | 3:L:609:GLU:OE1  | 2.52                     | 0.40              |
| 3:L:382:PHE:CE1  | 3:L:512:LEU:HD11 | 2.56                     | 0.40              |
| 4:M:283:MET:O    | 4:M:287:VAL:HG23 | 2.21                     | 0.40              |
| 1:S:65:ARG:HB2   | 1:S:222:GLU:HB3  | 2.02                     | 0.40              |
| 1:S:89:LEU:HD12  | 1:S:217:THR:HG22 | 2.03                     | 0.40              |
| 1:S:290:ILE:CG2  | 1:S:330:LEU:HD22 | 2.51                     | 0.40              |
| 1:S:317:GLN:C    | 1:S:319:LYS:H    | 2.30                     | 0.40              |
| 3:U:203:ILE:O    | 3:U:204:GLU:O    | 2.39                     | 0.40              |
| 3:U:498:GLU:C    | 3:U:500:ALA:N    | 2.79                     | 0.40              |
| 4:V:290:ILE:O    | 4:V:294:LEU:HB2  | 2.22                     | 0.40              |
| 1:1:186:THR:HA   | 1:1:189:MET:HE2  | 2.02                     | 0.40              |
| 1:1:343:ASN:O    | 1:1:346:ARG:HG2  | 2.21                     | 0.40              |
| 3:3:317:LEU:HD22 | 3:3:317:LEU:H    | 1.82                     | 0.40              |
| 1:A:65:ARG:NH2   | 1:A:268:MET:CE   | 2.83                     | 0.40              |
| 2:B:112:THR:HG22 | 2:B:117:PHE:H    | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:131:GLN:O    | 3:C:134:THR:HB   | 2.22                     | 0.40              |
| 3:C:236:LEU:HD23 | 3:C:236:LEU:HA   | 1.84                     | 0.40              |
| 3:C:286:ASN:ND2  | 3:C:286:ASN:C    | 2.76                     | 0.40              |
| 3:C:577:LEU:O    | 3:C:578:LYS:C    | 2.64                     | 0.40              |
| 4:D:40:VAL:HG13  | 4:D:404:MET:HG3  | 2.02                     | 0.40              |
| 4:D:63:HIS:HA    | 4:D:409:ARG:OXT  | 2.20                     | 0.40              |
| 4:D:239:LEU:HD22 | 4:D:244:VAL:CB   | 2.50                     | 0.40              |
| 4:D:298:GLU:CG   | 4:D:299:PRO:HD2  | 2.51                     | 0.40              |
| 6:F:165:GLU:HG2  | 7:G:148:ARG:NH1  | 2.35                     | 0.40              |
| 7:G:125:GLU:O    | 7:G:126:TYR:C    | 2.63                     | 0.40              |
| 1:J:67:GLY:HA2   | 1:J:324:GLY:O    | 2.20                     | 0.40              |
| 3:L:130:LEU:HD12 | 3:L:130:LEU:O    | 2.20                     | 0.40              |
| 3:L:243:ARG:HB3  | 3:L:275:LEU:CD1  | 2.52                     | 0.40              |
| 3:L:317:LEU:N    | 3:L:317:LEU:CD2  | 2.83                     | 0.40              |
| 3:L:414:SER:HA   | 3:L:461:TRP:CZ3  | 2.57                     | 0.40              |
| 4:M:233:GLY:O    | 4:M:235:THR:N    | 2.54                     | 0.40              |
| 4:M:286:SER:O    | 4:M:290:ILE:HG12 | 2.22                     | 0.40              |
| 5:N:25:LEU:N     | 5:N:25:LEU:HD22  | 2.36                     | 0.40              |
| 7:P:130:VAL:O    | 7:P:130:VAL:HG13 | 2.21                     | 0.40              |
| 1:S:160:LYS:HG3  | 1:S:161:ASN:N    | 2.35                     | 0.40              |
| 1:S:341:MET:HB2  | 1:S:371:PHE:CE1  | 2.57                     | 0.40              |
| 1:S:344:LEU:HD23 | 1:S:344:LEU:HA   | 1.80                     | 0.40              |
| 3:U:532:VAL:HG12 | 3:U:533:LEU:N    | 2.35                     | 0.40              |
| 3:U:750:ARG:HB2  | 3:U:753:VAL:CG2  | 2.52                     | 0.40              |
| 4:V:72:HIS:O     | 4:V:73:ARG:CD    | 2.49                     | 0.40              |
| 4:V:215:TYR:CD2  | 4:V:215:TYR:C    | 3.00                     | 0.40              |
| 1:1:154:ALA:C    | 1:1:156:GLY:H    | 2.29                     | 0.40              |
| 1:1:312:SER:C    | 1:1:314:GLU:H    | 2.28                     | 0.40              |
| 2:2:112:THR:OG1  | 2:2:113:PRO:HD2  | 2.21                     | 0.40              |
| 3:3:36:GLU:OE2   | 3:3:229:ILE:HG23 | 2.21                     | 0.40              |
| 3:3:474:ARG:CZ   | 3:3:516:VAL:HG21 | 2.46                     | 0.40              |
| 3:3:596:ARG:C    | 3:3:597:TYR:HD1  | 2.29                     | 0.40              |
| 3:3:713:ARG:HE   | 3:3:713:ARG:HB2  | 1.72                     | 0.40              |
| 4:4:234:LEU:O    | 4:4:239:LEU:CG   | 2.61                     | 0.40              |
| 5:5:48:PHE:CD2   | 5:5:77:LEU:HD21  | 2.56                     | 0.40              |
| 6:6:113:SER:HB3  | 7:9:96:LEU:HD13  | 2.04                     | 0.40              |
| 1:A:363:VAL:CG2  | 1:A:364:ALA:N    | 2.85                     | 0.40              |
| 2:B:26:ALA:O     | 2:B:29:PRO:HG2   | 2.21                     | 0.40              |
| 2:B:86:LEU:HD11  | 2:B:90:LEU:HD11  | 2.02                     | 0.40              |
| 3:C:55:PRO:CG    | 3:C:73:ILE:C     | 2.95                     | 0.40              |
| 3:C:244:ALA:HB3  | 3:C:249:MET:CE   | 2.44                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:281:GLU:HG3  | 3:C:288:ILE:HG22 | 2.04                     | 0.40              |
| 4:D:354:GLY:H    | 4:D:371:ARG:HB3  | 1.86                     | 0.40              |
| 5:E:40:HIS:CE1   | 5:E:44:MET:HE2   | 2.57                     | 0.40              |
| 6:F:152:MET:HE2  | 6:F:152:MET:HB3  | 1.51                     | 0.40              |
| 7:G:143:THR:H    | 7:G:146:GLN:HB2  | 1.87                     | 0.40              |
| 8:H:87:PRO:O     | 8:H:88:ARG:CB    | 2.69                     | 0.40              |
| 1:J:58:LYS:HA    | 1:J:73:GLY:HA3   | 2.02                     | 0.40              |
| 1:J:154:ALA:O    | 1:J:156:GLY:N    | 2.55                     | 0.40              |
| 1:J:158:LEU:HA   | 1:J:162:LEU:HD21 | 2.02                     | 0.40              |
| 1:J:271:THR:HG23 | 1:J:271:THR:H    | 1.50                     | 0.40              |
| 4:M:114:GLU:O    | 4:M:118:VAL:HG13 | 2.21                     | 0.40              |
| 4:M:163:VAL:HG13 | 4:M:164:THR:HG23 | 2.03                     | 0.40              |
| 6:O:114:SER:C    | 6:O:116:GLY:H    | 2.30                     | 0.40              |
| 8:Q:65:GLU:HA    | 8:Q:66:PRO:HD3   | 1.83                     | 0.40              |
| 1:S:125:ILE:O    | 1:S:126:ARG:HB2  | 2.20                     | 0.40              |
| 2:T:112:THR:OG1  | 2:T:113:PRO:HD2  | 2.21                     | 0.40              |
| 3:U:123:ASP:HB3  | 3:U:236:LEU:HD13 | 2.02                     | 0.40              |
| 3:U:164:VAL:HB   | 3:U:165:ASP:H    | 1.61                     | 0.40              |
| 3:U:258:LEU:HD12 | 3:U:294:GLY:HA2  | 2.03                     | 0.40              |
| 3:U:329:LEU:CD1  | 3:U:584:VAL:HG11 | 2.51                     | 0.40              |
| 3:U:469:ARG:HB2  | 3:U:470:PRO:CD   | 2.50                     | 0.40              |
| 3:U:577:LEU:O    | 3:U:578:LYS:C    | 2.65                     | 0.40              |
| 3:U:654:PHE:HE2  | 3:U:663:ALA:HB3  | 1.86                     | 0.40              |
| 4:V:215:TYR:C    | 4:V:215:TYR:HD2  | 2.30                     | 0.40              |
| 4:V:390:VAL:N    | 4:V:391:PRO:CD   | 2.84                     | 0.40              |
| 1:1:158:LEU:HA   | 1:1:162:LEU:HD21 | 2.03                     | 0.40              |
| 1:1:202:LYS:N    | 1:1:203:PRO:CD   | 2.85                     | 0.40              |
| 1:1:424:LEU:HD21 | 1:1:431:VAL:HG12 | 2.02                     | 0.40              |
| 3:3:695:ARG:NH1  | 3:3:717:TRP:CZ2  | 2.90                     | 0.40              |
| 5:5:49:LEU:HD13  | 5:5:74:LEU:HD23  | 2.04                     | 0.40              |
| 6:6:104:TRP:NE1  | 6:6:172:PRO:O    | 2.50                     | 0.40              |
| 6:6:163:TYR:CD1  | 7:9:152:ARG:HD2  | 2.56                     | 0.40              |
| 8:7:108:ILE:HA   | 8:7:109:PRO:HD3  | 1.94                     | 0.40              |
| 1:A:107:LEU:HD22 | 1:A:145:LEU:CD1  | 2.51                     | 0.40              |
| 3:C:180:ARG:O    | 3:C:181:CYS:C    | 2.64                     | 0.40              |
| 3:C:343:LEU:HD12 | 3:C:361:ALA:HB2  | 2.03                     | 0.40              |
| 3:C:368:HIS:CB   | 3:C:556:ALA:HB3  | 2.52                     | 0.40              |
| 3:C:734:VAL:HG12 | 3:C:735:ALA:N    | 2.36                     | 0.40              |
| 4:D:115:THR:HG22 | 4:D:297:LEU:HD23 | 2.02                     | 0.40              |
| 8:H:108:ILE:HA   | 8:H:109:PRO:HD3  | 1.92                     | 0.40              |
| 1:J:211:LEU:HG   | 1:J:212:TRP:CZ3  | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:115:HIS:ND1  | 3:L:116:PRO:HD2  | 2.37                     | 0.40              |
| 3:L:254:THR:HG23 | 3:L:255:THR:N    | 2.36                     | 0.40              |
| 3:L:703:GLN:O    | 3:L:705:VAL:N    | 2.54                     | 0.40              |
| 4:M:140:LEU:HD11 | 4:M:214:PHE:HB2  | 2.03                     | 0.40              |
| 4:M:203:GLU:O    | 4:M:207:LEU:HG   | 2.22                     | 0.40              |
| 4:M:344:VAL:HG23 | 4:M:344:VAL:O    | 2.21                     | 0.40              |
| 4:M:344:VAL:HA   | 4:M:345:PRO:HD2  | 1.96                     | 0.40              |
| 7:P:58:LEU:HD12  | 7:P:58:LEU:HA    | 1.76                     | 0.40              |
| 7:P:125:GLU:O    | 7:P:126:TYR:C    | 2.64                     | 0.40              |
| 7:P:150:ALA:HA   | 7:P:153:THR:HB   | 2.04                     | 0.40              |
| 1:S:158:LEU:HA   | 1:S:162:LEU:HD21 | 2.03                     | 0.40              |
| 1:S:267:PRO:O    | 1:S:270:THR:HG23 | 2.21                     | 0.40              |
| 2:T:136:VAL:HG21 | 2:T:163:LEU:HD13 | 2.04                     | 0.40              |
| 3:U:133:ARG:HA   | 3:U:136:GLU:HB2  | 2.04                     | 0.40              |
| 3:U:334:LYS:NZ   | 3:U:334:LYS:HB3  | 2.37                     | 0.40              |
| 3:U:459:MET:HG3  | 3:U:465:HIS:HB2  | 2.03                     | 0.40              |
| 3:U:583:VAL:HG23 | 3:U:583:VAL:O    | 2.21                     | 0.40              |
| 3:U:695:ARG:HA   | 3:U:696:PRO:HD2  | 1.92                     | 0.40              |
| 4:V:195:GLU:O    | 4:V:198:PRO:HD2  | 2.22                     | 0.40              |
| 4:V:285:GLU:OE1  | 4:V:288:LYS:HD3  | 2.21                     | 0.40              |
| 5:W:41:TYR:HA    | 5:W:44:MET:HE3   | 2.03                     | 0.40              |
| 5:W:137:THR:O    | 5:W:138:PRO:C    | 2.64                     | 0.40              |
| 6:X:145:GLU:H    | 6:X:145:GLU:CD   | 2.29                     | 0.40              |
| 7:Y:134:GLU:CD   | 7:Y:134:GLU:N    | 2.78                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles        |
|-----|-------|---------------|-----------|----------|----------|--------------------|
| 1   | 1     | 435/438 (99%) | 366 (84%) | 59 (14%) | 10 (2%)  | <b>5</b> <b>24</b> |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 435/438 (99%) | 359 (82%) | 65 (15%) | 11 (2%)  | 4           | 22  |
| 1   | J     | 435/438 (99%) | 363 (83%) | 62 (14%) | 10 (2%)  | 5           | 24  |
| 1   | S     | 435/438 (99%) | 362 (83%) | 62 (14%) | 11 (2%)  | 4           | 22  |
| 2   | 2     | 176/181 (97%) | 147 (84%) | 26 (15%) | 3 (2%)   | 7           | 30  |
| 2   | B     | 176/181 (97%) | 145 (82%) | 28 (16%) | 3 (2%)   | 7           | 30  |
| 2   | K     | 176/181 (97%) | 145 (82%) | 29 (16%) | 2 (1%)   | 11          | 39  |
| 2   | T     | 176/181 (97%) | 147 (84%) | 27 (15%) | 2 (1%)   | 11          | 39  |
| 3   | 3     | 748/783 (96%) | 628 (84%) | 96 (13%) | 24 (3%)  | 3           | 17  |
| 3   | C     | 748/783 (96%) | 632 (84%) | 93 (12%) | 23 (3%)  | 3           | 18  |
| 3   | L     | 748/783 (96%) | 630 (84%) | 93 (12%) | 25 (3%)  | 3           | 17  |
| 3   | U     | 748/783 (96%) | 633 (85%) | 93 (12%) | 22 (3%)  | 3           | 20  |
| 4   | 4     | 373/409 (91%) | 319 (86%) | 44 (12%) | 10 (3%)  | 4           | 21  |
| 4   | D     | 373/409 (91%) | 320 (86%) | 41 (11%) | 12 (3%)  | 3           | 17  |
| 4   | M     | 373/409 (91%) | 319 (86%) | 44 (12%) | 10 (3%)  | 4           | 21  |
| 4   | V     | 373/409 (91%) | 319 (86%) | 42 (11%) | 12 (3%)  | 3           | 17  |
| 5   | 5     | 194/207 (94%) | 162 (84%) | 21 (11%) | 11 (6%)  | 1           | 9   |
| 5   | E     | 194/207 (94%) | 160 (82%) | 23 (12%) | 11 (6%)  | 1           | 9   |
| 5   | N     | 194/207 (94%) | 160 (82%) | 23 (12%) | 11 (6%)  | 1           | 9   |
| 5   | W     | 194/207 (94%) | 157 (81%) | 26 (13%) | 11 (6%)  | 1           | 9   |
| 6   | 6     | 141/181 (78%) | 121 (86%) | 17 (12%) | 3 (2%)   | 5           | 26  |
| 6   | F     | 141/181 (78%) | 120 (85%) | 18 (13%) | 3 (2%)   | 5           | 26  |
| 6   | O     | 141/181 (78%) | 119 (84%) | 21 (15%) | 1 (1%)   | 18          | 49  |
| 6   | X     | 141/181 (78%) | 120 (85%) | 18 (13%) | 3 (2%)   | 5           | 26  |
| 7   | 9     | 152/182 (84%) | 127 (84%) | 23 (15%) | 2 (1%)   | 9           | 36  |
| 7   | G     | 152/182 (84%) | 128 (84%) | 22 (14%) | 2 (1%)   | 9           | 36  |
| 7   | P     | 152/182 (84%) | 128 (84%) | 22 (14%) | 2 (1%)   | 9           | 36  |
| 7   | Y     | 152/182 (84%) | 130 (86%) | 20 (13%) | 2 (1%)   | 9           | 36  |
| 8   | 7     | 125/129 (97%) | 114 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 8   | H     | 125/129 (97%) | 115 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 8   | Q     | 125/129 (97%) | 115 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 8   | Z     | 125/129 (97%) | 114 (91%) | 11 (9%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed    | Outliers | Percentiles |    |
|-----|-------|------------------|------------|------------|----------|-------------|----|
| All | All   | 9376/10040 (93%) | 7924 (84%) | 1200 (13%) | 252 (3%) | 4           | 21 |

All (252) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 4   | PRO  |
| 1   | 1     | 68  | ALA  |
| 1   | 1     | 81  | LYS  |
| 1   | 1     | 160 | LYS  |
| 1   | 1     | 234 | GLY  |
| 4   | 4     | 212 | PRO  |
| 5   | 5     | 160 | ARG  |
| 5   | 5     | 176 | GLY  |
| 1   | A     | 4   | PRO  |
| 1   | A     | 68  | ALA  |
| 1   | A     | 81  | LYS  |
| 1   | A     | 160 | LYS  |
| 1   | A     | 234 | GLY  |
| 4   | D     | 212 | PRO  |
| 4   | D     | 255 | SER  |
| 5   | E     | 160 | ARG  |
| 5   | E     | 176 | GLY  |
| 1   | J     | 4   | PRO  |
| 1   | J     | 68  | ALA  |
| 1   | J     | 81  | LYS  |
| 1   | J     | 160 | LYS  |
| 1   | J     | 234 | GLY  |
| 4   | M     | 212 | PRO  |
| 5   | N     | 160 | ARG  |
| 5   | N     | 176 | GLY  |
| 1   | S     | 4   | PRO  |
| 1   | S     | 81  | LYS  |
| 1   | S     | 160 | LYS  |
| 1   | S     | 234 | GLY  |
| 4   | V     | 212 | PRO  |
| 5   | W     | 160 | ARG  |
| 5   | W     | 176 | GLY  |
| 1   | 1     | 37  | GLY  |
| 1   | 1     | 155 | ARG  |
| 2   | 2     | 136 | VAL  |
| 3   | 3     | 6   | VAL  |
| 3   | 3     | 204 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 338 | GLY  |
| 3   | 3     | 365 | LYS  |
| 3   | 3     | 580 | LYS  |
| 3   | 3     | 690 | GLY  |
| 4   | 4     | 53  | LEU  |
| 4   | 4     | 219 | ARG  |
| 4   | 4     | 255 | SER  |
| 7   | 9     | 156 | PRO  |
| 1   | A     | 37  | GLY  |
| 1   | A     | 155 | ARG  |
| 3   | C     | 181 | CYS  |
| 3   | C     | 204 | GLU  |
| 3   | C     | 365 | LYS  |
| 3   | C     | 516 | VAL  |
| 3   | C     | 580 | LYS  |
| 3   | C     | 690 | GLY  |
| 4   | D     | 53  | LEU  |
| 4   | D     | 219 | ARG  |
| 5   | E     | 27  | VAL  |
| 5   | E     | 50  | ALA  |
| 1   | J     | 37  | GLY  |
| 1   | J     | 155 | ARG  |
| 2   | K     | 136 | VAL  |
| 3   | L     | 204 | GLU  |
| 3   | L     | 365 | LYS  |
| 3   | L     | 516 | VAL  |
| 3   | L     | 556 | ALA  |
| 3   | L     | 580 | LYS  |
| 3   | L     | 690 | GLY  |
| 4   | M     | 53  | LEU  |
| 4   | M     | 219 | ARG  |
| 4   | M     | 255 | SER  |
| 5   | N     | 27  | VAL  |
| 1   | S     | 37  | GLY  |
| 1   | S     | 68  | ALA  |
| 1   | S     | 155 | ARG  |
| 2   | T     | 136 | VAL  |
| 3   | U     | 181 | CYS  |
| 3   | U     | 204 | GLU  |
| 3   | U     | 338 | GLY  |
| 3   | U     | 365 | LYS  |
| 3   | U     | 556 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | U     | 580 | LYS  |
| 3   | U     | 690 | GLY  |
| 4   | V     | 53  | LEU  |
| 4   | V     | 219 | ARG  |
| 4   | V     | 255 | SER  |
| 5   | W     | 27  | VAL  |
| 5   | W     | 50  | ALA  |
| 1   | 1     | 38  | TYR  |
| 2   | 2     | 140 | PRO  |
| 3   | 3     | 119 | CYS  |
| 3   | 3     | 181 | CYS  |
| 3   | 3     | 516 | VAL  |
| 3   | 3     | 554 | LYS  |
| 3   | 3     | 556 | ALA  |
| 4   | 4     | 142 | ALA  |
| 5   | 5     | 50  | ALA  |
| 1   | A     | 38  | TYR  |
| 1   | A     | 154 | ALA  |
| 2   | B     | 136 | VAL  |
| 2   | B     | 140 | PRO  |
| 3   | C     | 139 | LEU  |
| 3   | C     | 338 | GLY  |
| 3   | C     | 554 | LYS  |
| 3   | C     | 556 | ALA  |
| 4   | D     | 142 | ALA  |
| 7   | G     | 156 | PRO  |
| 1   | J     | 38  | TYR  |
| 2   | K     | 140 | PRO  |
| 3   | L     | 6   | VAL  |
| 3   | L     | 119 | CYS  |
| 3   | L     | 139 | LEU  |
| 3   | L     | 181 | CYS  |
| 3   | L     | 338 | GLY  |
| 3   | L     | 554 | LYS  |
| 4   | M     | 142 | ALA  |
| 5   | N     | 50  | ALA  |
| 7   | P     | 156 | PRO  |
| 1   | S     | 38  | TYR  |
| 1   | S     | 154 | ALA  |
| 2   | T     | 140 | PRO  |
| 3   | U     | 554 | LYS  |
| 4   | V     | 142 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Y     | 156 | PRO  |
| 1   | 1     | 154 | ALA  |
| 3   | 3     | 139 | LEU  |
| 3   | 3     | 367 | PRO  |
| 5   | 5     | 27  | VAL  |
| 5   | 5     | 33  | ARG  |
| 5   | 5     | 138 | PRO  |
| 6   | 6     | 156 | LYS  |
| 3   | C     | 6   | VAL  |
| 3   | C     | 119 | CYS  |
| 3   | C     | 367 | PRO  |
| 4   | D     | 198 | PRO  |
| 5   | E     | 2   | ARG  |
| 5   | E     | 47  | ASN  |
| 5   | E     | 61  | PRO  |
| 5   | E     | 138 | PRO  |
| 3   | L     | 367 | PRO  |
| 3   | L     | 704 | ALA  |
| 5   | N     | 138 | PRO  |
| 3   | U     | 6   | VAL  |
| 3   | U     | 119 | CYS  |
| 3   | U     | 139 | LEU  |
| 3   | U     | 367 | PRO  |
| 3   | U     | 704 | ALA  |
| 4   | V     | 198 | PRO  |
| 5   | W     | 47  | ASN  |
| 5   | W     | 61  | PRO  |
| 5   | W     | 138 | PRO  |
| 2   | 2     | 116 | LEU  |
| 3   | 3     | 164 | VAL  |
| 3   | 3     | 704 | ALA  |
| 4   | 4     | 198 | PRO  |
| 4   | 4     | 381 | LEU  |
| 5   | 5     | 2   | ARG  |
| 5   | 5     | 47  | ASN  |
| 5   | 5     | 61  | PRO  |
| 5   | 5     | 65  | PRO  |
| 3   | C     | 164 | VAL  |
| 3   | C     | 704 | ALA  |
| 4   | D     | 381 | LEU  |
| 5   | E     | 33  | ARG  |
| 5   | E     | 35  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 65  | PRO  |
| 1   | J     | 154 | ALA  |
| 3   | L     | 285 | VAL  |
| 3   | L     | 453 | PRO  |
| 3   | L     | 563 | ALA  |
| 4   | M     | 198 | PRO  |
| 4   | M     | 381 | LEU  |
| 5   | N     | 2   | ARG  |
| 5   | N     | 35  | LYS  |
| 5   | N     | 47  | ASN  |
| 5   | N     | 61  | PRO  |
| 5   | N     | 65  | PRO  |
| 3   | U     | 164 | VAL  |
| 3   | U     | 285 | VAL  |
| 3   | U     | 516 | VAL  |
| 4   | V     | 314 | ARG  |
| 4   | V     | 381 | LEU  |
| 5   | W     | 33  | ARG  |
| 5   | W     | 188 | SER  |
| 6   | X     | 156 | LYS  |
| 3   | 3     | 285 | VAL  |
| 3   | 3     | 303 | GLN  |
| 3   | 3     | 453 | PRO  |
| 3   | 3     | 563 | ALA  |
| 4   | 4     | 211 | SER  |
| 5   | 5     | 35  | LYS  |
| 1   | A     | 166 | ASP  |
| 2   | B     | 116 | LEU  |
| 3   | C     | 203 | ILE  |
| 3   | C     | 285 | VAL  |
| 3   | C     | 453 | PRO  |
| 3   | C     | 471 | GLY  |
| 4   | D     | 211 | SER  |
| 6   | F     | 156 | LYS  |
| 3   | L     | 164 | VAL  |
| 3   | L     | 203 | ILE  |
| 3   | L     | 303 | GLN  |
| 4   | M     | 106 | GLY  |
| 1   | S     | 166 | ASP  |
| 3   | U     | 453 | PRO  |
| 4   | V     | 237 | GLY  |
| 5   | W     | 35  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | W     | 65  | PRO  |
| 1   | 1     | 204 | PRO  |
| 3   | 3     | 203 | ILE  |
| 4   | 4     | 270 | GLY  |
| 6   | 6     | 77  | VAL  |
| 3   | C     | 549 | VAL  |
| 3   | C     | 765 | PRO  |
| 6   | F     | 77  | VAL  |
| 6   | O     | 77  | VAL  |
| 1   | S     | 204 | PRO  |
| 3   | U     | 203 | ILE  |
| 3   | U     | 471 | GLY  |
| 6   | X     | 77  | VAL  |
| 3   | 3     | 471 | GLY  |
| 3   | 3     | 549 | VAL  |
| 4   | 4     | 106 | GLY  |
| 1   | A     | 204 | PRO  |
| 4   | D     | 237 | GLY  |
| 4   | D     | 270 | GLY  |
| 6   | F     | 100 | PRO  |
| 3   | L     | 471 | GLY  |
| 3   | L     | 549 | VAL  |
| 4   | M     | 211 | SER  |
| 4   | M     | 270 | GLY  |
| 3   | U     | 549 | VAL  |
| 3   | U     | 765 | PRO  |
| 4   | V     | 211 | SER  |
| 4   | V     | 270 | GLY  |
| 3   | 3     | 626 | PRO  |
| 3   | 3     | 765 | PRO  |
| 7   | 9     | 81  | VAL  |
| 3   | C     | 470 | PRO  |
| 1   | J     | 204 | PRO  |
| 3   | L     | 219 | PRO  |
| 3   | L     | 765 | PRO  |
| 5   | N     | 99  | PRO  |
| 6   | 6     | 100 | PRO  |
| 3   | C     | 626 | PRO  |
| 4   | D     | 106 | GLY  |
| 3   | L     | 626 | PRO  |
| 4   | V     | 106 | GLY  |
| 7   | Y     | 81  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 177 | GLY  |
| 7   | G     | 81  | VAL  |
| 7   | P     | 81  | VAL  |
| 3   | U     | 219 | PRO  |
| 6   | X     | 100 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | 1     | 355/356 (100%) | 318 (90%) | 37 (10%) | 7           | 24 |
| 1   | A     | 355/356 (100%) | 320 (90%) | 35 (10%) | 7           | 27 |
| 1   | J     | 355/356 (100%) | 316 (89%) | 39 (11%) | 6           | 23 |
| 1   | S     | 355/356 (100%) | 318 (90%) | 37 (10%) | 7           | 24 |
| 2   | 2     | 150/152 (99%)  | 131 (87%) | 19 (13%) | 4           | 18 |
| 2   | B     | 150/152 (99%)  | 131 (87%) | 19 (13%) | 4           | 18 |
| 2   | K     | 150/152 (99%)  | 131 (87%) | 19 (13%) | 4           | 18 |
| 2   | T     | 150/152 (99%)  | 133 (89%) | 17 (11%) | 5           | 21 |
| 3   | 3     | 607/628 (97%)  | 541 (89%) | 66 (11%) | 6           | 23 |
| 3   | C     | 607/628 (97%)  | 541 (89%) | 66 (11%) | 6           | 23 |
| 3   | L     | 607/628 (97%)  | 538 (89%) | 69 (11%) | 5           | 21 |
| 3   | U     | 607/628 (97%)  | 541 (89%) | 66 (11%) | 6           | 23 |
| 4   | 4     | 325/355 (92%)  | 288 (89%) | 37 (11%) | 5           | 21 |
| 4   | D     | 325/355 (92%)  | 288 (89%) | 37 (11%) | 5           | 21 |
| 4   | M     | 325/355 (92%)  | 288 (89%) | 37 (11%) | 5           | 21 |
| 4   | V     | 325/355 (92%)  | 288 (89%) | 37 (11%) | 5           | 21 |
| 5   | 5     | 167/175 (95%)  | 147 (88%) | 20 (12%) | 5           | 20 |
| 5   | E     | 167/175 (95%)  | 146 (87%) | 21 (13%) | 4           | 18 |
| 5   | N     | 167/175 (95%)  | 147 (88%) | 20 (12%) | 5           | 20 |
| 5   | W     | 167/175 (95%)  | 147 (88%) | 20 (12%) | 5           | 20 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 6   | 6     | 118/149 (79%)   | 103 (87%)  | 15 (13%)  | 4           | 18 |
| 6   | F     | 118/149 (79%)   | 102 (86%)  | 16 (14%)  | 3           | 16 |
| 6   | O     | 118/149 (79%)   | 103 (87%)  | 15 (13%)  | 4           | 18 |
| 6   | X     | 118/149 (79%)   | 101 (86%)  | 17 (14%)  | 3           | 14 |
| 7   | 9     | 126/150 (84%)   | 111 (88%)  | 15 (12%)  | 5           | 20 |
| 7   | G     | 126/150 (84%)   | 112 (89%)  | 14 (11%)  | 6           | 22 |
| 7   | P     | 126/150 (84%)   | 111 (88%)  | 15 (12%)  | 5           | 20 |
| 7   | Y     | 126/150 (84%)   | 112 (89%)  | 14 (11%)  | 6           | 22 |
| 8   | 7     | 104/106 (98%)   | 96 (92%)   | 8 (8%)    | 12          | 37 |
| 8   | H     | 104/106 (98%)   | 96 (92%)   | 8 (8%)    | 12          | 37 |
| 8   | Q     | 104/106 (98%)   | 96 (92%)   | 8 (8%)    | 12          | 37 |
| 8   | Z     | 104/106 (98%)   | 97 (93%)   | 7 (7%)    | 15          | 42 |
| All | All   | 7808/8284 (94%) | 6938 (89%) | 870 (11%) | 6           | 22 |

All (870) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 10  | ASP  |
| 1   | 1     | 28  | THR  |
| 1   | 1     | 29  | LEU  |
| 1   | 1     | 39  | GLU  |
| 1   | 1     | 49  | THR  |
| 1   | 1     | 104 | ARG  |
| 1   | 1     | 114 | LEU  |
| 1   | 1     | 128 | THR  |
| 1   | 1     | 129 | VAL  |
| 1   | 1     | 155 | ARG  |
| 1   | 1     | 161 | ASN  |
| 1   | 1     | 168 | SER  |
| 1   | 1     | 184 | GLU  |
| 1   | 1     | 186 | THR  |
| 1   | 1     | 217 | THR  |
| 1   | 1     | 228 | VAL  |
| 1   | 1     | 243 | THR  |
| 1   | 1     | 249 | MET  |
| 1   | 1     | 253 | GLN  |
| 1   | 1     | 254 | ILE  |
| 1   | 1     | 255 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 270 | THR  |
| 1   | 1     | 271 | THR  |
| 1   | 1     | 284 | LEU  |
| 1   | 1     | 295 | SER  |
| 1   | 1     | 303 | THR  |
| 1   | 1     | 342 | TRP  |
| 1   | 1     | 346 | ARG  |
| 1   | 1     | 363 | VAL  |
| 1   | 1     | 368 | VAL  |
| 1   | 1     | 370 | LEU  |
| 1   | 1     | 374 | ILE  |
| 1   | 1     | 397 | ARG  |
| 1   | 1     | 414 | LEU  |
| 1   | 1     | 419 | ASP  |
| 1   | 1     | 437 | TRP  |
| 1   | 1     | 438 | ARG  |
| 2   | 2     | 5   | ASP  |
| 2   | 2     | 7   | LYS  |
| 2   | 2     | 31  | LEU  |
| 2   | 2     | 35  | GLN  |
| 2   | 2     | 45  | ARG  |
| 2   | 2     | 46  | ILE  |
| 2   | 2     | 53  | VAL  |
| 2   | 2     | 61  | MET  |
| 2   | 2     | 106 | ILE  |
| 2   | 2     | 114 | ASP  |
| 2   | 2     | 122 | VAL  |
| 2   | 2     | 139 | GLU  |
| 2   | 2     | 140 | PRO  |
| 2   | 2     | 146 | THR  |
| 2   | 2     | 150 | LEU  |
| 2   | 2     | 153 | LEU  |
| 2   | 2     | 163 | LEU  |
| 2   | 2     | 172 | CYS  |
| 2   | 2     | 176 | VAL  |
| 3   | 3     | 11  | VAL  |
| 3   | 3     | 32  | LEU  |
| 3   | 3     | 42  | ILE  |
| 3   | 3     | 46  | ARG  |
| 3   | 3     | 73  | ILE  |
| 3   | 3     | 85  | THR  |
| 3   | 3     | 89  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 94  | ASP  |
| 3   | 3     | 95  | THR  |
| 3   | 3     | 97  | SER  |
| 3   | 3     | 99  | VAL  |
| 3   | 3     | 109 | GLU  |
| 3   | 3     | 121 | THR  |
| 3   | 3     | 124 | LYS  |
| 3   | 3     | 133 | ARG  |
| 3   | 3     | 135 | VAL  |
| 3   | 3     | 188 | VAL  |
| 3   | 3     | 192 | GLU  |
| 3   | 3     | 207 | VAL  |
| 3   | 3     | 209 | THR  |
| 3   | 3     | 218 | LEU  |
| 3   | 3     | 239 | THR  |
| 3   | 3     | 269 | THR  |
| 3   | 3     | 284 | GLU  |
| 3   | 3     | 286 | ASN  |
| 3   | 3     | 317 | LEU  |
| 3   | 3     | 321 | THR  |
| 3   | 3     | 334 | LYS  |
| 3   | 3     | 337 | ARG  |
| 3   | 3     | 368 | HIS  |
| 3   | 3     | 369 | LEU  |
| 3   | 3     | 381 | LEU  |
| 3   | 3     | 382 | PHE  |
| 3   | 3     | 387 | LEU  |
| 3   | 3     | 408 | ILE  |
| 3   | 3     | 440 | ARG  |
| 3   | 3     | 445 | THR  |
| 3   | 3     | 450 | LEU  |
| 3   | 3     | 459 | MET  |
| 3   | 3     | 460 | LYS  |
| 3   | 3     | 464 | ILE  |
| 3   | 3     | 473 | GLU  |
| 3   | 3     | 501 | LYS  |
| 3   | 3     | 507 | LEU  |
| 3   | 3     | 512 | LEU  |
| 3   | 3     | 514 | ASP  |
| 3   | 3     | 515 | THR  |
| 3   | 3     | 523 | LEU  |
| 3   | 3     | 542 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 577 | LEU  |
| 3   | 3     | 578 | LYS  |
| 3   | 3     | 593 | LEU  |
| 3   | 3     | 617 | LEU  |
| 3   | 3     | 625 | SER  |
| 3   | 3     | 644 | LEU  |
| 3   | 3     | 655 | ARG  |
| 3   | 3     | 676 | LEU  |
| 3   | 3     | 683 | LEU  |
| 3   | 3     | 684 | ARG  |
| 3   | 3     | 705 | VAL  |
| 3   | 3     | 715 | GLU  |
| 3   | 3     | 716 | LEU  |
| 3   | 3     | 738 | THR  |
| 3   | 3     | 761 | SER  |
| 3   | 3     | 771 | VAL  |
| 3   | 3     | 776 | LEU  |
| 4   | 4     | 40  | VAL  |
| 4   | 4     | 44  | MET  |
| 4   | 4     | 48  | SER  |
| 4   | 4     | 59  | ILE  |
| 4   | 4     | 69  | THR  |
| 4   | 4     | 99  | LEU  |
| 4   | 4     | 101 | VAL  |
| 4   | 4     | 109 | VAL  |
| 4   | 4     | 116 | ILE  |
| 4   | 4     | 118 | VAL  |
| 4   | 4     | 120 | LEU  |
| 4   | 4     | 129 | HIS  |
| 4   | 4     | 133 | LEU  |
| 4   | 4     | 143 | LEU  |
| 4   | 4     | 152 | GLU  |
| 4   | 4     | 163 | VAL  |
| 4   | 4     | 168 | PHE  |
| 4   | 4     | 170 | HIS  |
| 4   | 4     | 182 | LEU  |
| 4   | 4     | 200 | ARG  |
| 4   | 4     | 201 | ILE  |
| 4   | 4     | 213 | ILE  |
| 4   | 4     | 221 | VAL  |
| 4   | 4     | 234 | LEU  |
| 4   | 4     | 239 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 262 | PHE  |
| 4   | 4     | 272 | VAL  |
| 4   | 4     | 296 | ARG  |
| 4   | 4     | 303 | ARG  |
| 4   | 4     | 309 | ILE  |
| 4   | 4     | 310 | THR  |
| 4   | 4     | 314 | ARG  |
| 4   | 4     | 319 | THR  |
| 4   | 4     | 333 | GLU  |
| 4   | 4     | 371 | ARG  |
| 4   | 4     | 380 | SER  |
| 4   | 4     | 407 | VAL  |
| 5   | 5     | 1   | MET  |
| 5   | 5     | 5   | ARG  |
| 5   | 5     | 25  | LEU  |
| 5   | 5     | 27  | VAL  |
| 5   | 5     | 38  | MET  |
| 5   | 5     | 51  | ASP  |
| 5   | 5     | 52  | ILE  |
| 5   | 5     | 53  | VAL  |
| 5   | 5     | 66  | GLU  |
| 5   | 5     | 80  | TRP  |
| 5   | 5     | 81  | LYS  |
| 5   | 5     | 84  | ASP  |
| 5   | 5     | 90  | VAL  |
| 5   | 5     | 105 | THR  |
| 5   | 5     | 124 | ILE  |
| 5   | 5     | 135 | ILE  |
| 5   | 5     | 142 | GLU  |
| 5   | 5     | 146 | LEU  |
| 5   | 5     | 175 | THR  |
| 5   | 5     | 193 | ARG  |
| 6   | 6     | 19  | ILE  |
| 6   | 6     | 27  | LEU  |
| 6   | 6     | 40  | THR  |
| 6   | 6     | 45  | CYS  |
| 6   | 6     | 53  | SER  |
| 6   | 6     | 57  | ARG  |
| 6   | 6     | 74  | GLN  |
| 6   | 6     | 83  | ARG  |
| 6   | 6     | 84  | LEU  |
| 6   | 6     | 121 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 6     | 124 | VAL  |
| 6   | 6     | 131 | VAL  |
| 6   | 6     | 147 | LEU  |
| 6   | 6     | 153 | GLN  |
| 6   | 6     | 163 | TYR  |
| 7   | 9     | 26  | TYR  |
| 7   | 9     | 33  | LEU  |
| 7   | 9     | 36  | ARG  |
| 7   | 9     | 42  | VAL  |
| 7   | 9     | 58  | LEU  |
| 7   | 9     | 85  | GLU  |
| 7   | 9     | 97  | ARG  |
| 7   | 9     | 99  | ILE  |
| 7   | 9     | 101 | CYS  |
| 7   | 9     | 134 | GLU  |
| 7   | 9     | 137 | LEU  |
| 7   | 9     | 140 | VAL  |
| 7   | 9     | 153 | THR  |
| 7   | 9     | 157 | VAL  |
| 7   | 9     | 159 | VAL  |
| 8   | 7     | 34  | GLU  |
| 8   | 7     | 43  | ARG  |
| 8   | 7     | 52  | THR  |
| 8   | 7     | 53  | THR  |
| 8   | 7     | 54  | ILE  |
| 8   | 7     | 63  | LEU  |
| 8   | 7     | 73  | SER  |
| 8   | 7     | 82  | ILE  |
| 1   | A     | 10  | ASP  |
| 1   | A     | 28  | THR  |
| 1   | A     | 29  | LEU  |
| 1   | A     | 39  | GLU  |
| 1   | A     | 49  | THR  |
| 1   | A     | 96  | SER  |
| 1   | A     | 104 | ARG  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 128 | THR  |
| 1   | A     | 129 | VAL  |
| 1   | A     | 155 | ARG  |
| 1   | A     | 161 | ASN  |
| 1   | A     | 168 | SER  |
| 1   | A     | 184 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 211 | LEU  |
| 1   | A     | 217 | THR  |
| 1   | A     | 243 | THR  |
| 1   | A     | 249 | MET  |
| 1   | A     | 253 | GLN  |
| 1   | A     | 254 | ILE  |
| 1   | A     | 255 | SER  |
| 1   | A     | 270 | THR  |
| 1   | A     | 271 | THR  |
| 1   | A     | 295 | SER  |
| 1   | A     | 303 | THR  |
| 1   | A     | 342 | TRP  |
| 1   | A     | 346 | ARG  |
| 1   | A     | 363 | VAL  |
| 1   | A     | 368 | VAL  |
| 1   | A     | 374 | ILE  |
| 1   | A     | 397 | ARG  |
| 1   | A     | 414 | LEU  |
| 1   | A     | 419 | ASP  |
| 1   | A     | 437 | TRP  |
| 1   | A     | 438 | ARG  |
| 2   | B     | 5   | ASP  |
| 2   | B     | 7   | LYS  |
| 2   | B     | 31  | LEU  |
| 2   | B     | 35  | GLN  |
| 2   | B     | 45  | ARG  |
| 2   | B     | 46  | ILE  |
| 2   | B     | 53  | VAL  |
| 2   | B     | 61  | MET  |
| 2   | B     | 106 | ILE  |
| 2   | B     | 114 | ASP  |
| 2   | B     | 122 | VAL  |
| 2   | B     | 139 | GLU  |
| 2   | B     | 140 | PRO  |
| 2   | B     | 146 | THR  |
| 2   | B     | 150 | LEU  |
| 2   | B     | 153 | LEU  |
| 2   | B     | 163 | LEU  |
| 2   | B     | 172 | CYS  |
| 2   | B     | 176 | VAL  |
| 3   | C     | 11  | VAL  |
| 3   | C     | 32  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 42  | ILE  |
| 3   | C     | 46  | ARG  |
| 3   | C     | 73  | ILE  |
| 3   | C     | 85  | THR  |
| 3   | C     | 89  | ASP  |
| 3   | C     | 94  | ASP  |
| 3   | C     | 95  | THR  |
| 3   | C     | 97  | SER  |
| 3   | C     | 99  | VAL  |
| 3   | C     | 109 | GLU  |
| 3   | C     | 121 | THR  |
| 3   | C     | 124 | LYS  |
| 3   | C     | 133 | ARG  |
| 3   | C     | 135 | VAL  |
| 3   | C     | 188 | VAL  |
| 3   | C     | 192 | GLU  |
| 3   | C     | 203 | ILE  |
| 3   | C     | 207 | VAL  |
| 3   | C     | 209 | THR  |
| 3   | C     | 218 | LEU  |
| 3   | C     | 239 | THR  |
| 3   | C     | 269 | THR  |
| 3   | C     | 274 | LEU  |
| 3   | C     | 284 | GLU  |
| 3   | C     | 286 | ASN  |
| 3   | C     | 317 | LEU  |
| 3   | C     | 321 | THR  |
| 3   | C     | 334 | LYS  |
| 3   | C     | 337 | ARG  |
| 3   | C     | 368 | HIS  |
| 3   | C     | 369 | LEU  |
| 3   | C     | 381 | LEU  |
| 3   | C     | 382 | PHE  |
| 3   | C     | 387 | LEU  |
| 3   | C     | 408 | ILE  |
| 3   | C     | 440 | ARG  |
| 3   | C     | 445 | THR  |
| 3   | C     | 450 | LEU  |
| 3   | C     | 459 | MET  |
| 3   | C     | 464 | ILE  |
| 3   | C     | 473 | GLU  |
| 3   | C     | 501 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 512 | LEU  |
| 3   | C     | 514 | ASP  |
| 3   | C     | 523 | LEU  |
| 3   | C     | 542 | ARG  |
| 3   | C     | 577 | LEU  |
| 3   | C     | 578 | LYS  |
| 3   | C     | 593 | LEU  |
| 3   | C     | 617 | LEU  |
| 3   | C     | 625 | SER  |
| 3   | C     | 644 | LEU  |
| 3   | C     | 655 | ARG  |
| 3   | C     | 671 | GLU  |
| 3   | C     | 676 | LEU  |
| 3   | C     | 683 | LEU  |
| 3   | C     | 684 | ARG  |
| 3   | C     | 705 | VAL  |
| 3   | C     | 715 | GLU  |
| 3   | C     | 716 | LEU  |
| 3   | C     | 738 | THR  |
| 3   | C     | 761 | SER  |
| 3   | C     | 771 | VAL  |
| 3   | C     | 776 | LEU  |
| 4   | D     | 40  | VAL  |
| 4   | D     | 44  | MET  |
| 4   | D     | 48  | SER  |
| 4   | D     | 59  | ILE  |
| 4   | D     | 69  | THR  |
| 4   | D     | 99  | LEU  |
| 4   | D     | 101 | VAL  |
| 4   | D     | 109 | VAL  |
| 4   | D     | 116 | ILE  |
| 4   | D     | 118 | VAL  |
| 4   | D     | 120 | LEU  |
| 4   | D     | 129 | HIS  |
| 4   | D     | 133 | LEU  |
| 4   | D     | 143 | LEU  |
| 4   | D     | 152 | GLU  |
| 4   | D     | 163 | VAL  |
| 4   | D     | 168 | PHE  |
| 4   | D     | 170 | HIS  |
| 4   | D     | 182 | LEU  |
| 4   | D     | 200 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 201 | ILE  |
| 4   | D     | 213 | ILE  |
| 4   | D     | 221 | VAL  |
| 4   | D     | 234 | LEU  |
| 4   | D     | 239 | LEU  |
| 4   | D     | 262 | PHE  |
| 4   | D     | 272 | VAL  |
| 4   | D     | 296 | ARG  |
| 4   | D     | 303 | ARG  |
| 4   | D     | 309 | ILE  |
| 4   | D     | 310 | THR  |
| 4   | D     | 314 | ARG  |
| 4   | D     | 319 | THR  |
| 4   | D     | 333 | GLU  |
| 4   | D     | 371 | ARG  |
| 4   | D     | 380 | SER  |
| 4   | D     | 407 | VAL  |
| 5   | E     | 1   | MET  |
| 5   | E     | 5   | ARG  |
| 5   | E     | 25  | LEU  |
| 5   | E     | 27  | VAL  |
| 5   | E     | 38  | MET  |
| 5   | E     | 51  | ASP  |
| 5   | E     | 52  | ILE  |
| 5   | E     | 53  | VAL  |
| 5   | E     | 66  | GLU  |
| 5   | E     | 80  | TRP  |
| 5   | E     | 81  | LYS  |
| 5   | E     | 84  | ASP  |
| 5   | E     | 90  | VAL  |
| 5   | E     | 105 | THR  |
| 5   | E     | 124 | ILE  |
| 5   | E     | 135 | ILE  |
| 5   | E     | 142 | GLU  |
| 5   | E     | 146 | LEU  |
| 5   | E     | 161 | GLU  |
| 5   | E     | 175 | THR  |
| 5   | E     | 193 | ARG  |
| 6   | F     | 19  | ILE  |
| 6   | F     | 27  | LEU  |
| 6   | F     | 40  | THR  |
| 6   | F     | 45  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 53  | SER  |
| 6   | F     | 57  | ARG  |
| 6   | F     | 74  | GLN  |
| 6   | F     | 78  | MET  |
| 6   | F     | 83  | ARG  |
| 6   | F     | 84  | LEU  |
| 6   | F     | 121 | TYR  |
| 6   | F     | 124 | VAL  |
| 6   | F     | 131 | VAL  |
| 6   | F     | 147 | LEU  |
| 6   | F     | 153 | GLN  |
| 6   | F     | 163 | TYR  |
| 7   | G     | 26  | TYR  |
| 7   | G     | 33  | LEU  |
| 7   | G     | 36  | ARG  |
| 7   | G     | 42  | VAL  |
| 7   | G     | 58  | LEU  |
| 7   | G     | 85  | GLU  |
| 7   | G     | 97  | ARG  |
| 7   | G     | 99  | ILE  |
| 7   | G     | 101 | CYS  |
| 7   | G     | 134 | GLU  |
| 7   | G     | 140 | VAL  |
| 7   | G     | 153 | THR  |
| 7   | G     | 157 | VAL  |
| 7   | G     | 159 | VAL  |
| 8   | H     | 34  | GLU  |
| 8   | H     | 43  | ARG  |
| 8   | H     | 52  | THR  |
| 8   | H     | 53  | THR  |
| 8   | H     | 54  | ILE  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 73  | SER  |
| 8   | H     | 82  | ILE  |
| 1   | J     | 10  | ASP  |
| 1   | J     | 28  | THR  |
| 1   | J     | 29  | LEU  |
| 1   | J     | 39  | GLU  |
| 1   | J     | 49  | THR  |
| 1   | J     | 104 | ARG  |
| 1   | J     | 106 | ILE  |
| 1   | J     | 114 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 128 | THR  |
| 1   | J     | 129 | VAL  |
| 1   | J     | 155 | ARG  |
| 1   | J     | 161 | ASN  |
| 1   | J     | 168 | SER  |
| 1   | J     | 184 | GLU  |
| 1   | J     | 203 | PRO  |
| 1   | J     | 211 | LEU  |
| 1   | J     | 217 | THR  |
| 1   | J     | 233 | ARG  |
| 1   | J     | 243 | THR  |
| 1   | J     | 249 | MET  |
| 1   | J     | 253 | GLN  |
| 1   | J     | 254 | ILE  |
| 1   | J     | 255 | SER  |
| 1   | J     | 270 | THR  |
| 1   | J     | 271 | THR  |
| 1   | J     | 291 | ILE  |
| 1   | J     | 295 | SER  |
| 1   | J     | 303 | THR  |
| 1   | J     | 342 | TRP  |
| 1   | J     | 346 | ARG  |
| 1   | J     | 363 | VAL  |
| 1   | J     | 368 | VAL  |
| 1   | J     | 370 | LEU  |
| 1   | J     | 374 | ILE  |
| 1   | J     | 397 | ARG  |
| 1   | J     | 414 | LEU  |
| 1   | J     | 419 | ASP  |
| 1   | J     | 437 | TRP  |
| 1   | J     | 438 | ARG  |
| 2   | K     | 5   | ASP  |
| 2   | K     | 7   | LYS  |
| 2   | K     | 31  | LEU  |
| 2   | K     | 35  | GLN  |
| 2   | K     | 45  | ARG  |
| 2   | K     | 46  | ILE  |
| 2   | K     | 53  | VAL  |
| 2   | K     | 61  | MET  |
| 2   | K     | 106 | ILE  |
| 2   | K     | 114 | ASP  |
| 2   | K     | 122 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 139 | GLU  |
| 2   | K     | 140 | PRO  |
| 2   | K     | 146 | THR  |
| 2   | K     | 150 | LEU  |
| 2   | K     | 153 | LEU  |
| 2   | K     | 163 | LEU  |
| 2   | K     | 172 | CYS  |
| 2   | K     | 176 | VAL  |
| 3   | L     | 11  | VAL  |
| 3   | L     | 32  | LEU  |
| 3   | L     | 42  | ILE  |
| 3   | L     | 46  | ARG  |
| 3   | L     | 73  | ILE  |
| 3   | L     | 85  | THR  |
| 3   | L     | 89  | ASP  |
| 3   | L     | 94  | ASP  |
| 3   | L     | 95  | THR  |
| 3   | L     | 97  | SER  |
| 3   | L     | 99  | VAL  |
| 3   | L     | 109 | GLU  |
| 3   | L     | 121 | THR  |
| 3   | L     | 124 | LYS  |
| 3   | L     | 133 | ARG  |
| 3   | L     | 135 | VAL  |
| 3   | L     | 188 | VAL  |
| 3   | L     | 192 | GLU  |
| 3   | L     | 203 | ILE  |
| 3   | L     | 207 | VAL  |
| 3   | L     | 209 | THR  |
| 3   | L     | 218 | LEU  |
| 3   | L     | 229 | ILE  |
| 3   | L     | 239 | THR  |
| 3   | L     | 269 | THR  |
| 3   | L     | 274 | LEU  |
| 3   | L     | 284 | GLU  |
| 3   | L     | 286 | ASN  |
| 3   | L     | 317 | LEU  |
| 3   | L     | 321 | THR  |
| 3   | L     | 334 | LYS  |
| 3   | L     | 337 | ARG  |
| 3   | L     | 368 | HIS  |
| 3   | L     | 369 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L     | 381 | LEU  |
| 3   | L     | 382 | PHE  |
| 3   | L     | 387 | LEU  |
| 3   | L     | 408 | ILE  |
| 3   | L     | 440 | ARG  |
| 3   | L     | 445 | THR  |
| 3   | L     | 450 | LEU  |
| 3   | L     | 459 | MET  |
| 3   | L     | 460 | LYS  |
| 3   | L     | 464 | ILE  |
| 3   | L     | 473 | GLU  |
| 3   | L     | 501 | LYS  |
| 3   | L     | 512 | LEU  |
| 3   | L     | 514 | ASP  |
| 3   | L     | 515 | THR  |
| 3   | L     | 523 | LEU  |
| 3   | L     | 542 | ARG  |
| 3   | L     | 577 | LEU  |
| 3   | L     | 578 | LYS  |
| 3   | L     | 593 | LEU  |
| 3   | L     | 617 | LEU  |
| 3   | L     | 625 | SER  |
| 3   | L     | 644 | LEU  |
| 3   | L     | 655 | ARG  |
| 3   | L     | 671 | GLU  |
| 3   | L     | 676 | LEU  |
| 3   | L     | 683 | LEU  |
| 3   | L     | 684 | ARG  |
| 3   | L     | 705 | VAL  |
| 3   | L     | 715 | GLU  |
| 3   | L     | 716 | LEU  |
| 3   | L     | 738 | THR  |
| 3   | L     | 761 | SER  |
| 3   | L     | 771 | VAL  |
| 3   | L     | 776 | LEU  |
| 4   | M     | 40  | VAL  |
| 4   | M     | 44  | MET  |
| 4   | M     | 48  | SER  |
| 4   | M     | 59  | ILE  |
| 4   | M     | 69  | THR  |
| 4   | M     | 99  | LEU  |
| 4   | M     | 101 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | M     | 109 | VAL  |
| 4   | M     | 116 | ILE  |
| 4   | M     | 118 | VAL  |
| 4   | M     | 120 | LEU  |
| 4   | M     | 129 | HIS  |
| 4   | M     | 133 | LEU  |
| 4   | M     | 143 | LEU  |
| 4   | M     | 152 | GLU  |
| 4   | M     | 163 | VAL  |
| 4   | M     | 168 | PHE  |
| 4   | M     | 170 | HIS  |
| 4   | M     | 182 | LEU  |
| 4   | M     | 200 | ARG  |
| 4   | M     | 201 | ILE  |
| 4   | M     | 213 | ILE  |
| 4   | M     | 221 | VAL  |
| 4   | M     | 234 | LEU  |
| 4   | M     | 239 | LEU  |
| 4   | M     | 262 | PHE  |
| 4   | M     | 272 | VAL  |
| 4   | M     | 296 | ARG  |
| 4   | M     | 303 | ARG  |
| 4   | M     | 309 | ILE  |
| 4   | M     | 310 | THR  |
| 4   | M     | 314 | ARG  |
| 4   | M     | 319 | THR  |
| 4   | M     | 333 | GLU  |
| 4   | M     | 371 | ARG  |
| 4   | M     | 380 | SER  |
| 4   | M     | 407 | VAL  |
| 5   | N     | 1   | MET  |
| 5   | N     | 5   | ARG  |
| 5   | N     | 25  | LEU  |
| 5   | N     | 27  | VAL  |
| 5   | N     | 38  | MET  |
| 5   | N     | 51  | ASP  |
| 5   | N     | 52  | ILE  |
| 5   | N     | 53  | VAL  |
| 5   | N     | 66  | GLU  |
| 5   | N     | 80  | TRP  |
| 5   | N     | 81  | LYS  |
| 5   | N     | 84  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | N     | 90  | VAL  |
| 5   | N     | 105 | THR  |
| 5   | N     | 124 | ILE  |
| 5   | N     | 135 | ILE  |
| 5   | N     | 142 | GLU  |
| 5   | N     | 146 | LEU  |
| 5   | N     | 175 | THR  |
| 5   | N     | 193 | ARG  |
| 6   | O     | 19  | ILE  |
| 6   | O     | 27  | LEU  |
| 6   | O     | 40  | THR  |
| 6   | O     | 45  | CYS  |
| 6   | O     | 53  | SER  |
| 6   | O     | 57  | ARG  |
| 6   | O     | 74  | GLN  |
| 6   | O     | 83  | ARG  |
| 6   | O     | 84  | LEU  |
| 6   | O     | 121 | TYR  |
| 6   | O     | 124 | VAL  |
| 6   | O     | 131 | VAL  |
| 6   | O     | 147 | LEU  |
| 6   | O     | 153 | GLN  |
| 6   | O     | 163 | TYR  |
| 7   | P     | 26  | TYR  |
| 7   | P     | 33  | LEU  |
| 7   | P     | 36  | ARG  |
| 7   | P     | 42  | VAL  |
| 7   | P     | 58  | LEU  |
| 7   | P     | 85  | GLU  |
| 7   | P     | 97  | ARG  |
| 7   | P     | 99  | ILE  |
| 7   | P     | 101 | CYS  |
| 7   | P     | 134 | GLU  |
| 7   | P     | 137 | LEU  |
| 7   | P     | 140 | VAL  |
| 7   | P     | 153 | THR  |
| 7   | P     | 157 | VAL  |
| 7   | P     | 159 | VAL  |
| 8   | Q     | 34  | GLU  |
| 8   | Q     | 43  | ARG  |
| 8   | Q     | 52  | THR  |
| 8   | Q     | 53  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | Q     | 54  | ILE  |
| 8   | Q     | 63  | LEU  |
| 8   | Q     | 73  | SER  |
| 8   | Q     | 82  | ILE  |
| 1   | S     | 10  | ASP  |
| 1   | S     | 28  | THR  |
| 1   | S     | 29  | LEU  |
| 1   | S     | 39  | GLU  |
| 1   | S     | 49  | THR  |
| 1   | S     | 96  | SER  |
| 1   | S     | 104 | ARG  |
| 1   | S     | 106 | ILE  |
| 1   | S     | 114 | LEU  |
| 1   | S     | 128 | THR  |
| 1   | S     | 129 | VAL  |
| 1   | S     | 155 | ARG  |
| 1   | S     | 161 | ASN  |
| 1   | S     | 168 | SER  |
| 1   | S     | 184 | GLU  |
| 1   | S     | 186 | THR  |
| 1   | S     | 203 | PRO  |
| 1   | S     | 211 | LEU  |
| 1   | S     | 217 | THR  |
| 1   | S     | 249 | MET  |
| 1   | S     | 253 | GLN  |
| 1   | S     | 254 | ILE  |
| 1   | S     | 255 | SER  |
| 1   | S     | 270 | THR  |
| 1   | S     | 271 | THR  |
| 1   | S     | 295 | SER  |
| 1   | S     | 303 | THR  |
| 1   | S     | 342 | TRP  |
| 1   | S     | 346 | ARG  |
| 1   | S     | 363 | VAL  |
| 1   | S     | 368 | VAL  |
| 1   | S     | 370 | LEU  |
| 1   | S     | 374 | ILE  |
| 1   | S     | 397 | ARG  |
| 1   | S     | 414 | LEU  |
| 1   | S     | 419 | ASP  |
| 1   | S     | 438 | ARG  |
| 2   | T     | 5   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | T     | 7   | LYS  |
| 2   | T     | 31  | LEU  |
| 2   | T     | 35  | GLN  |
| 2   | T     | 45  | ARG  |
| 2   | T     | 53  | VAL  |
| 2   | T     | 61  | MET  |
| 2   | T     | 106 | ILE  |
| 2   | T     | 114 | ASP  |
| 2   | T     | 122 | VAL  |
| 2   | T     | 139 | GLU  |
| 2   | T     | 146 | THR  |
| 2   | T     | 150 | LEU  |
| 2   | T     | 153 | LEU  |
| 2   | T     | 163 | LEU  |
| 2   | T     | 172 | CYS  |
| 2   | T     | 176 | VAL  |
| 3   | U     | 11  | VAL  |
| 3   | U     | 32  | LEU  |
| 3   | U     | 42  | ILE  |
| 3   | U     | 46  | ARG  |
| 3   | U     | 73  | ILE  |
| 3   | U     | 85  | THR  |
| 3   | U     | 89  | ASP  |
| 3   | U     | 94  | ASP  |
| 3   | U     | 95  | THR  |
| 3   | U     | 97  | SER  |
| 3   | U     | 99  | VAL  |
| 3   | U     | 109 | GLU  |
| 3   | U     | 121 | THR  |
| 3   | U     | 124 | LYS  |
| 3   | U     | 133 | ARG  |
| 3   | U     | 135 | VAL  |
| 3   | U     | 188 | VAL  |
| 3   | U     | 192 | GLU  |
| 3   | U     | 207 | VAL  |
| 3   | U     | 209 | THR  |
| 3   | U     | 218 | LEU  |
| 3   | U     | 239 | THR  |
| 3   | U     | 269 | THR  |
| 3   | U     | 274 | LEU  |
| 3   | U     | 284 | GLU  |
| 3   | U     | 286 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | U     | 317 | LEU  |
| 3   | U     | 321 | THR  |
| 3   | U     | 334 | LYS  |
| 3   | U     | 337 | ARG  |
| 3   | U     | 368 | HIS  |
| 3   | U     | 369 | LEU  |
| 3   | U     | 381 | LEU  |
| 3   | U     | 382 | PHE  |
| 3   | U     | 387 | LEU  |
| 3   | U     | 408 | ILE  |
| 3   | U     | 440 | ARG  |
| 3   | U     | 445 | THR  |
| 3   | U     | 450 | LEU  |
| 3   | U     | 459 | MET  |
| 3   | U     | 460 | LYS  |
| 3   | U     | 464 | ILE  |
| 3   | U     | 473 | GLU  |
| 3   | U     | 501 | LYS  |
| 3   | U     | 512 | LEU  |
| 3   | U     | 514 | ASP  |
| 3   | U     | 515 | THR  |
| 3   | U     | 523 | LEU  |
| 3   | U     | 542 | ARG  |
| 3   | U     | 578 | LYS  |
| 3   | U     | 593 | LEU  |
| 3   | U     | 617 | LEU  |
| 3   | U     | 625 | SER  |
| 3   | U     | 644 | LEU  |
| 3   | U     | 655 | ARG  |
| 3   | U     | 676 | LEU  |
| 3   | U     | 683 | LEU  |
| 3   | U     | 684 | ARG  |
| 3   | U     | 705 | VAL  |
| 3   | U     | 715 | GLU  |
| 3   | U     | 716 | LEU  |
| 3   | U     | 738 | THR  |
| 3   | U     | 743 | VAL  |
| 3   | U     | 761 | SER  |
| 3   | U     | 771 | VAL  |
| 3   | U     | 776 | LEU  |
| 4   | V     | 40  | VAL  |
| 4   | V     | 44  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | V     | 48  | SER  |
| 4   | V     | 59  | ILE  |
| 4   | V     | 69  | THR  |
| 4   | V     | 99  | LEU  |
| 4   | V     | 101 | VAL  |
| 4   | V     | 109 | VAL  |
| 4   | V     | 116 | ILE  |
| 4   | V     | 118 | VAL  |
| 4   | V     | 120 | LEU  |
| 4   | V     | 129 | HIS  |
| 4   | V     | 133 | LEU  |
| 4   | V     | 143 | LEU  |
| 4   | V     | 152 | GLU  |
| 4   | V     | 163 | VAL  |
| 4   | V     | 168 | PHE  |
| 4   | V     | 170 | HIS  |
| 4   | V     | 182 | LEU  |
| 4   | V     | 200 | ARG  |
| 4   | V     | 201 | ILE  |
| 4   | V     | 213 | ILE  |
| 4   | V     | 221 | VAL  |
| 4   | V     | 234 | LEU  |
| 4   | V     | 239 | LEU  |
| 4   | V     | 262 | PHE  |
| 4   | V     | 272 | VAL  |
| 4   | V     | 296 | ARG  |
| 4   | V     | 303 | ARG  |
| 4   | V     | 309 | ILE  |
| 4   | V     | 310 | THR  |
| 4   | V     | 314 | ARG  |
| 4   | V     | 319 | THR  |
| 4   | V     | 333 | GLU  |
| 4   | V     | 371 | ARG  |
| 4   | V     | 380 | SER  |
| 4   | V     | 407 | VAL  |
| 5   | W     | 1   | MET  |
| 5   | W     | 5   | ARG  |
| 5   | W     | 25  | LEU  |
| 5   | W     | 27  | VAL  |
| 5   | W     | 38  | MET  |
| 5   | W     | 51  | ASP  |
| 5   | W     | 52  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | W     | 53  | VAL  |
| 5   | W     | 66  | GLU  |
| 5   | W     | 80  | TRP  |
| 5   | W     | 81  | LYS  |
| 5   | W     | 84  | ASP  |
| 5   | W     | 90  | VAL  |
| 5   | W     | 105 | THR  |
| 5   | W     | 124 | ILE  |
| 5   | W     | 135 | ILE  |
| 5   | W     | 142 | GLU  |
| 5   | W     | 146 | LEU  |
| 5   | W     | 175 | THR  |
| 5   | W     | 193 | ARG  |
| 6   | X     | 19  | ILE  |
| 6   | X     | 27  | LEU  |
| 6   | X     | 40  | THR  |
| 6   | X     | 45  | CYS  |
| 6   | X     | 53  | SER  |
| 6   | X     | 57  | ARG  |
| 6   | X     | 74  | GLN  |
| 6   | X     | 78  | MET  |
| 6   | X     | 83  | ARG  |
| 6   | X     | 84  | LEU  |
| 6   | X     | 121 | TYR  |
| 6   | X     | 123 | ILE  |
| 6   | X     | 124 | VAL  |
| 6   | X     | 131 | VAL  |
| 6   | X     | 147 | LEU  |
| 6   | X     | 153 | GLN  |
| 6   | X     | 163 | TYR  |
| 7   | Y     | 26  | TYR  |
| 7   | Y     | 33  | LEU  |
| 7   | Y     | 36  | ARG  |
| 7   | Y     | 42  | VAL  |
| 7   | Y     | 58  | LEU  |
| 7   | Y     | 85  | GLU  |
| 7   | Y     | 97  | ARG  |
| 7   | Y     | 99  | ILE  |
| 7   | Y     | 101 | CYS  |
| 7   | Y     | 134 | GLU  |
| 7   | Y     | 137 | LEU  |
| 7   | Y     | 153 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Y     | 157 | VAL  |
| 7   | Y     | 159 | VAL  |
| 8   | Z     | 34  | GLU  |
| 8   | Z     | 43  | ARG  |
| 8   | Z     | 52  | THR  |
| 8   | Z     | 54  | ILE  |
| 8   | Z     | 63  | LEU  |
| 8   | Z     | 73  | SER  |
| 8   | Z     | 82  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 86  | GLN  |
| 1   | 1     | 92  | ASN  |
| 1   | 1     | 198 | ASN  |
| 1   | 1     | 288 | GLN  |
| 3   | 3     | 104 | GLN  |
| 3   | 3     | 428 | HIS  |
| 3   | 3     | 613 | HIS  |
| 3   | 3     | 661 | GLN  |
| 3   | 3     | 733 | GLN  |
| 4   | 4     | 72  | HIS  |
| 4   | 4     | 166 | GLN  |
| 4   | 4     | 199 | HIS  |
| 5   | 5     | 129 | HIS  |
| 5   | 5     | 144 | HIS  |
| 6   | 6     | 34  | ASN  |
| 6   | 6     | 153 | GLN  |
| 8   | 7     | 94  | HIS  |
| 1   | A     | 86  | GLN  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 174 | HIS  |
| 1   | A     | 198 | ASN  |
| 1   | A     | 219 | ASN  |
| 3   | C     | 38  | HIS  |
| 3   | C     | 104 | GLN  |
| 3   | C     | 246 | ASN  |
| 3   | C     | 428 | HIS  |
| 3   | C     | 468 | HIS  |
| 3   | C     | 613 | HIS  |
| 3   | C     | 661 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 733 | GLN  |
| 4   | D     | 72  | HIS  |
| 4   | D     | 166 | GLN  |
| 4   | D     | 199 | HIS  |
| 5   | E     | 129 | HIS  |
| 6   | F     | 34  | ASN  |
| 6   | F     | 153 | GLN  |
| 8   | H     | 94  | HIS  |
| 1   | J     | 86  | GLN  |
| 1   | J     | 92  | ASN  |
| 1   | J     | 198 | ASN  |
| 1   | J     | 219 | ASN  |
| 3   | L     | 104 | GLN  |
| 3   | L     | 183 | HIS  |
| 3   | L     | 368 | HIS  |
| 3   | L     | 424 | HIS  |
| 3   | L     | 468 | HIS  |
| 3   | L     | 613 | HIS  |
| 3   | L     | 661 | GLN  |
| 3   | L     | 733 | GLN  |
| 4   | M     | 72  | HIS  |
| 4   | M     | 166 | GLN  |
| 4   | M     | 169 | HIS  |
| 4   | M     | 245 | ASN  |
| 4   | M     | 377 | ASN  |
| 5   | N     | 129 | HIS  |
| 6   | O     | 34  | ASN  |
| 6   | O     | 153 | GLN  |
| 6   | O     | 155 | GLN  |
| 8   | Q     | 94  | HIS  |
| 1   | S     | 86  | GLN  |
| 1   | S     | 92  | ASN  |
| 1   | S     | 198 | ASN  |
| 1   | S     | 219 | ASN  |
| 3   | U     | 104 | GLN  |
| 3   | U     | 246 | ASN  |
| 3   | U     | 428 | HIS  |
| 3   | U     | 613 | HIS  |
| 3   | U     | 661 | GLN  |
| 3   | U     | 733 | GLN  |
| 4   | V     | 72  | HIS  |
| 4   | V     | 166 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | V     | 169 | HIS  |
| 4   | V     | 170 | HIS  |
| 4   | V     | 199 | HIS  |
| 4   | V     | 377 | ASN  |
| 5   | W     | 129 | HIS  |
| 6   | X     | 34  | ASN  |
| 6   | X     | 153 | GLN  |
| 8   | Z     | 94  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 16 are monoatomic - leaving 40 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 9   | SF4  | 1     | 439 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 9   | SF4  | F     | 182 | 6    | 0,12,12      | -    | -           | -           |      |             |
| 10  | FMN  | S     | 440 | -    | 33,33,33     | 1.19 | 3 (9%)      | 48,50,50    | 1.94 | 14 (29%)    |
| 9   | SF4  | G     | 183 | 7    | 0,12,12      | -    | -           | -           |      |             |
| 11  | FES  | L     | 787 | 3    | 0,4,4        | -    | -           | -           |      |             |
| 9   | SF4  | 6     | 182 | 6    | 0,12,12      | -    | -           | -           |      |             |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | SF4  | C     | 784 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | O     | 182 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | B     | 182 | 2    | 0,4,4        | -    | -        | -           |      |          |
| 11  | FES  | U     | 787 | 3    | 0,4,4        | -    | -        | -           |      |          |
| 11  | FES  | K     | 182 | 2    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | C     | 785 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | A     | 439 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | U     | 786 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 10  | FMN  | J     | 440 | -    | 33,33,33     | 1.24 | 3 (9%)   | 48,50,50    | 1.73 | 11 (22%) |
| 11  | FES  | 2     | 182 | 2    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | L     | 785 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | X     | 182 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | Y     | 183 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | 3     | 785 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | U     | 785 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 10  | FMN  | 1     | 440 | -    | 33,33,33     | 1.23 | 3 (9%)   | 48,50,50    | 2.07 | 13 (27%) |
| 9   | SF4  | J     | 439 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | L     | 784 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | S     | 439 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | 3     | 787 | 3    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | P     | 183 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | C     | 787 | 3    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | L     | 786 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | 9     | 184 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | Y     | 184 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 10  | FMN  | A     | 440 | -    | 33,33,33     | 1.25 | 4 (12%)  | 48,50,50    | 1.81 | 11 (22%) |
| 9   | SF4  | 3     | 784 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | U     | 784 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | 9     | 183 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | G     | 184 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | P     | 184 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | 3     | 786 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | C     | 786 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | T     | 182 | 2    | 0,4,4        | -    | -        | -           |      |          |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 9   | SF4  | 1     | 439 | 1    | -       | -        | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 9   | SF4  | F     | 182 | 6    | -       | -          | 0/6/5/5 |
| 10  | FMN  | S     | 440 | -    | -       | 2/18/18/18 | 0/3/3/3 |
| 9   | SF4  | G     | 183 | 7    | -       | -          | 0/6/5/5 |
| 11  | FES  | L     | 787 | 3    | -       | -          | 0/1/1/1 |
| 9   | SF4  | 6     | 182 | 6    | -       | -          | 0/6/5/5 |
| 9   | SF4  | C     | 784 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | O     | 182 | 6    | -       | -          | 0/6/5/5 |
| 11  | FES  | B     | 182 | 2    | -       | -          | 0/1/1/1 |
| 11  | FES  | U     | 787 | 3    | -       | -          | 0/1/1/1 |
| 11  | FES  | K     | 182 | 2    | -       | -          | 0/1/1/1 |
| 9   | SF4  | C     | 785 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | A     | 439 | 1    | -       | -          | 0/6/5/5 |
| 9   | SF4  | U     | 786 | 3    | -       | -          | 0/6/5/5 |
| 10  | FMN  | J     | 440 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 11  | FES  | 2     | 182 | 2    | -       | -          | 0/1/1/1 |
| 9   | SF4  | L     | 785 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | X     | 182 | 6    | -       | -          | 0/6/5/5 |
| 9   | SF4  | Y     | 183 | 7    | -       | -          | 0/6/5/5 |
| 9   | SF4  | 3     | 785 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | U     | 785 | 3    | -       | -          | 0/6/5/5 |
| 10  | FMN  | 1     | 440 | -    | -       | 6/18/18/18 | 0/3/3/3 |
| 9   | SF4  | J     | 439 | 1    | -       | -          | 0/6/5/5 |
| 9   | SF4  | L     | 784 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | S     | 439 | 1    | -       | -          | 0/6/5/5 |
| 11  | FES  | 3     | 787 | 3    | -       | -          | 0/1/1/1 |
| 9   | SF4  | P     | 183 | 7    | -       | -          | 0/6/5/5 |
| 11  | FES  | C     | 787 | 3    | -       | -          | 0/1/1/1 |
| 9   | SF4  | L     | 786 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | 9     | 184 | 7    | -       | -          | 0/6/5/5 |
| 9   | SF4  | Y     | 184 | 7    | -       | -          | 0/6/5/5 |
| 10  | FMN  | A     | 440 | -    | -       | 7/18/18/18 | 0/3/3/3 |
| 9   | SF4  | 3     | 784 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | U     | 784 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | 9     | 183 | 7    | -       | -          | 0/6/5/5 |
| 9   | SF4  | G     | 184 | 7    | -       | -          | 0/6/5/5 |
| 9   | SF4  | P     | 184 | 7    | -       | -          | 0/6/5/5 |
| 9   | SF4  | 3     | 786 | 3    | -       | -          | 0/6/5/5 |
| 9   | SF4  | C     | 786 | 3    | -       | -          | 0/6/5/5 |
| 11  | FES  | T     | 182 | 2    | -       | -          | 0/1/1/1 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | A     | 440 | FMN  | C4A-N5  | 4.15  | 1.39        | 1.30     |
| 10  | 1     | 440 | FMN  | C4A-N5  | 3.95  | 1.39        | 1.30     |
| 10  | S     | 440 | FMN  | C4A-N5  | 3.84  | 1.39        | 1.30     |
| 10  | J     | 440 | FMN  | C4A-N5  | 3.69  | 1.38        | 1.30     |
| 10  | A     | 440 | FMN  | C10-N1  | 2.73  | 1.38        | 1.33     |
| 10  | J     | 440 | FMN  | C10-N1  | 2.64  | 1.38        | 1.33     |
| 10  | S     | 440 | FMN  | C10-N1  | 2.60  | 1.38        | 1.33     |
| 10  | 1     | 440 | FMN  | C10-N1  | 2.57  | 1.38        | 1.33     |
| 10  | A     | 440 | FMN  | C1'-C2' | -2.42 | 1.49        | 1.52     |
| 10  | 1     | 440 | FMN  | C9A-N10 | -2.34 | 1.37        | 1.41     |
| 10  | S     | 440 | FMN  | C9A-N10 | -2.30 | 1.37        | 1.41     |
| 10  | A     | 440 | FMN  | C9A-N10 | -2.18 | 1.37        | 1.41     |
| 10  | J     | 440 | FMN  | C9A-N10 | -2.04 | 1.37        | 1.41     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | 1     | 440 | FMN  | C5'-C4'-C3' | -8.32 | 96.52       | 112.22   |
| 10  | S     | 440 | FMN  | C5'-C4'-C3' | -6.77 | 99.44       | 112.22   |
| 10  | A     | 440 | FMN  | C1'-C2'-C3' | -6.27 | 92.66       | 109.66   |
| 10  | J     | 440 | FMN  | C1'-C2'-C3' | -5.90 | 93.67       | 109.66   |
| 10  | A     | 440 | FMN  | C5'-C4'-C3' | -5.25 | 102.32      | 112.22   |
| 10  | 1     | 440 | FMN  | C1'-C2'-C3' | -5.09 | 95.86       | 109.66   |
| 10  | S     | 440 | FMN  | C1'-C2'-C3' | -4.61 | 97.17       | 109.66   |
| 10  | S     | 440 | FMN  | C4'-C3'-C2' | 3.89  | 120.05      | 113.57   |
| 10  | J     | 440 | FMN  | C5'-C4'-C3' | -3.45 | 105.70      | 112.22   |
| 10  | 1     | 440 | FMN  | C4'-C3'-C2' | 3.42  | 119.26      | 113.57   |
| 10  | 1     | 440 | FMN  | C9A-C5A-N5  | -3.26 | 118.99      | 122.45   |
| 10  | J     | 440 | FMN  | O4'-C4'-C5' | 3.24  | 117.14      | 109.99   |
| 10  | 1     | 440 | FMN  | C4-N3-C2    | -3.02 | 120.28      | 125.64   |
| 10  | A     | 440 | FMN  | C10-C4A-N5  | -2.94 | 118.81      | 124.81   |
| 10  | J     | 440 | FMN  | C4-N3-C2    | -2.88 | 120.52      | 125.64   |
| 10  | S     | 440 | FMN  | O5'-C5'-C4' | 2.81  | 116.86      | 109.36   |
| 10  | S     | 440 | FMN  | C9A-C5A-N5  | -2.79 | 119.49      | 122.45   |
| 10  | J     | 440 | FMN  | C9A-C5A-N5  | -2.76 | 119.53      | 122.45   |
| 10  | J     | 440 | FMN  | C10-C4A-N5  | -2.72 | 119.26      | 124.81   |
| 10  | 1     | 440 | FMN  | C10-C4A-N5  | -2.69 | 119.31      | 124.81   |
| 10  | S     | 440 | FMN  | C4-N3-C2    | -2.69 | 120.87      | 125.64   |
| 10  | S     | 440 | FMN  | C10-C4A-N5  | -2.66 | 119.38      | 124.81   |
| 10  | A     | 440 | FMN  | C9A-C5A-N5  | -2.64 | 119.65      | 122.45   |
| 10  | A     | 440 | FMN  | C4-C4A-N5   | 2.64  | 121.86      | 118.21   |
| 10  | S     | 440 | FMN  | O4-C4-C4A   | -2.59 | 119.70      | 126.53   |
| 10  | 1     | 440 | FMN  | C4A-C4-N3   | 2.56  | 119.76      | 113.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | 1     | 440 | FMN  | C5A-C9A-N10 | 2.54  | 120.26      | 117.97   |
| 10  | A     | 440 | FMN  | C4A-C10-N10 | 2.43  | 119.96      | 116.48   |
| 10  | 1     | 440 | FMN  | C9-C9A-N10  | -2.43 | 118.59      | 121.85   |
| 10  | 1     | 440 | FMN  | O4-C4-C4A   | -2.39 | 120.22      | 126.53   |
| 10  | J     | 440 | FMN  | O4-C4-C4A   | -2.39 | 120.23      | 126.53   |
| 10  | S     | 440 | FMN  | C4A-C4-N3   | 2.39  | 119.33      | 113.25   |
| 10  | S     | 440 | FMN  | C4A-C10-N10 | 2.38  | 119.88      | 116.48   |
| 10  | 1     | 440 | FMN  | C4-C4A-N5   | 2.30  | 121.39      | 118.21   |
| 10  | J     | 440 | FMN  | C4A-C4-N3   | 2.25  | 118.97      | 113.25   |
| 10  | S     | 440 | FMN  | C9-C9A-N10  | -2.24 | 118.84      | 121.85   |
| 10  | S     | 440 | FMN  | O2'-C2'-C3' | 2.22  | 114.45      | 109.25   |
| 10  | S     | 440 | FMN  | C5A-C9A-N10 | 2.21  | 119.96      | 117.97   |
| 10  | A     | 440 | FMN  | C9-C9A-N10  | -2.21 | 118.89      | 121.85   |
| 10  | J     | 440 | FMN  | C2'-C1'-N10 | 2.21  | 120.62      | 110.20   |
| 10  | A     | 440 | FMN  | O4-C4-C4A   | -2.14 | 120.88      | 126.53   |
| 10  | S     | 440 | FMN  | C4-C4A-N5   | 2.12  | 121.14      | 118.21   |
| 10  | A     | 440 | FMN  | O3P-P-O5'   | 2.11  | 112.17      | 106.67   |
| 10  | 1     | 440 | FMN  | O2'-C2'-C3' | 2.08  | 114.12      | 109.25   |
| 10  | J     | 440 | FMN  | C5A-C9A-N10 | 2.04  | 119.81      | 117.97   |
| 10  | J     | 440 | FMN  | C4A-C10-N10 | 2.03  | 119.38      | 116.48   |
| 10  | A     | 440 | FMN  | C5A-C9A-N10 | 2.01  | 119.79      | 117.97   |
| 10  | 1     | 440 | FMN  | C4A-C10-N10 | 2.01  | 119.36      | 116.48   |
| 10  | A     | 440 | FMN  | C4-N3-C2    | -2.01 | 122.08      | 125.64   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | 1     | 440 | FMN  | N10-C1'-C2'-O2' |
| 10  | 1     | 440 | FMN  | N10-C1'-C2'-C3' |
| 10  | 1     | 440 | FMN  | C1'-C2'-C3'-O3' |
| 10  | 1     | 440 | FMN  | C1'-C2'-C3'-C4' |
| 10  | A     | 440 | FMN  | N10-C1'-C2'-O2' |
| 10  | A     | 440 | FMN  | N10-C1'-C2'-C3' |
| 10  | A     | 440 | FMN  | C3'-C4'-C5'-O5' |
| 10  | A     | 440 | FMN  | O4'-C4'-C5'-O5' |
| 10  | A     | 440 | FMN  | C5'-O5'-P-O1P   |
| 10  | A     | 440 | FMN  | C5'-O5'-P-O2P   |
| 10  | A     | 440 | FMN  | C5'-O5'-P-O3P   |
| 10  | J     | 440 | FMN  | N10-C1'-C2'-O2' |
| 10  | J     | 440 | FMN  | N10-C1'-C2'-C3' |
| 10  | J     | 440 | FMN  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | J     | 440 | FMN  | O4'-C4'-C5'-O5' |
| 10  | S     | 440 | FMN  | N10-C1'-C2'-O2' |
| 10  | S     | 440 | FMN  | N10-C1'-C2'-C3' |
| 10  | 1     | 440 | FMN  | O2'-C2'-C3'-C4' |
| 10  | 1     | 440 | FMN  | O2'-C2'-C3'-O3' |
| 10  | J     | 440 | FMN  | O3'-C3'-C4'-C5' |

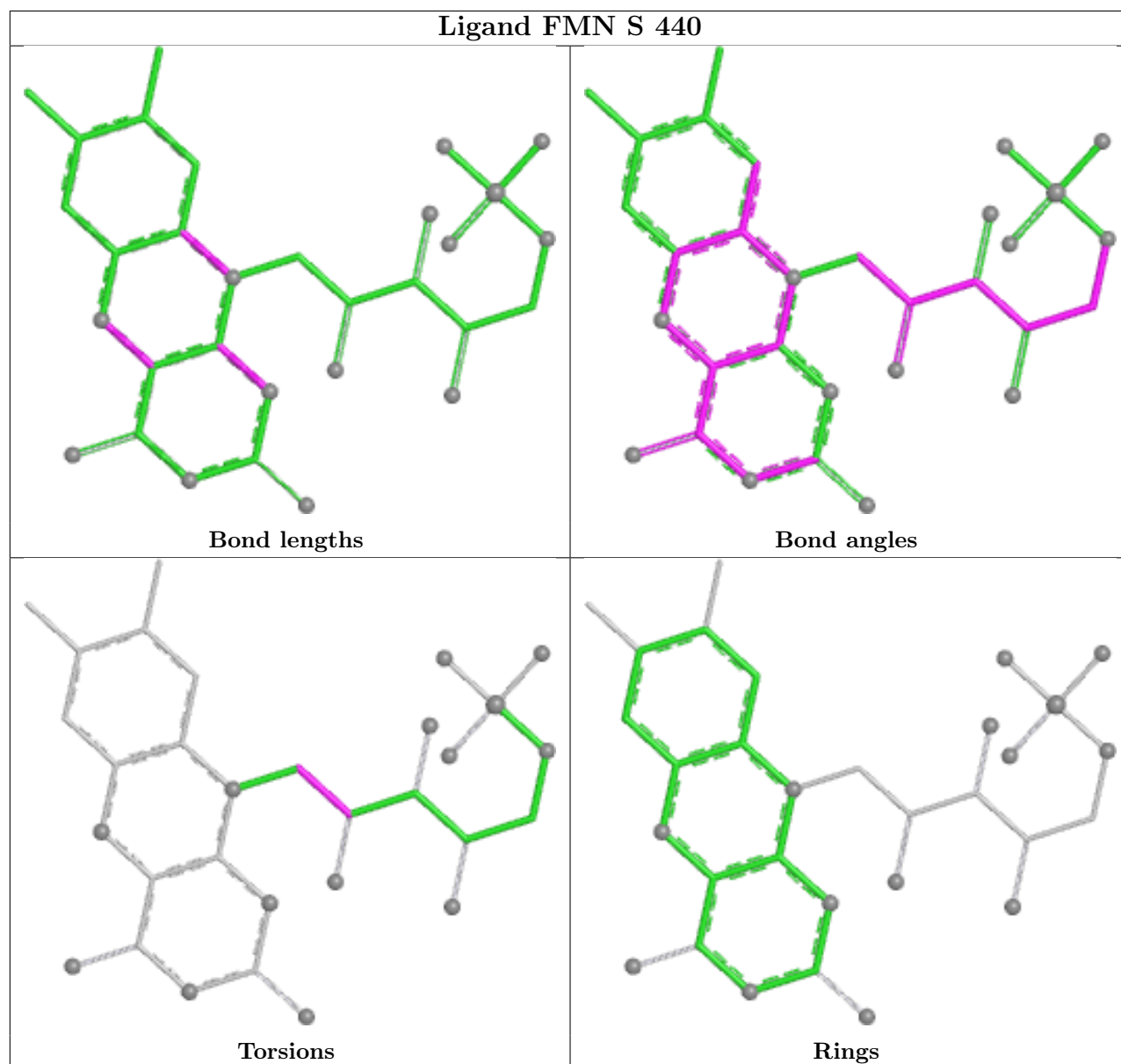
There are no ring outliers.

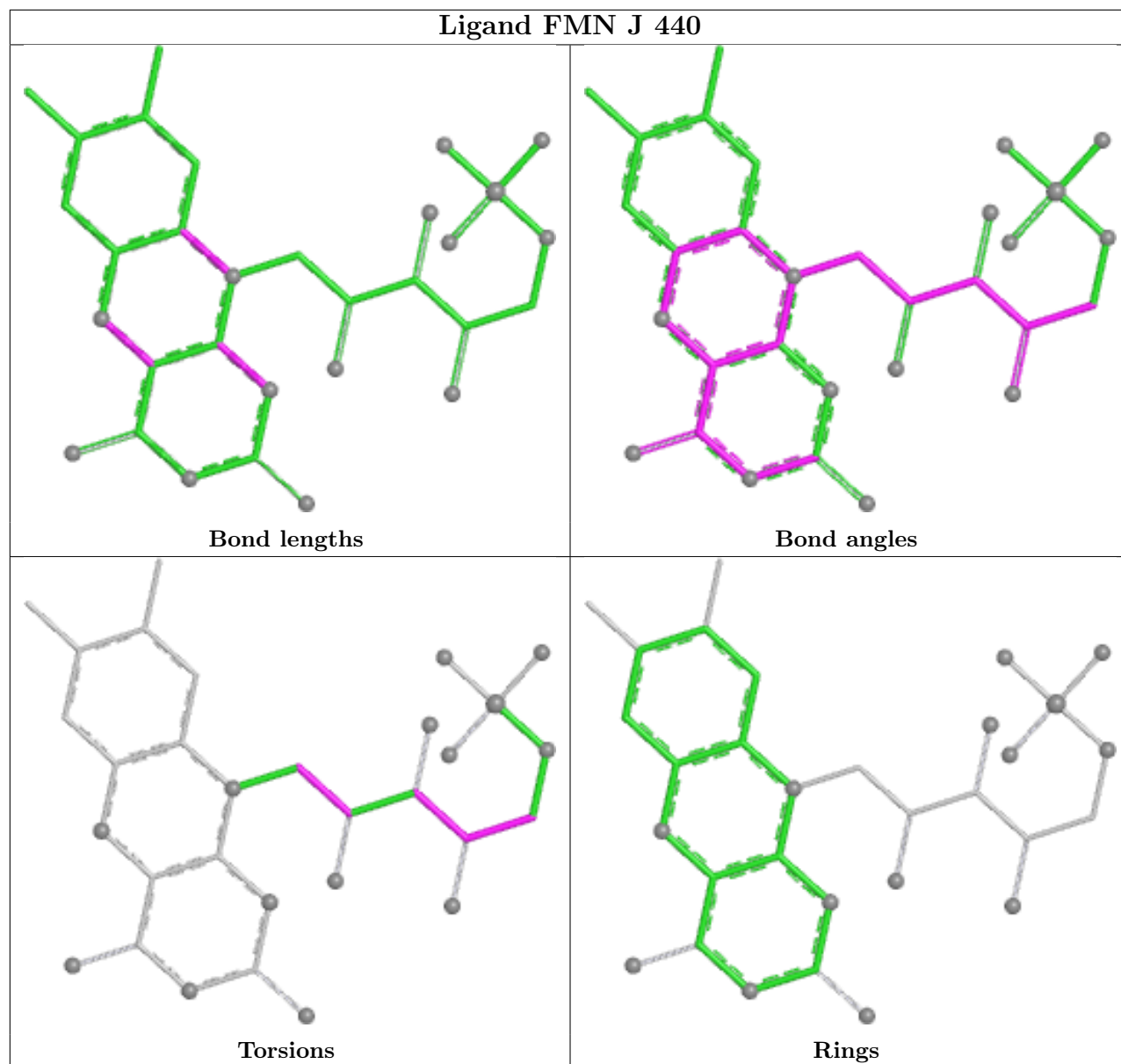
29 monomers are involved in 58 short contacts:

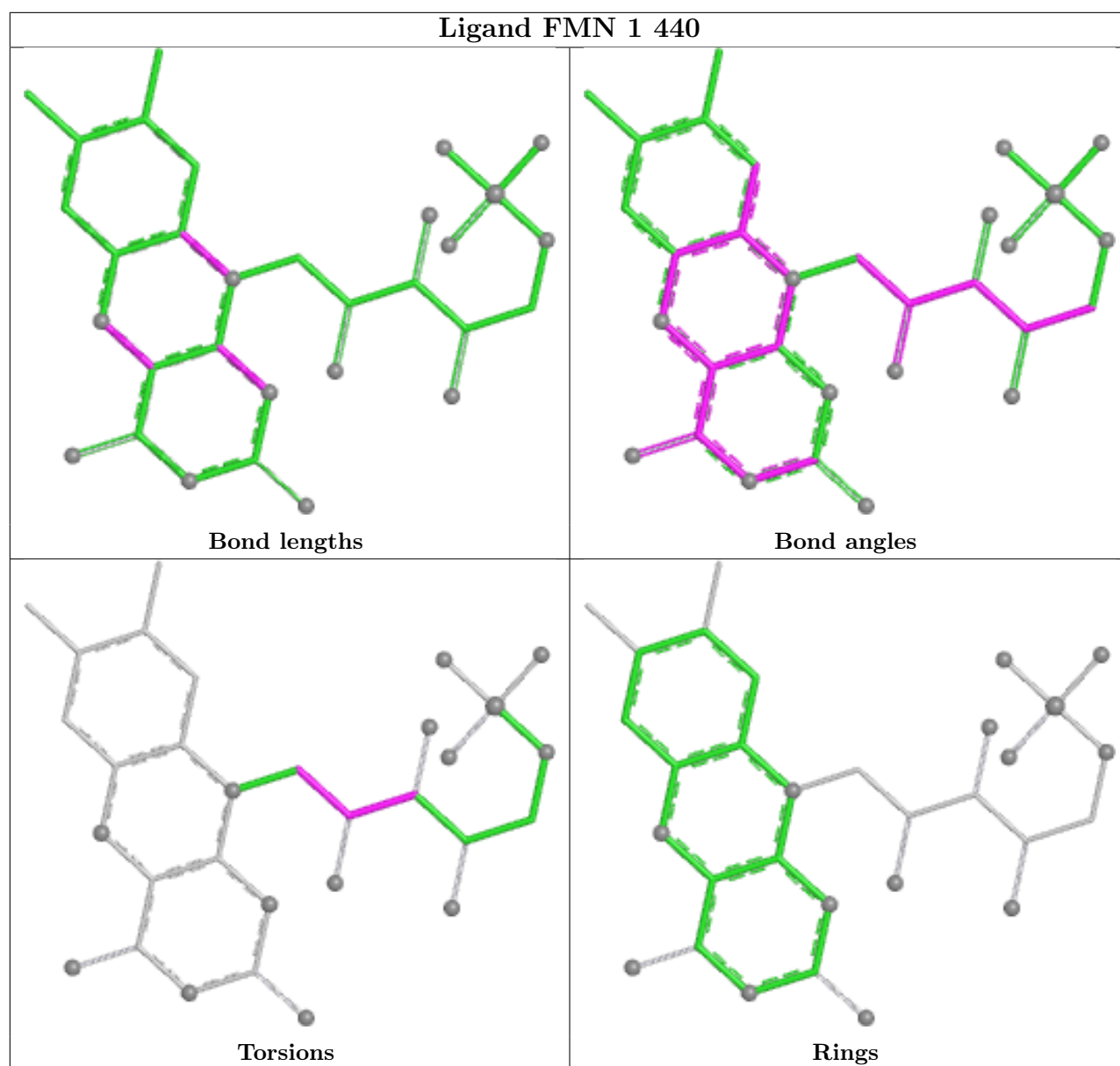
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | F     | 182 | SF4  | 3       | 0            |
| 10  | S     | 440 | FMN  | 6       | 0            |
| 9   | G     | 183 | SF4  | 1       | 0            |
| 9   | 6     | 182 | SF4  | 2       | 0            |
| 9   | O     | 182 | SF4  | 2       | 0            |
| 11  | B     | 182 | FES  | 1       | 0            |
| 11  | K     | 182 | FES  | 1       | 0            |
| 9   | C     | 785 | SF4  | 1       | 0            |
| 9   | A     | 439 | SF4  | 1       | 0            |
| 10  | J     | 440 | FMN  | 8       | 0            |
| 11  | 2     | 182 | FES  | 1       | 0            |
| 9   | L     | 785 | SF4  | 1       | 0            |
| 9   | X     | 182 | SF4  | 3       | 0            |
| 9   | 3     | 785 | SF4  | 1       | 0            |
| 9   | U     | 785 | SF4  | 1       | 0            |
| 10  | 1     | 440 | FMN  | 7       | 0            |
| 9   | L     | 784 | SF4  | 1       | 0            |
| 9   | P     | 183 | SF4  | 1       | 0            |
| 11  | C     | 787 | FES  | 1       | 0            |
| 9   | L     | 786 | SF4  | 1       | 0            |
| 9   | 9     | 184 | SF4  | 1       | 0            |
| 10  | A     | 440 | FMN  | 6       | 0            |
| 9   | 3     | 784 | SF4  | 1       | 0            |
| 9   | U     | 784 | SF4  | 1       | 0            |
| 9   | 9     | 183 | SF4  | 1       | 0            |
| 9   | G     | 184 | SF4  | 1       | 0            |
| 9   | P     | 184 | SF4  | 1       | 0            |
| 9   | 3     | 786 | SF4  | 1       | 0            |
| 11  | T     | 182 | FES  | 1       | 0            |

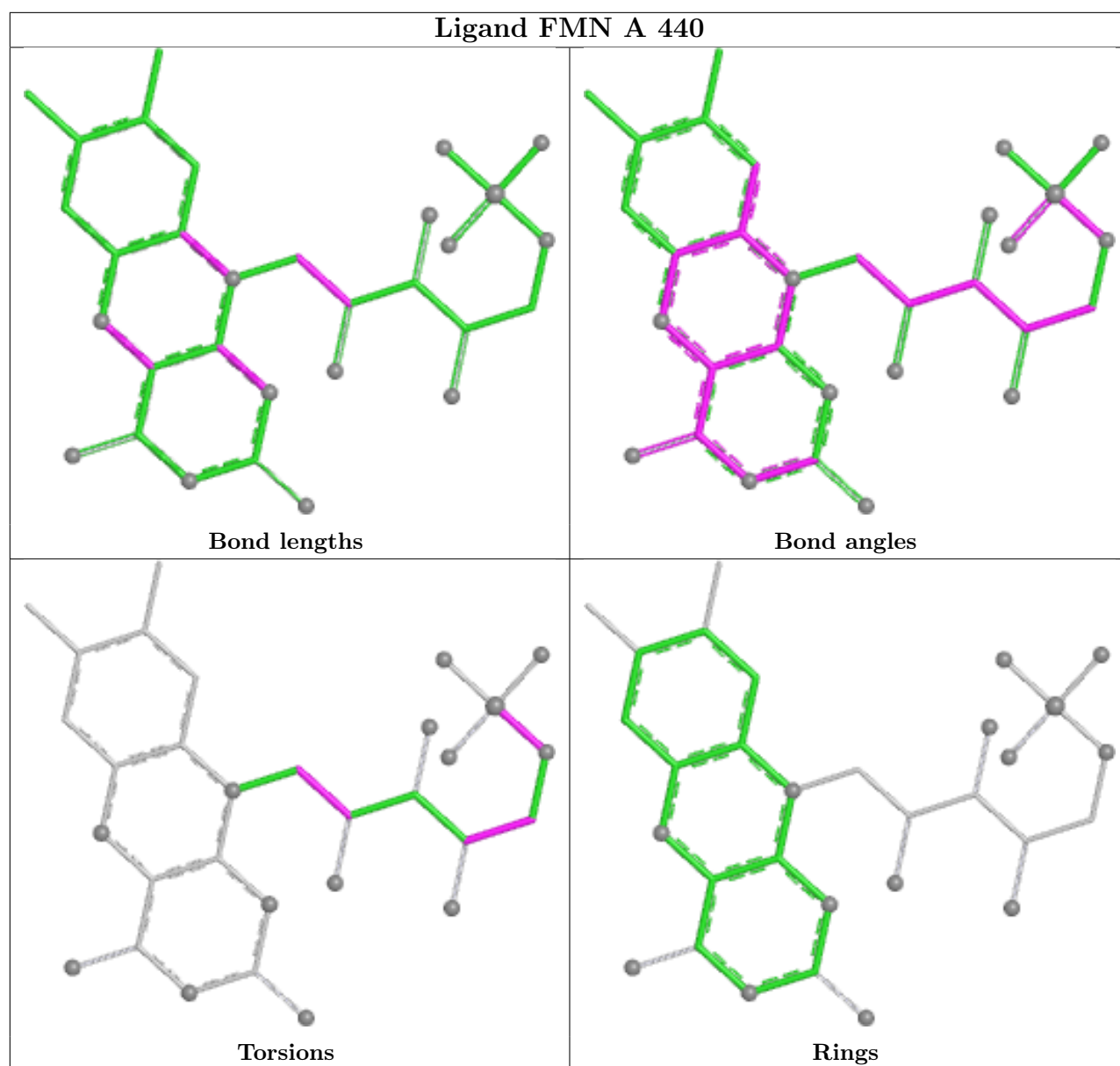
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|-----------|-----------------------|-------|
| 1   | 1     | 437/438 (99%) | -1.75  | 0 100 100 | 38, 59, 83, 110       | 0     |
| 1   | A     | 437/438 (99%) | -1.73  | 0 100 100 | 40, 60, 84, 110       | 0     |
| 1   | J     | 437/438 (99%) | -1.73  | 0 100 100 | 39, 59, 83, 110       | 0     |
| 1   | S     | 437/438 (99%) | -1.77  | 0 100 100 | 39, 60, 83, 111       | 0     |
| 2   | 2     | 178/181 (98%) | -1.74  | 0 100 100 | 43, 63, 93, 135       | 0     |
| 2   | B     | 178/181 (98%) | -1.70  | 0 100 100 | 43, 64, 94, 134       | 0     |
| 2   | K     | 178/181 (98%) | -1.73  | 0 100 100 | 43, 63, 93, 136       | 0     |
| 2   | T     | 178/181 (98%) | -1.75  | 0 100 100 | 43, 64, 94, 134       | 0     |
| 3   | 3     | 754/783 (96%) | -1.71  | 0 100 100 | 36, 74, 112, 133      | 0     |
| 3   | C     | 754/783 (96%) | -1.72  | 0 100 100 | 36, 75, 113, 134      | 0     |
| 3   | L     | 754/783 (96%) | -1.69  | 0 100 100 | 37, 75, 114, 133      | 0     |
| 3   | U     | 754/783 (96%) | -1.72  | 0 100 100 | 36, 75, 113, 134      | 0     |
| 4   | 4     | 377/409 (92%) | -1.68  | 0 100 100 | 38, 78, 112, 129      | 0     |
| 4   | D     | 377/409 (92%) | -1.72  | 0 100 100 | 38, 77, 112, 129      | 0     |
| 4   | M     | 377/409 (92%) | -1.68  | 0 100 100 | 38, 78, 112, 129      | 0     |
| 4   | V     | 377/409 (92%) | -1.67  | 0 100 100 | 39, 78, 112, 130      | 0     |
| 5   | 5     | 196/207 (94%) | -1.66  | 0 100 100 | 50, 83, 120, 132      | 0     |
| 5   | E     | 196/207 (94%) | -1.67  | 0 100 100 | 51, 83, 120, 132      | 0     |
| 5   | N     | 196/207 (94%) | -1.68  | 0 100 100 | 50, 83, 120, 132      | 0     |
| 5   | W     | 196/207 (94%) | -1.61  | 0 100 100 | 52, 84, 120, 133      | 0     |
| 6   | 6     | 145/181 (80%) | -1.69  | 0 100 100 | 51, 71, 104, 125      | 0     |
| 6   | F     | 145/181 (80%) | -1.64  | 0 100 100 | 49, 71, 105, 125      | 0     |
| 6   | O     | 145/181 (80%) | -1.62  | 0 100 100 | 50, 71, 105, 125      | 0     |
| 6   | X     | 145/181 (80%) | -1.61  | 0 100 100 | 51, 72, 105, 125      | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2 | OWAB(Å <sup>2</sup> ) | Q<0.9 |                  |   |
|-----|-------|------------------|--------|---------|-----------------------|-------|------------------|---|
| 7   | 9     | 154/182 (84%)    | -1.78  | 0       | 100                   | 100   | 37, 59, 96, 136  | 0 |
| 7   | G     | 154/182 (84%)    | -1.74  | 0       | 100                   | 100   | 37, 58, 95, 135  | 0 |
| 7   | P     | 154/182 (84%)    | -1.79  | 0       | 100                   | 100   | 37, 59, 95, 136  | 0 |
| 7   | Y     | 154/182 (84%)    | -1.72  | 0       | 100                   | 100   | 37, 60, 96, 136  | 0 |
| 8   | 7     | 127/129 (98%)    | -1.79  | 0       | 100                   | 100   | 49, 66, 101, 119 | 0 |
| 8   | H     | 127/129 (98%)    | -1.78  | 0       | 100                   | 100   | 48, 66, 101, 120 | 0 |
| 8   | Q     | 127/129 (98%)    | -1.76  | 0       | 100                   | 100   | 48, 66, 102, 120 | 0 |
| 8   | Z     | 127/129 (98%)    | -1.77  | 0       | 100                   | 100   | 48, 67, 101, 119 | 0 |
| All | All   | 9472/10040 (94%) | -1.71  | 0       | 100                   | 100   | 36, 69, 111, 136 | 0 |

There are no RSRZ outliers to report.

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 12  | CA   | T     | 202 | 1/1   | 0.97 | 0.03 | 100,100,100,100            | 0     |
| 12  | CA   | B     | 202 | 1/1   | 0.98 | 0.02 | 108,108,108,108            | 0     |
| 10  | FMN  | A     | 440 | 31/31 | 0.99 | 0.04 | 48,60,64,66                | 0     |
| 10  | FMN  | J     | 440 | 31/31 | 0.99 | 0.04 | 42,53,60,63                | 0     |
| 9   | SF4  | 6     | 182 | 8/8   | 1.00 | 0.01 | 24,37,69,69                | 0     |
| 9   | SF4  | 9     | 183 | 8/8   | 1.00 | 0.01 | 12,19,45,48                | 0     |
| 9   | SF4  | 9     | 184 | 8/8   | 1.00 | 0.01 | 7,27,44,48                 | 0     |
| 9   | SF4  | A     | 439 | 8/8   | 1.00 | 0.01 | 13,26,49,50                | 0     |
| 9   | SF4  | C     | 784 | 8/8   | 1.00 | 0.01 | 13,18,40,40                | 0     |

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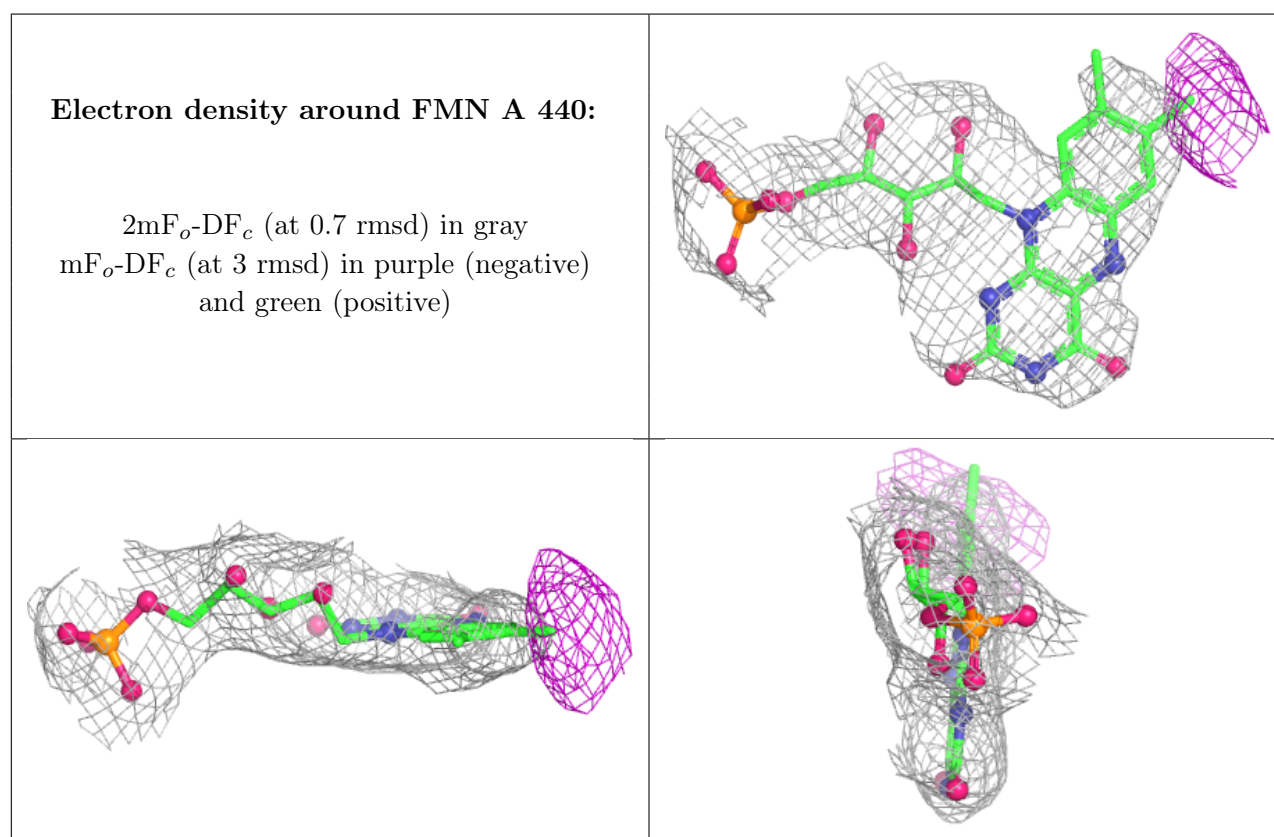
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 9   | SF4  | C     | 785 | 8/8   | 1.00 | 0.01 | 12,22,39,40                 | 0     |
| 9   | SF4  | C     | 786 | 8/8   | 1.00 | 0.01 | 21,34,56,59                 | 0     |
| 9   | SF4  | F     | 182 | 8/8   | 1.00 | 0.01 | 18,31,51,62                 | 0     |
| 9   | SF4  | G     | 183 | 8/8   | 1.00 | 0.01 | 11,18,42,46                 | 0     |
| 9   | SF4  | G     | 184 | 8/8   | 1.00 | 0.01 | 12,15,39,39                 | 0     |
| 9   | SF4  | J     | 439 | 8/8   | 1.00 | 0.01 | 8,25,43,44                  | 0     |
| 9   | SF4  | L     | 784 | 8/8   | 1.00 | 0.01 | 11,17,34,42                 | 0     |
| 9   | SF4  | L     | 785 | 8/8   | 1.00 | 0.02 | 11,18,39,39                 | 0     |
| 9   | SF4  | L     | 786 | 8/8   | 1.00 | 0.01 | 30,39,61,62                 | 0     |
| 9   | SF4  | O     | 182 | 8/8   | 1.00 | 0.01 | 18,27,54,59                 | 0     |
| 9   | SF4  | P     | 183 | 8/8   | 1.00 | 0.01 | 10,16,42,46                 | 0     |
| 9   | SF4  | P     | 184 | 8/8   | 1.00 | 0.02 | 1,19,41,41                  | 0     |
| 9   | SF4  | S     | 439 | 8/8   | 1.00 | 0.01 | 19,27,49,51                 | 0     |
| 9   | SF4  | U     | 784 | 8/8   | 1.00 | 0.01 | 15,26,43,43                 | 0     |
| 9   | SF4  | U     | 785 | 8/8   | 1.00 | 0.02 | 19,27,43,43                 | 0     |
| 9   | SF4  | U     | 786 | 8/8   | 1.00 | 0.01 | 21,33,51,58                 | 0     |
| 9   | SF4  | X     | 182 | 8/8   | 1.00 | 0.01 | 39,56,81,89                 | 0     |
| 9   | SF4  | Y     | 183 | 8/8   | 1.00 | 0.01 | 17,35,53,57                 | 0     |
| 9   | SF4  | Y     | 184 | 8/8   | 1.00 | 0.01 | 19,29,51,57                 | 0     |
| 10  | FMN  | 1     | 440 | 31/31 | 1.00 | 0.03 | 48,54,62,68                 | 0     |
| 9   | SF4  | 1     | 439 | 8/8   | 1.00 | 0.01 | 13,24,43,45                 | 0     |
| 9   | SF4  | 3     | 784 | 8/8   | 1.00 | 0.01 | 12,16,36,38                 | 0     |
| 10  | FMN  | S     | 440 | 31/31 | 1.00 | 0.02 | 53,60,65,66                 | 0     |
| 11  | FES  | 2     | 182 | 4/4   | 1.00 | 0.01 | 11,18,41,42                 | 0     |
| 11  | FES  | 3     | 787 | 4/4   | 1.00 | 0.01 | 17,20,34,47                 | 0     |
| 11  | FES  | B     | 182 | 4/4   | 1.00 | 0.01 | 15,29,43,48                 | 0     |
| 11  | FES  | C     | 787 | 4/4   | 1.00 | 0.01 | 22,23,31,43                 | 0     |
| 11  | FES  | K     | 182 | 4/4   | 1.00 | 0.01 | 14,22,42,44                 | 0     |
| 11  | FES  | L     | 787 | 4/4   | 1.00 | 0.01 | 16,17,33,41                 | 0     |
| 11  | FES  | T     | 182 | 4/4   | 1.00 | 0.02 | 18,26,47,47                 | 0     |
| 11  | FES  | U     | 787 | 4/4   | 1.00 | 0.01 | 22,28,34,45                 | 0     |
| 12  | CA   | 2     | 202 | 1/1   | 1.00 | 0.03 | 58,58,58,58                 | 0     |
| 12  | CA   | 3     | 788 | 1/1   | 1.00 | 0.01 | 43,43,43,43                 | 0     |
| 12  | CA   | 3     | 789 | 1/1   | 1.00 | 0.01 | 50,50,50,50                 | 0     |
| 12  | CA   | 9     | 201 | 1/1   | 1.00 | 0.05 | 37,37,37,37                 | 0     |
| 9   | SF4  | 3     | 785 | 8/8   | 1.00 | 0.01 | 8,18,36,38                  | 0     |
| 12  | CA   | C     | 788 | 1/1   | 1.00 | 0.01 | 46,46,46,46                 | 0     |
| 12  | CA   | G     | 201 | 1/1   | 1.00 | 0.02 | 43,43,43,43                 | 0     |
| 12  | CA   | H     | 203 | 1/1   | 1.00 | 0.03 | 55,55,55,55                 | 0     |
| 12  | CA   | K     | 202 | 1/1   | 1.00 | 0.03 | 66,66,66,66                 | 0     |
| 12  | CA   | L     | 788 | 1/1   | 1.00 | 0.01 | 50,50,50,50                 | 0     |
| 12  | CA   | L     | 789 | 1/1   | 1.00 | 0.01 | 62,62,62,62                 | 0     |

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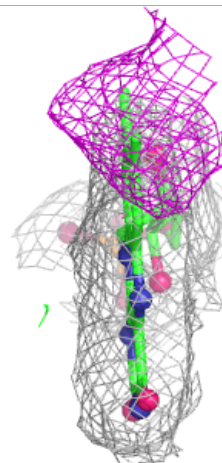
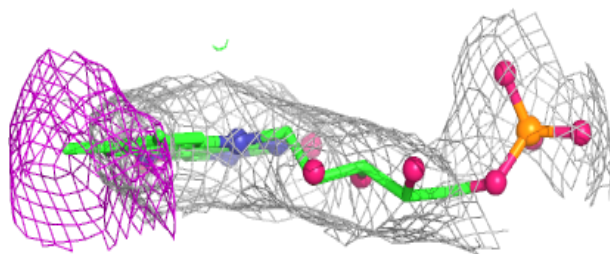
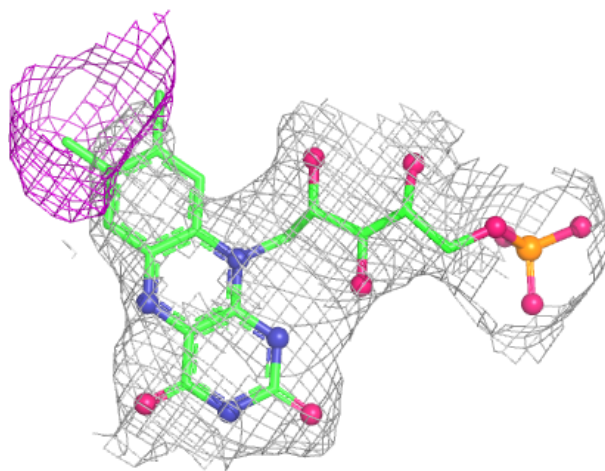
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 12  | CA   | P     | 201 | 1/1   | 1.00 | 0.04 | 40,40,40,40                 | 0     |
| 9   | SF4  | 3     | 786 | 8/8   | 1.00 | 0.01 | 16,27,50,50                 | 0     |
| 12  | CA   | U     | 788 | 1/1   | 1.00 | 0.01 | 50,50,50,50                 | 0     |
| 12  | CA   | Y     | 201 | 1/1   | 1.00 | 0.03 | 41,41,41,41                 | 0     |
| 12  | CA   | Z     | 203 | 1/1   | 1.00 | 0.03 | 60,60,60,60                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



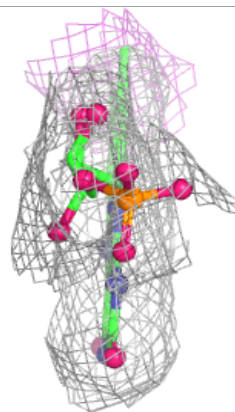
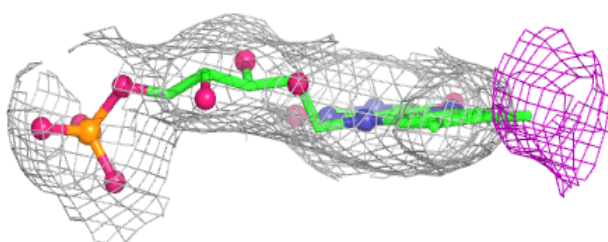
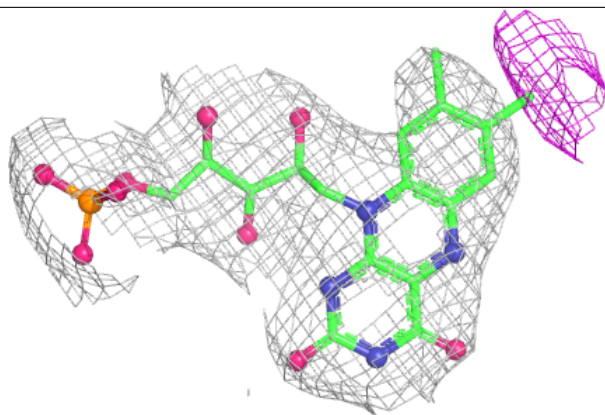
**Electron density around FMN J 440:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

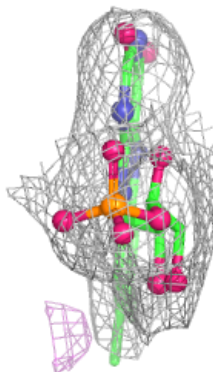
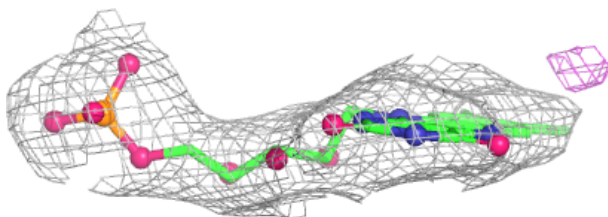
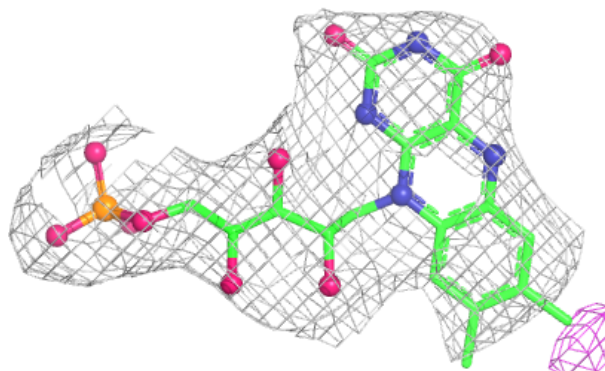


**Electron density around FMN 1 440:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FMN S 440:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.