



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:10 AM GMT

PDB ID : 1E7P  
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINO-  
GENES  
Authors : Lancaster, C.R.D.; Kroeger, A.  
Deposited on : 2000-09-01  
Resolution : 3.10 Å(reported)

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

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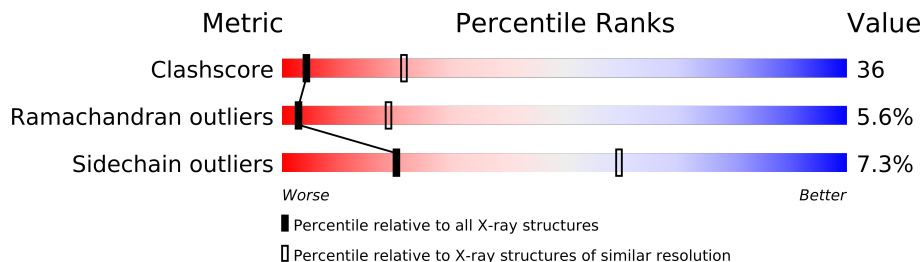
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 79885                       | 1078 (3.16-3.04)                                      |
| Ramachandran outliers | 78287                       | 1044 (3.16-3.04)                                      |
| Sidechain outliers    | 78261                       | 1044 (3.16-3.04)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 656    |                  |
| 1   | D     | 656    |                  |
| 1   | G     | 656    |                  |
| 1   | J     | 656    |                  |
| 2   | B     | 239    |                  |
| 2   | E     | 239    |                  |
| 2   | H     | 239    |                  |
| 2   | K     | 239    |                  |
| 3   | C     | 256    |                  |
| 3   | F     | 256    |                  |
| 3   | I     | 256    |                  |
| 3   | L     | 256    |                  |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 37080 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 655      | Total | C    | N   | O   | S  | 33      | 0       | 0     |
|     |       |          | 5094  | 3190 | 910 | 962 | 32 |         |         |       |
| 1   | D     | 655      | Total | C    | N   | O   | S  | 33      | 0       | 0     |
|     |       |          | 5094  | 3190 | 910 | 962 | 32 |         |         |       |
| 1   | G     | 655      | Total | C    | N   | O   | S  | 33      | 0       | 0     |
|     |       |          | 5094  | 3190 | 910 | 962 | 32 |         |         |       |
| 1   | J     | 655      | Total | C    | N   | O   | S  | 33      | 0       | 0     |
|     |       |          | 5094  | 3190 | 910 | 962 | 32 |         |         |       |

- Molecule 2 is a protein called FUMARATE REDUCTASE IRON-SULFUR PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 239      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1894  | 1194 | 322 | 355 | 23 |         |         |       |
| 2   | E     | 239      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1894  | 1194 | 322 | 355 | 23 |         |         |       |
| 2   | H     | 239      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1894  | 1194 | 322 | 355 | 23 |         |         |       |
| 2   | K     | 239      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1894  | 1194 | 322 | 355 | 23 |         |         |       |

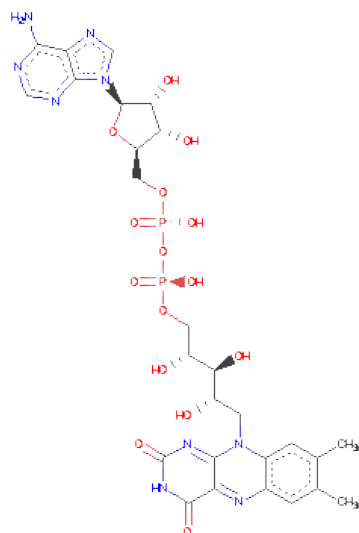
- Molecule 3 is a protein called FUMARATE REDUCTASE CYTOCHROME B SUBUNIT.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 254      | Total | C    | N   | O   | S  | 24      | 0       | 0     |
|     |       |          | 2081  | 1388 | 334 | 345 | 14 |         |         |       |
| 3   | F     | 254      | Total | C    | N   | O   | S  | 24      | 0       | 0     |
|     |       |          | 2081  | 1388 | 334 | 345 | 14 |         |         |       |
| 3   | I     | 254      | Total | C    | N   | O   | S  | 24      | 0       | 0     |
|     |       |          | 2081  | 1388 | 334 | 345 | 14 |         |         |       |
| 3   | L     | 254      | Total | C    | N   | O   | S  | 24      | 0       | 0     |
|     |       |          | 2081  | 1388 | 334 | 345 | 14 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

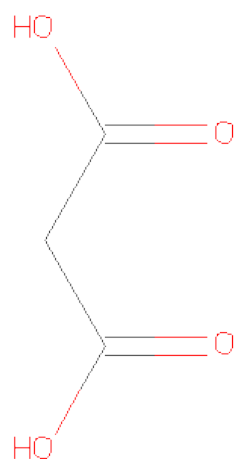
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 66      | GLN      | GLU    | ENGINEERED MUTATION | UNP P17413 |
| F     | 66      | GLN      | GLU    | ENGINEERED MUTATION | UNP P17413 |
| I     | 66      | GLN      | GLU    | ENGINEERED MUTATION | UNP P17413 |
| L     | 66      | GLN      | GLU    | ENGINEERED MUTATION | UNP P17413 |

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 4   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 4   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 4   | J     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula:  $C_3H_4O_4$ ).

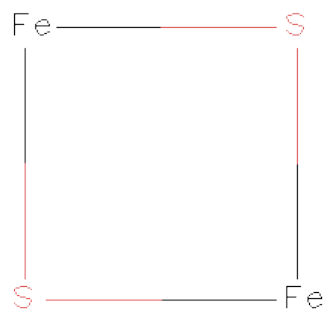


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 3 | 4 |         |         |
| 5   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 3 | 4 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 3 | 4 |         |         |
| 5   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 3 | 4 |         |         |

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

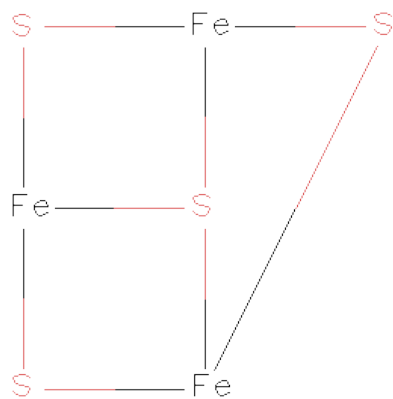
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | G     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | J     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | D     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



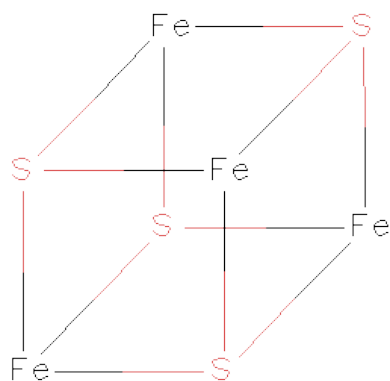
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 7   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 7   | E     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 7   | H     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 7   | K     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



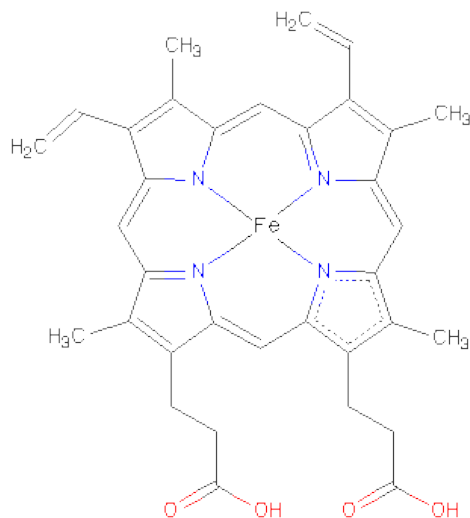
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |
| 8   | E     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |
| 8   | H     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |
| 8   | K     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |

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



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | E     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | H     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | K     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

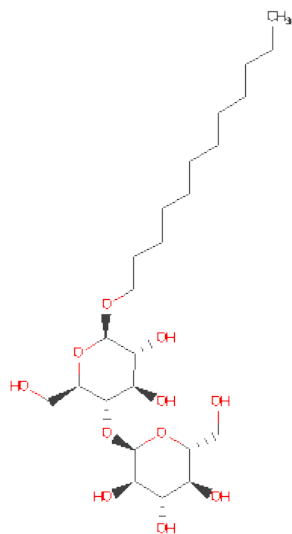
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 10  | C     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | C     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | F     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | F     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | I     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | I     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | L     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | L     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 11 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).





| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 11  | C     | 1        | Total | C  | O  | 17      | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 11  | F     | 1        | Total | C  | O  | 17      | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 11  | I     | 1        | Total | C  | O  | 17      | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 11  | L     | 1        | Total | C  | O  | 17      | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

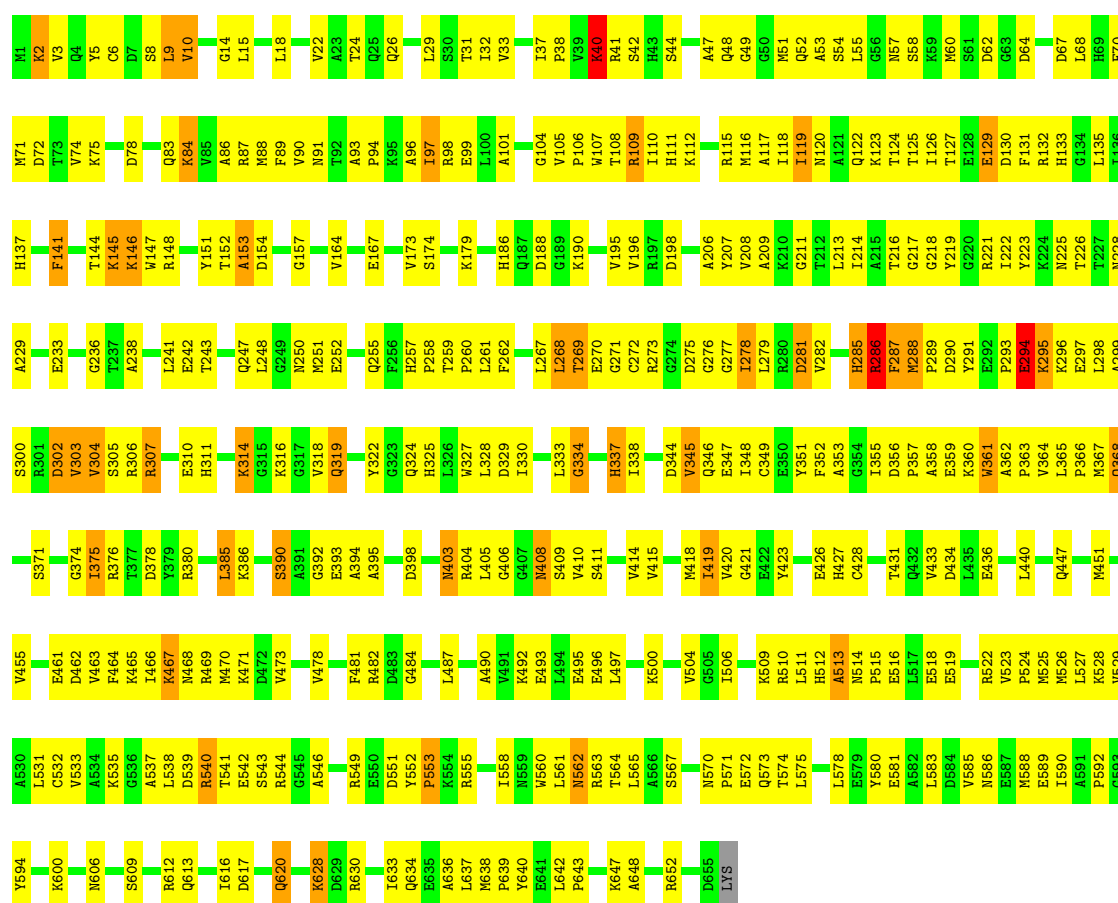
### 3 Residue-property plots

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

Note EDS was not executed.

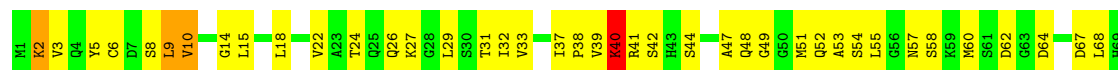
#### • Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT

Chain A:



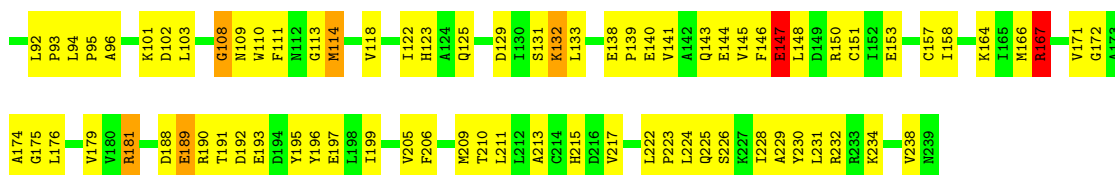
#### • Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT

Chain D:



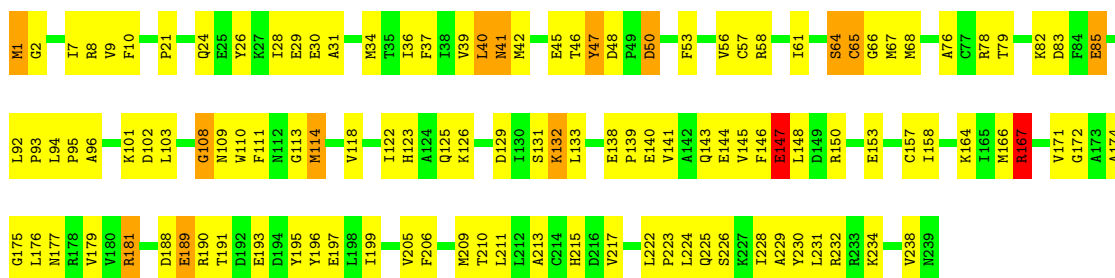






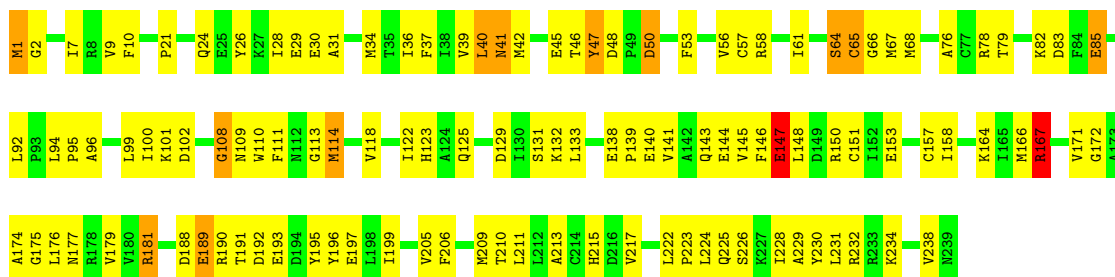
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain H:



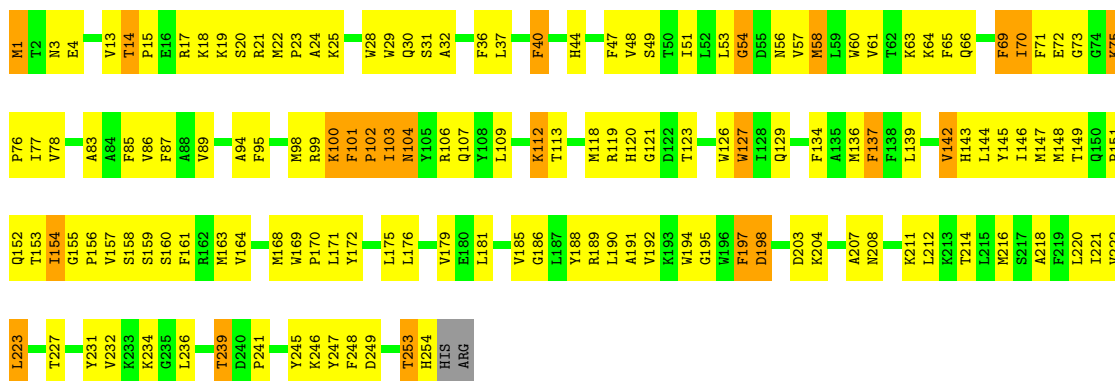
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain K:



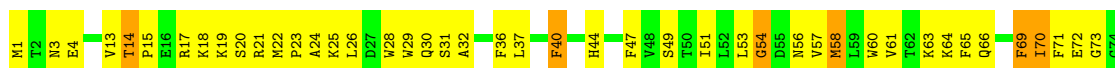
• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain C:



• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

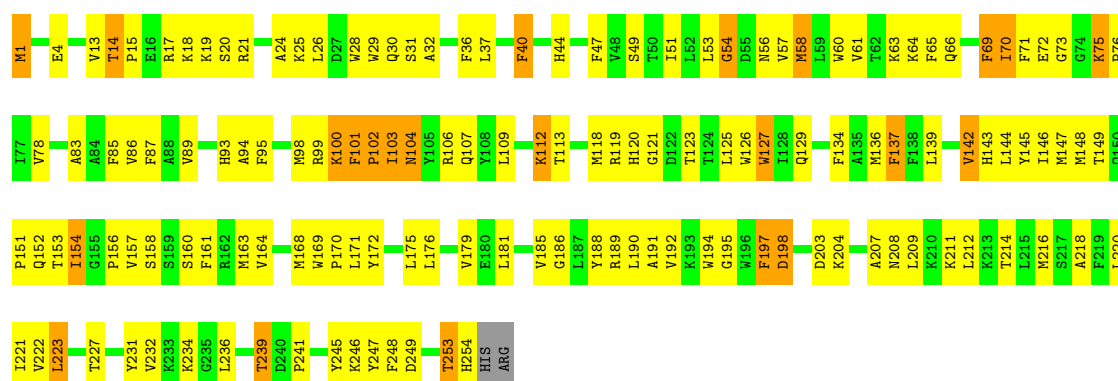
Chain F:





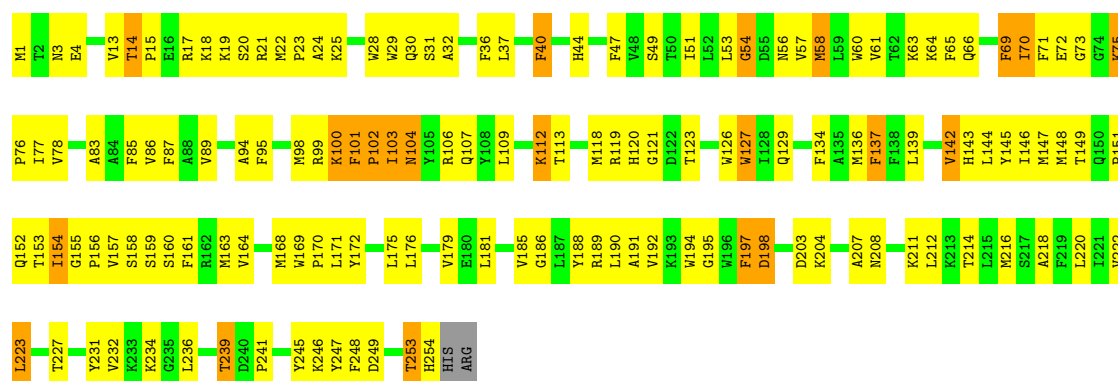
• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain I:



• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain L:



## 4 Data and refinement statistics

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

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | P 1 21 1                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 81.07Å 290.24Å 153.61Å<br>90.00° 95.73° 90.00° | Depositor |
| Resolution (Å)   | 30.00 – 3.10                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 80.8 (30.00-3.10)                              | Depositor |
| $R_{merge}$  | (Not available)                                | Depositor |
| $R_{sym}$  | 0.06   | Depositor |
| Refinement program                                       | CNS 1.0  | Depositor |
| R, $R_{free}$  | 0.283 , 0.291                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 37080  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 84.0   | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLA, NA, SF4, LMT, F3S, FES, HEM, FAD

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | A     | 0.58         | 0/5190      | 0.73        | 0/6996         |
| 1   | D     | 0.58         | 0/5190      | 0.73        | 0/6996         |
| 1   | G     | 0.58         | 0/5190      | 0.73        | 0/6996         |
| 1   | J     | 0.58         | 0/5190      | 0.73        | 0/6996         |
| 2   | B     | 0.47         | 0/1931      | 0.70        | 1/2604 (0.0%)  |
| 2   | E     | 0.47         | 0/1931      | 0.70        | 1/2604 (0.0%)  |
| 2   | H     | 0.47         | 0/1931      | 0.70        | 1/2604 (0.0%)  |
| 2   | K     | 0.47         | 0/1931      | 0.70        | 1/2604 (0.0%)  |
| 3   | C     | 0.60         | 0/2147      | 0.67        | 1/2904 (0.0%)  |
| 3   | F     | 0.60         | 0/2147      | 0.67        | 1/2904 (0.0%)  |
| 3   | I     | 0.60         | 0/2147      | 0.67        | 1/2904 (0.0%)  |
| 3   | L     | 0.60         | 0/2147      | 0.67        | 1/2904 (0.0%)  |
| All | All   | 0.56         | 0/37072     | 0.71        | 8/50016 (0.0%) |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | L     | 102 | PRO  | N-CA-C | -5.31 | 98.30       | 112.10   |
| 3   | F     | 102 | PRO  | N-CA-C | -5.30 | 98.31       | 112.10   |
| 3   | C     | 102 | PRO  | N-CA-C | -5.30 | 98.32       | 112.10   |
| 3   | I     | 102 | PRO  | N-CA-C | -5.30 | 98.32       | 112.10   |
| 2   | H     | 167 | ARG  | N-CA-C | -5.14 | 97.13       | 111.00   |
| 2   | E     | 167 | ARG  | N-CA-C | -5.13 | 97.15       | 111.00   |
| 2   | K     | 167 | ARG  | N-CA-C | -5.13 | 97.15       | 111.00   |
| 2   | B     | 167 | ARG  | N-CA-C | -5.12 | 97.16       | 111.00   |

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5094  | 0        | 5069     | 407     | 11           |
| 1   | D     | 5094  | 0        | 5069     | 408     | 16           |
| 1   | G     | 5094  | 0        | 5069     | 416     | 13           |
| 1   | J     | 5094  | 0        | 5069     | 413     | 14           |
| 2   | B     | 1894  | 0        | 1861     | 105     | 0            |
| 2   | E     | 1894  | 0        | 1861     | 106     | 0            |
| 2   | H     | 1894  | 0        | 1861     | 107     | 0            |
| 2   | K     | 1894  | 0        | 1861     | 103     | 0            |
| 3   | C     | 2081  | 0        | 2103     | 163     | 0            |
| 3   | F     | 2081  | 0        | 2103     | 163     | 0            |
| 3   | I     | 2081  | 0        | 2103     | 166     | 0            |
| 3   | L     | 2081  | 0        | 2103     | 162     | 0            |
| 4   | A     | 53    | 0        | 29       | 4       | 0            |
| 4   | D     | 53    | 0        | 29       | 4       | 0            |
| 4   | G     | 53    | 0        | 29       | 4       | 0            |
| 4   | J     | 53    | 0        | 29       | 4       | 0            |
| 5   | A     | 7     | 0        | 2        | 5       | 0            |
| 5   | D     | 7     | 0        | 2        | 5       | 0            |
| 5   | G     | 7     | 0        | 2        | 6       | 0            |
| 5   | J     | 7     | 0        | 2        | 5       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | G     | 1     | 0        | 0        | 0       | 0            |
| 6   | J     | 1     | 0        | 0        | 0       | 0            |
| 7   | B     | 4     | 0        | 0        | 0       | 0            |
| 7   | E     | 4     | 0        | 0        | 0       | 0            |
| 7   | H     | 4     | 0        | 0        | 0       | 0            |
| 7   | K     | 4     | 0        | 0        | 0       | 0            |
| 8   | B     | 7     | 0        | 0        | 2       | 0            |
| 8   | E     | 7     | 0        | 0        | 2       | 0            |
| 8   | H     | 7     | 0        | 0        | 2       | 0            |
| 8   | K     | 7     | 0        | 0        | 2       | 0            |
| 9   | B     | 8     | 0        | 0        | 0       | 0            |
| 9   | E     | 8     | 0        | 0        | 0       | 0            |
| 9   | H     | 8     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | K     | 8     | 0        | 0        | 0       | 0            |
| 10  | C     | 86    | 0        | 60       | 11      | 0            |
| 10  | F     | 86    | 0        | 60       | 12      | 0            |
| 10  | I     | 86    | 0        | 60       | 11      | 0            |
| 10  | L     | 86    | 0        | 60       | 11      | 0            |
| 11  | C     | 35    | 0        | 46       | 3       | 0            |
| 11  | F     | 35    | 0        | 46       | 3       | 0            |
| 11  | I     | 35    | 0        | 46       | 3       | 0            |
| 11  | L     | 35    | 0        | 46       | 3       | 0            |
| All | All   | 37080 | 0        | 36680    | 2632    | 27           |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (2632) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:216:THR:HG21 | 1:D:236:GLY:HA3  | 1.32        | 1.12     |
| 1:J:327:TRP:HB3  | 1:J:361:TRP:HB2  | 1.30        | 1.11     |
| 1:G:216:THR:HG21 | 1:G:236:GLY:HA3  | 1.32        | 1.09     |
| 3:L:152:GLN:HE21 | 3:L:153:THR:HG23 | 1.18        | 1.07     |
| 1:J:216:THR:HG21 | 1:J:236:GLY:HA3  | 1.32        | 1.06     |
| 1:G:327:TRP:HB3  | 1:G:361:TRP:HB2  | 1.30        | 1.06     |
| 1:D:327:TRP:HB3  | 1:D:361:TRP:HB2  | 1.30        | 1.06     |
| 3:C:152:GLN:HE21 | 3:C:153:THR:HG23 | 1.18        | 1.06     |
| 1:A:216:THR:HG21 | 1:A:236:GLY:HA3  | 1.32        | 1.05     |
| 1:A:327:TRP:HB3  | 1:A:361:TRP:HB2  | 1.30        | 1.05     |
| 3:I:152:GLN:HE21 | 3:I:153:THR:HG23 | 1.18        | 1.04     |
| 3:F:152:GLN:HE21 | 3:F:153:THR:HG23 | 1.18        | 1.04     |
| 3:L:30:GLN:HE22  | 3:L:100:LYS:HE3  | 1.26        | 1.01     |
| 3:C:30:GLN:HE22  | 3:C:100:LYS:HE3  | 1.26        | 1.00     |
| 3:I:30:GLN:HE22  | 3:I:100:LYS:HE3  | 1.26        | 0.99     |
| 3:F:30:GLN:HE22  | 3:F:100:LYS:HE3  | 1.26        | 0.99     |
| 1:J:281:ASP:HB2  | 1:J:285:HIS:CD2  | 2.01        | 0.96     |
| 3:F:142:VAL:HG21 | 3:F:171:LEU:HD11 | 1.48        | 0.95     |
| 1:A:281:ASP:HB2  | 1:A:285:HIS:CD2  | 2.01        | 0.95     |
| 1:A:269:THR:HG22 | 1:A:345:VAL:HG21 | 1.49        | 0.95     |
| 3:I:142:VAL:HG21 | 3:I:171:LEU:HD11 | 1.48        | 0.95     |
| 1:G:281:ASP:HB2  | 1:G:285:HIS:CD2  | 2.01        | 0.95     |
| 1:D:269:THR:HG22 | 1:D:345:VAL:HG21 | 1.49        | 0.95     |
| 1:D:281:ASP:HB2  | 1:D:285:HIS:CD2  | 2.01        | 0.94     |
| 3:L:142:VAL:HG21 | 3:L:171:LEU:HD11 | 1.48        | 0.94     |
| 1:G:269:THR:HG22 | 1:G:345:VAL:HG21 | 1.49        | 0.94     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:I:142:VAL:HG23 | 3:I:143:HIS:H    | 1.33        | 0.94     |
| 3:F:142:VAL:HG23 | 3:F:143:HIS:H    | 1.33        | 0.93     |
| 1:J:48:GLN:HG3   | 1:J:267:LEU:HD23 | 1.51        | 0.93     |
| 1:A:48:GLN:HG3   | 1:A:267:LEU:HD23 | 1.51        | 0.93     |
| 1:A:307:ARG:H    | 1:A:307:ARG:NH1  | 1.66        | 0.93     |
| 1:J:47:ALA:HB3   | 1:J:157:GLY:HA3  | 1.51        | 0.93     |
| 1:D:307:ARG:H    | 1:D:307:ARG:NH1  | 1.67        | 0.93     |
| 1:J:269:THR:HG22 | 1:J:345:VAL:HG21 | 1.49        | 0.93     |
| 1:A:47:ALA:HB3   | 1:A:157:GLY:HA3  | 1.51        | 0.93     |
| 1:D:288:MET:HB3  | 1:D:289:PRO:CD   | 1.99        | 0.92     |
| 3:C:142:VAL:HG21 | 3:C:171:LEU:HD11 | 1.48        | 0.92     |
| 1:G:48:GLN:HG3   | 1:G:267:LEU:HD23 | 1.51        | 0.92     |
| 1:A:286:ARG:HD2  | 1:A:288:MET:HE3  | 1.52        | 0.92     |
| 1:G:288:MET:HB3  | 1:G:289:PRO:CD   | 1.99        | 0.91     |
| 1:G:307:ARG:NH1  | 1:G:307:ARG:H    | 1.67        | 0.91     |
| 3:C:142:VAL:HG23 | 3:C:143:HIS:H    | 1.33        | 0.91     |
| 3:L:142:VAL:HG23 | 3:L:143:HIS:H    | 1.33        | 0.91     |
| 1:D:48:GLN:HG3   | 1:D:267:LEU:HD23 | 1.51        | 0.91     |
| 1:A:288:MET:HB3  | 1:A:289:PRO:CD   | 1.99        | 0.91     |
| 1:J:288:MET:HB3  | 1:J:289:PRO:CD   | 1.99        | 0.91     |
| 1:A:119:ILE:HG22 | 1:A:120:ASN:H    | 1.35        | 0.91     |
| 1:J:307:ARG:H    | 1:J:307:ARG:NH1  | 1.66        | 0.90     |
| 1:G:279:LEU:HD23 | 1:G:328:LEU:HD13 | 1.54        | 0.90     |
| 1:J:404:ARG:HE   | 1:J:409:SER:HB2  | 1.36        | 0.90     |
| 1:G:47:ALA:HB3   | 1:G:157:GLY:HA3  | 1.51        | 0.90     |
| 1:D:47:ALA:HB3   | 1:D:157:GLY:HA3  | 1.51        | 0.90     |
| 1:G:404:ARG:HE   | 1:G:409:SER:HB2  | 1.36        | 0.90     |
| 1:D:344:ASP:O    | 1:D:348:ILE:HG12 | 1.71        | 0.90     |
| 1:D:346:GLN:HA   | 1:D:357:PRO:HG2  | 1.54        | 0.90     |
| 1:A:344:ASP:O    | 1:A:348:ILE:HG12 | 1.71        | 0.90     |
| 1:A:346:GLN:HA   | 1:A:357:PRO:HG2  | 1.54        | 0.90     |
| 1:D:119:ILE:HG22 | 1:D:120:ASN:H    | 1.35        | 0.90     |
| 1:J:346:GLN:HA   | 1:J:357:PRO:HG2  | 1.54        | 0.90     |
| 1:A:107:TRP:HA   | 1:A:152:THR:HG22 | 1.53        | 0.90     |
| 1:A:404:ARG:HE   | 1:A:409:SER:HB2  | 1.36        | 0.90     |
| 1:J:307:ARG:N    | 1:J:307:ARG:HH11 | 1.70        | 0.90     |
| 1:A:279:LEU:HD23 | 1:A:328:LEU:HD13 | 1.54        | 0.90     |
| 1:J:258:PRO:HA   | 1:J:366:PRO:HG3  | 1.54        | 0.89     |
| 1:J:119:ILE:HG22 | 1:J:120:ASN:H    | 1.35        | 0.89     |
| 1:D:279:LEU:HD23 | 1:D:328:LEU:HD13 | 1.54        | 0.89     |
| 1:J:107:TRP:HA   | 1:J:152:THR:HG22 | 1.53        | 0.89     |
| 1:G:307:ARG:HH11 | 1:G:307:ARG:N    | 1.70        | 0.89     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:344:ASP:O    | 1:J:348:ILE:HG12 | 1.72        | 0.89     |
| 1:G:344:ASP:O    | 1:G:348:ILE:HG12 | 1.71        | 0.89     |
| 1:G:346:GLN:HA   | 1:G:357:PRO:HG2  | 1.54        | 0.89     |
| 1:D:258:PRO:HA   | 1:D:366:PRO:HG3  | 1.54        | 0.89     |
| 1:D:307:ARG:HH11 | 1:D:307:ARG:N    | 1.70        | 0.89     |
| 3:I:142:VAL:HG12 | 3:L:142:VAL:HA   | 1.52        | 0.89     |
| 1:G:119:ILE:HG22 | 1:G:120:ASN:H    | 1.36        | 0.89     |
| 1:D:107:TRP:HA   | 1:D:152:THR:HG22 | 1.53        | 0.88     |
| 1:A:258:PRO:HA   | 1:A:366:PRO:HG3  | 1.54        | 0.88     |
| 3:I:142:VAL:HA   | 3:L:142:VAL:HG12 | 1.54        | 0.88     |
| 1:G:258:PRO:HA   | 1:G:366:PRO:HG3  | 1.54        | 0.88     |
| 1:J:279:LEU:HD23 | 1:J:328:LEU:HD13 | 1.54        | 0.88     |
| 1:A:307:ARG:N    | 1:A:307:ARG:HH11 | 1.70        | 0.88     |
| 3:C:142:VAL:HG12 | 3:F:142:VAL:HA   | 1.53        | 0.88     |
| 1:D:404:ARG:HE   | 1:D:409:SER:HB2  | 1.36        | 0.88     |
| 1:G:107:TRP:HA   | 1:G:152:THR:HG22 | 1.53        | 0.88     |
| 3:C:142:VAL:HA   | 3:F:142:VAL:HG12 | 1.54        | 0.87     |
| 3:C:30:GLN:NE2   | 3:C:100:LYS:HE3  | 1.90        | 0.87     |
| 3:F:30:GLN:NE2   | 3:F:100:LYS:HE3  | 1.90        | 0.87     |
| 2:K:138:GLU:HB2  | 2:K:141:VAL:HG23 | 1.56        | 0.87     |
| 3:I:30:GLN:NE2   | 3:I:100:LYS:HE3  | 1.90        | 0.86     |
| 1:J:286:ARG:HD2  | 1:J:288:MET:HE3  | 1.57        | 0.86     |
| 1:G:286:ARG:HD2  | 1:G:288:MET:HE3  | 1.58        | 0.86     |
| 1:J:262:PHE:HB3  | 1:J:363:PRO:O    | 1.76        | 0.86     |
| 1:A:262:PHE:HB3  | 1:A:363:PRO:O    | 1.76        | 0.85     |
| 1:J:482:ARG:HB3  | 1:J:487:LEU:HD11 | 1.58        | 0.85     |
| 2:H:138:GLU:HB2  | 2:H:141:VAL:HG23 | 1.56        | 0.85     |
| 1:A:482:ARG:HB3  | 1:A:487:LEU:HD11 | 1.58        | 0.85     |
| 2:E:138:GLU:HB2  | 2:E:141:VAL:HG23 | 1.56        | 0.85     |
| 1:D:262:PHE:HB3  | 1:D:363:PRO:O    | 1.76        | 0.85     |
| 1:D:482:ARG:HB3  | 1:D:487:LEU:HD11 | 1.58        | 0.85     |
| 2:B:138:GLU:HB2  | 2:B:141:VAL:HG23 | 1.56        | 0.85     |
| 1:G:262:PHE:HB3  | 1:G:363:PRO:O    | 1.77        | 0.85     |
| 3:L:30:GLN:NE2   | 3:L:100:LYS:HE3  | 1.90        | 0.85     |
| 3:C:253:THR:HG22 | 3:C:254:HIS:H    | 1.42        | 0.84     |
| 1:G:287:PHE:CE1  | 1:G:291:TYR:HB2  | 2.13        | 0.84     |
| 1:D:287:PHE:CE1  | 1:D:291:TYR:HB2  | 2.13        | 0.84     |
| 1:J:287:PHE:HB3  | 1:J:296:LYS:HZ2  | 1.43        | 0.84     |
| 1:A:287:PHE:CE1  | 1:A:291:TYR:HB2  | 2.13        | 0.83     |
| 3:F:253:THR:HG22 | 3:F:254:HIS:H    | 1.41        | 0.83     |
| 1:G:482:ARG:HB3  | 1:G:487:LEU:HD11 | 1.58        | 0.83     |
| 3:L:253:THR:HG22 | 3:L:254:HIS:H    | 1.41        | 0.83     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:225:ASN:HB3  | 1:J:367:MET:HE2  | 1.61        | 0.83     |
| 1:J:287:PHE:CE1  | 1:J:291:TYR:HB2  | 2.13        | 0.83     |
| 3:F:100:LYS:HG2  | 10:F:302:HEM:O1A | 1.79        | 0.83     |
| 3:I:66:GLN:HB3   | 3:I:75:LYS:H     | 1.44        | 0.82     |
| 3:C:100:LYS:HG2  | 10:C:301:HEM:O1A | 1.79        | 0.82     |
| 3:F:66:GLN:HB3   | 3:F:75:LYS:H     | 1.45        | 0.82     |
| 1:D:286:ARG:HD2  | 1:D:288:MET:HE3  | 1.62        | 0.82     |
| 3:I:253:THR:HG22 | 3:I:254:HIS:H    | 1.41        | 0.82     |
| 1:D:87:ARG:HD2   | 1:D:640:TYR:CE2  | 2.15        | 0.81     |
| 1:J:87:ARG:HD2   | 1:J:640:TYR:CE2  | 2.15        | 0.81     |
| 1:G:87:ARG:HD2   | 1:G:640:TYR:CE2  | 2.15        | 0.81     |
| 1:A:87:ARG:HD2   | 1:A:640:TYR:CE2  | 2.15        | 0.81     |
| 1:G:252:GLU:HA   | 1:G:533:VAL:HG13 | 1.63        | 0.81     |
| 1:A:118:ILE:HD13 | 1:A:123:LYS:HE3  | 1.63        | 0.81     |
| 1:J:118:ILE:HD13 | 1:J:123:LYS:HE3  | 1.63        | 0.81     |
| 1:J:83:GLN:NE2   | 1:J:588:MET:HB3  | 1.95        | 0.81     |
| 1:D:83:GLN:NE2   | 1:D:588:MET:HB3  | 1.95        | 0.81     |
| 1:D:287:PHE:HB3  | 1:D:296:LYS:NZ   | 1.96        | 0.81     |
| 3:C:66:GLN:HB3   | 3:C:75:LYS:H     | 1.44        | 0.81     |
| 3:I:100:LYS:HG2  | 10:I:301:HEM:O1A | 1.79        | 0.81     |
| 3:L:100:LYS:HG2  | 10:L:302:HEM:O1A | 1.79        | 0.80     |
| 1:A:83:GLN:NE2   | 1:A:588:MET:HB3  | 1.95        | 0.80     |
| 3:F:142:VAL:HG23 | 3:F:143:HIS:N    | 1.96        | 0.80     |
| 1:G:83:GLN:NE2   | 1:G:588:MET:HB3  | 1.95        | 0.80     |
| 1:J:252:GLU:HA   | 1:J:533:VAL:HG13 | 1.63        | 0.80     |
| 3:I:142:VAL:HG23 | 3:I:143:HIS:N    | 1.96        | 0.80     |
| 1:J:87:ARG:HB3   | 1:J:640:TYR:CD2  | 2.17        | 0.80     |
| 1:D:118:ILE:HD13 | 1:D:123:LYS:HE3  | 1.63        | 0.80     |
| 1:A:287:PHE:HB3  | 1:A:296:LYS:NZ   | 1.96        | 0.80     |
| 3:L:66:GLN:HB3   | 3:L:75:LYS:H     | 1.45        | 0.80     |
| 1:J:287:PHE:HB3  | 1:J:296:LYS:NZ   | 1.96        | 0.80     |
| 3:L:142:VAL:HG23 | 3:L:143:HIS:N    | 1.96        | 0.80     |
| 1:A:225:ASN:HB3  | 1:A:367:MET:HE2  | 1.63        | 0.80     |
| 1:D:252:GLU:HA   | 1:D:533:VAL:HG13 | 1.63        | 0.80     |
| 1:G:87:ARG:HB3   | 1:G:640:TYR:CD2  | 2.17        | 0.79     |
| 1:A:252:GLU:HA   | 1:A:533:VAL:HG13 | 1.63        | 0.79     |
| 1:G:208:VAL:HG11 | 1:G:440:LEU:HD11 | 1.64        | 0.79     |
| 1:J:208:VAL:HG11 | 1:J:440:LEU:HD11 | 1.64        | 0.79     |
| 1:G:287:PHE:HB3  | 1:G:296:LYS:NZ   | 1.96        | 0.79     |
| 1:D:208:VAL:HG11 | 1:D:440:LEU:HD11 | 1.64        | 0.79     |
| 1:A:216:THR:CG2  | 1:A:236:GLY:HA3  | 2.13        | 0.79     |
| 3:C:142:VAL:HG23 | 3:C:143:HIS:N    | 1.96        | 0.79     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:87:ARG:HB3   | 1:D:640:TYR:CD2  | 2.17        | 0.79     |
| 1:G:118:ILE:HD13 | 1:G:123:LYS:HE3  | 1.63        | 0.78     |
| 1:A:208:VAL:HG11 | 1:A:440:LEU:HD11 | 1.64        | 0.78     |
| 1:A:83:GLN:HE21  | 1:A:588:MET:HB3  | 1.48        | 0.78     |
| 1:J:87:ARG:HD2   | 1:J:640:TYR:HE2  | 1.48        | 0.78     |
| 1:G:87:ARG:HD2   | 1:G:640:TYR:HE2  | 1.48        | 0.78     |
| 1:A:87:ARG:HB3   | 1:A:640:TYR:CD2  | 2.17        | 0.78     |
| 3:C:36:PHE:HD2   | 3:C:89:VAL:HG11  | 1.49        | 0.78     |
| 1:D:87:ARG:HD2   | 1:D:640:TYR:HE2  | 1.48        | 0.78     |
| 1:J:216:THR:CG2  | 1:J:236:GLY:HA3  | 2.13        | 0.77     |
| 1:J:83:GLN:HE21  | 1:J:588:MET:HB3  | 1.48        | 0.77     |
| 1:D:360:LYS:CG   | 1:D:361:TRP:H    | 1.97        | 0.77     |
| 1:A:360:LYS:CG   | 1:A:361:TRP:H    | 1.97        | 0.77     |
| 1:G:241:LEU:HB2  | 1:G:248:LEU:HD21 | 1.66        | 0.77     |
| 1:J:307:ARG:H    | 1:J:307:ARG:HH11 | 0.84        | 0.77     |
| 1:D:327:TRP:CB   | 1:D:361:TRP:HB2  | 2.14        | 0.77     |
| 2:K:179:VAL:HG21 | 2:K:199:ILE:HD13 | 1.67        | 0.77     |
| 1:G:360:LYS:CG   | 1:G:361:TRP:H    | 1.97        | 0.77     |
| 3:L:36:PHE:HD2   | 3:L:89:VAL:HG11  | 1.49        | 0.77     |
| 1:J:360:LYS:CG   | 1:J:361:TRP:H    | 1.97        | 0.76     |
| 2:H:179:VAL:HG21 | 2:H:199:ILE:HD13 | 1.67        | 0.76     |
| 1:A:612:ARG:O    | 1:A:616:ILE:HG13 | 1.86        | 0.76     |
| 1:G:83:GLN:HE21  | 1:G:588:MET:HB3  | 1.48        | 0.76     |
| 1:A:241:LEU:HB2  | 1:A:248:LEU:HD21 | 1.66        | 0.76     |
| 2:B:179:VAL:HG21 | 2:B:199:ILE:HD13 | 1.67        | 0.76     |
| 3:L:69:PHE:HD1   | 3:L:70:ILE:HG13  | 1.50        | 0.76     |
| 1:D:241:LEU:HB2  | 1:D:248:LEU:HD21 | 1.66        | 0.76     |
| 1:D:216:THR:CG2  | 1:D:236:GLY:HA3  | 2.13        | 0.76     |
| 1:J:612:ARG:O    | 1:J:616:ILE:HG13 | 1.86        | 0.76     |
| 1:J:241:LEU:HB2  | 1:J:248:LEU:HD21 | 1.66        | 0.76     |
| 1:D:83:GLN:HE21  | 1:D:588:MET:HB3  | 1.48        | 0.76     |
| 1:J:294:GLU:O    | 1:J:295:LYS:HG2  | 1.86        | 0.76     |
| 1:D:404:ARG:NE   | 1:D:409:SER:HB2  | 2.00        | 0.76     |
| 3:F:36:PHE:HD2   | 3:F:89:VAL:HG11  | 1.49        | 0.76     |
| 1:G:540:ARG:HH22 | 1:G:562:ASN:ND2  | 1.84        | 0.76     |
| 1:D:294:GLU:O    | 1:D:295:LYS:HG2  | 1.86        | 0.76     |
| 1:G:404:ARG:NE   | 1:G:409:SER:HB2  | 2.00        | 0.76     |
| 1:A:404:ARG:NE   | 1:A:409:SER:HB2  | 2.00        | 0.76     |
| 1:G:294:GLU:O    | 1:G:295:LYS:HG2  | 1.86        | 0.76     |
| 3:C:179:VAL:HG21 | 10:C:302:HEM:HAC | 1.66        | 0.76     |
| 1:J:404:ARG:NE   | 1:J:409:SER:HB2  | 2.00        | 0.76     |
| 3:F:69:PHE:HD1   | 3:F:70:ILE:HG13  | 1.50        | 0.76     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:225:ASN:HB3  | 1:D:367:MET:HE2  | 1.66        | 0.76     |
| 3:I:179:VAL:HG21 | 10:I:302:HEM:HAC | 1.66        | 0.76     |
| 1:G:612:ARG:O    | 1:G:616:ILE:HG13 | 1.86        | 0.76     |
| 3:I:69:PHE:HD1   | 3:I:70:ILE:HG13  | 1.50        | 0.75     |
| 3:C:29:TRP:HA    | 3:C:32:ALA:HB3   | 1.68        | 0.75     |
| 1:J:540:ARG:HH22 | 1:J:562:ASN:ND2  | 1.84        | 0.75     |
| 1:G:327:TRP:CB   | 1:G:361:TRP:HB2  | 2.14        | 0.75     |
| 1:D:540:ARG:HH22 | 1:D:562:ASN:ND2  | 1.84        | 0.75     |
| 3:C:69:PHE:HD1   | 3:C:70:ILE:HG13  | 1.50        | 0.75     |
| 3:I:36:PHE:HD2   | 3:I:89:VAL:HG11  | 1.49        | 0.75     |
| 1:J:286:ARG:HD2  | 1:J:288:MET:CE   | 2.17        | 0.75     |
| 3:L:179:VAL:HG21 | 10:L:303:HEM:HAC | 1.66        | 0.75     |
| 3:F:179:VAL:HG21 | 10:F:303:HEM:HAC | 1.66        | 0.75     |
| 1:A:294:GLU:O    | 1:A:295:LYS:HG2  | 1.86        | 0.75     |
| 1:A:87:ARG:HD2   | 1:A:640:TYR:HE2  | 1.48        | 0.75     |
| 1:D:286:ARG:HD2  | 1:D:288:MET:CE   | 2.17        | 0.75     |
| 1:A:286:ARG:HD2  | 1:A:288:MET:CE   | 2.17        | 0.74     |
| 1:G:286:ARG:HD2  | 1:G:288:MET:CE   | 2.17        | 0.74     |
| 3:I:134:PHE:O    | 3:I:137:PHE:HB2  | 1.87        | 0.74     |
| 1:A:540:ARG:HH22 | 1:A:562:ASN:ND2  | 1.84        | 0.74     |
| 3:F:134:PHE:O    | 3:F:137:PHE:HB2  | 1.87        | 0.74     |
| 1:G:225:ASN:HB3  | 1:G:367:MET:HE2  | 1.67        | 0.74     |
| 3:C:134:PHE:O    | 3:C:137:PHE:HB2  | 1.87        | 0.74     |
| 3:L:29:TRP:HA    | 3:L:32:ALA:HB3   | 1.68        | 0.74     |
| 1:J:277:GLY:HA3  | 1:J:330:ILE:HG22 | 1.70        | 0.74     |
| 1:J:327:TRP:CB   | 1:J:361:TRP:HB2  | 2.14        | 0.74     |
| 1:A:327:TRP:CB   | 1:A:361:TRP:HB2  | 2.14        | 0.74     |
| 2:E:179:VAL:HG21 | 2:E:199:ILE:HD13 | 1.67        | 0.74     |
| 1:G:277:GLY:HA3  | 1:G:330:ILE:HG22 | 1.70        | 0.74     |
| 3:F:76:PRO:HB2   | 3:F:151:PRO:HG2  | 1.70        | 0.74     |
| 1:G:216:THR:CG2  | 1:G:236:GLY:HA3  | 2.13        | 0.74     |
| 1:D:612:ARG:O    | 1:D:616:ILE:HG13 | 1.86        | 0.74     |
| 1:G:307:ARG:HH11 | 1:G:307:ARG:H    | 0.84        | 0.74     |
| 3:I:29:TRP:HA    | 3:I:32:ALA:HB3   | 1.68        | 0.74     |
| 3:F:152:GLN:NE2  | 3:F:153:THR:HG23 | 2.00        | 0.73     |
| 3:F:29:TRP:HA    | 3:F:32:ALA:HB3   | 1.68        | 0.73     |
| 3:L:134:PHE:O    | 3:L:137:PHE:HB2  | 1.87        | 0.73     |
| 3:L:76:PRO:HB2   | 3:L:151:PRO:HG2  | 1.70        | 0.73     |
| 3:C:76:PRO:HB2   | 3:C:151:PRO:HG2  | 1.70        | 0.73     |
| 3:L:152:GLN:NE2  | 3:L:153:THR:HG23 | 2.00        | 0.73     |
| 1:G:282:VAL:HG21 | 1:G:316:LYS:O    | 1.89        | 0.73     |
| 1:D:307:ARG:HH11 | 1:D:307:ARG:H    | 0.84        | 0.73     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:282:VAL:HG22 | 1:G:318:VAL:HG12 | 1.71        | 0.73     |
| 1:G:141:PHE:CZ   | 5:G:702:MLA:HC22 | 2.24        | 0.72     |
| 1:A:141:PHE:CZ   | 5:A:702:MLA:HC22 | 2.24        | 0.72     |
| 3:F:249:ASP:HA   | 3:F:254:HIS:HB3  | 1.71        | 0.72     |
| 3:L:249:ASP:HA   | 3:L:254:HIS:HB3  | 1.71        | 0.72     |
| 1:J:141:PHE:CZ   | 5:J:702:MLA:HC22 | 2.24        | 0.72     |
| 3:I:249:ASP:HA   | 3:I:254:HIS:HB3  | 1.71        | 0.72     |
| 1:J:282:VAL:HG21 | 1:J:316:LYS:O    | 1.89        | 0.72     |
| 1:G:327:TRP:HA   | 1:G:362:ALA:O    | 1.90        | 0.72     |
| 3:C:249:ASP:HA   | 3:C:254:HIS:HB3  | 1.71        | 0.72     |
| 1:A:282:VAL:HG22 | 1:A:318:VAL:HG12 | 1.71        | 0.72     |
| 1:D:2:LYS:HB2    | 1:D:2:LYS:NZ     | 2.05        | 0.72     |
| 1:D:282:VAL:HG21 | 1:D:316:LYS:O    | 1.88        | 0.72     |
| 1:J:48:GLN:CG    | 1:J:267:LEU:HD23 | 2.19        | 0.72     |
| 3:F:142:VAL:HG21 | 3:F:171:LEU:CD1  | 2.20        | 0.72     |
| 3:F:36:PHE:CD2   | 3:F:89:VAL:HG11  | 2.25        | 0.72     |
| 1:D:282:VAL:HG22 | 1:D:318:VAL:HG12 | 1.71        | 0.72     |
| 1:D:277:GLY:HA3  | 1:D:330:ILE:HG22 | 1.70        | 0.72     |
| 1:A:307:ARG:HH11 | 1:A:307:ARG:H    | 0.84        | 0.72     |
| 1:A:277:GLY:HA3  | 1:A:330:ILE:HG22 | 1.70        | 0.72     |
| 1:J:2:LYS:HB2    | 1:J:2:LYS:NZ     | 2.05        | 0.72     |
| 1:A:2:LYS:HB2    | 1:A:2:LYS:NZ     | 2.05        | 0.72     |
| 3:C:36:PHE:CD2   | 3:C:89:VAL:HG11  | 2.25        | 0.72     |
| 1:D:327:TRP:HA   | 1:D:362:ALA:O    | 1.90        | 0.72     |
| 3:I:36:PHE:CD2   | 3:I:89:VAL:HG11  | 2.25        | 0.72     |
| 1:D:141:PHE:CZ   | 5:D:702:MLA:HC22 | 2.24        | 0.71     |
| 1:D:48:GLN:CG    | 1:D:267:LEU:HD23 | 2.19        | 0.71     |
| 1:A:282:VAL:HG21 | 1:A:316:LYS:O    | 1.89        | 0.71     |
| 2:B:58:ARG:HG2   | 2:B:58:ARG:O     | 1.89        | 0.71     |
| 1:J:299:ALA:HB1  | 1:J:303:VAL:HG11 | 1.72        | 0.71     |
| 1:J:282:VAL:HG22 | 1:J:318:VAL:HG12 | 1.71        | 0.71     |
| 1:A:327:TRP:HA   | 1:A:362:ALA:O    | 1.90        | 0.71     |
| 3:L:36:PHE:CD2   | 3:L:89:VAL:HG11  | 2.25        | 0.71     |
| 1:G:469:ARG:O    | 1:G:473:VAL:HG23 | 1.90        | 0.71     |
| 3:I:142:VAL:HG21 | 3:I:171:LEU:CD1  | 2.20        | 0.71     |
| 1:D:314:LYS:HZ2  | 1:D:314:LYS:HB2  | 1.56        | 0.71     |
| 1:A:52:GLN:HG3   | 1:A:148:ARG:HG3  | 1.73        | 0.71     |
| 2:H:167:ARG:HH11 | 2:H:167:ARG:HG3  | 1.56        | 0.71     |
| 1:J:327:TRP:HA   | 1:J:362:ALA:O    | 1.90        | 0.71     |
| 1:D:287:PHE:HB3  | 1:D:296:LYS:HZ2  | 1.53        | 0.71     |
| 1:A:48:GLN:CG    | 1:A:267:LEU:HD23 | 2.19        | 0.71     |
| 1:G:252:GLU:HB2  | 1:G:537:ALA:HB2  | 1.72        | 0.71     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:252:GLU:HB2  | 1:D:537:ALA:HB2  | 1.72        | 0.71     |
| 1:A:252:GLU:HB2  | 1:A:537:ALA:HB2  | 1.72        | 0.71     |
| 1:G:48:GLN:CG    | 1:G:267:LEU:HD23 | 2.20        | 0.71     |
| 1:A:299:ALA:HB1  | 1:A:303:VAL:HG11 | 1.72        | 0.71     |
| 1:D:469:ARG:O    | 1:D:473:VAL:HG23 | 1.90        | 0.71     |
| 2:E:58:ARG:O     | 2:E:58:ARG:HG2   | 1.89        | 0.71     |
| 1:G:52:GLN:HG3   | 1:G:148:ARG:HG3  | 1.73        | 0.71     |
| 1:J:469:ARG:O    | 1:J:473:VAL:HG23 | 1.90        | 0.71     |
| 3:I:76:PRO:HB2   | 3:I:151:PRO:HG2  | 1.70        | 0.71     |
| 2:E:167:ARG:HG3  | 2:E:167:ARG:HH11 | 1.55        | 0.71     |
| 3:C:139:LEU:O    | 3:C:142:VAL:HG22 | 1.91        | 0.71     |
| 3:L:139:LEU:O    | 3:L:142:VAL:HG22 | 1.91        | 0.71     |
| 2:H:58:ARG:O     | 2:H:58:ARG:HG2   | 1.89        | 0.71     |
| 3:F:4:GLU:HB3    | 3:F:15:PRO:HG2   | 1.73        | 0.70     |
| 1:A:300:SER:O    | 1:A:304:VAL:HG23 | 1.91        | 0.70     |
| 3:I:139:LEU:O    | 3:I:142:VAL:HG22 | 1.91        | 0.70     |
| 3:L:142:VAL:CG2  | 3:L:143:HIS:H    | 2.04        | 0.70     |
| 1:D:558:ILE:HA   | 1:D:606:ASN:HD22 | 1.56        | 0.70     |
| 2:B:167:ARG:HH11 | 2:B:167:ARG:HG3  | 1.56        | 0.70     |
| 1:G:299:ALA:HB3  | 1:G:304:VAL:HG22 | 1.74        | 0.70     |
| 3:L:146:ILE:C    | 3:L:148:MET:H    | 1.95        | 0.70     |
| 1:J:558:ILE:HA   | 1:J:606:ASN:HD22 | 1.56        | 0.70     |
| 1:D:52:GLN:HE22  | 1:D:144:THR:HG21 | 1.56        | 0.70     |
| 1:J:9:LEU:HD23   | 1:J:10:VAL:H     | 1.56        | 0.70     |
| 1:G:2:LYS:HB2    | 1:G:2:LYS:NZ     | 2.05        | 0.70     |
| 1:J:252:GLU:HB2  | 1:J:537:ALA:HB2  | 1.72        | 0.70     |
| 3:F:18:LYS:HE3   | 3:F:21:ARG:HH12  | 1.57        | 0.70     |
| 1:A:9:LEU:HD23   | 1:A:10:VAL:H     | 1.56        | 0.70     |
| 1:J:414:VAL:O    | 1:J:418:MET:HG3  | 1.92        | 0.70     |
| 3:F:189:ARG:HG3  | 3:F:189:ARG:HH11 | 1.57        | 0.70     |
| 1:J:299:ALA:HB3  | 1:J:304:VAL:HG22 | 1.74        | 0.70     |
| 3:I:146:ILE:C    | 3:I:148:MET:H    | 1.95        | 0.70     |
| 1:D:52:GLN:HG3   | 1:D:148:ARG:HG3  | 1.73        | 0.70     |
| 1:J:562:ASN:H    | 1:J:562:ASN:HD22 | 1.40        | 0.70     |
| 3:C:146:ILE:C    | 3:C:148:MET:H    | 1.95        | 0.70     |
| 3:F:146:ILE:C    | 3:F:148:MET:H    | 1.95        | 0.70     |
| 3:F:139:LEU:O    | 3:F:142:VAL:HG22 | 1.91        | 0.70     |
| 3:C:4:GLU:HB3    | 3:C:15:PRO:HG2   | 1.73        | 0.70     |
| 2:K:167:ARG:HH11 | 2:K:167:ARG:HG3  | 1.56        | 0.70     |
| 1:D:300:SER:O    | 1:D:304:VAL:HG23 | 1.91        | 0.70     |
| 1:G:52:GLN:HE22  | 1:G:144:THR:HG21 | 1.56        | 0.70     |
| 1:J:52:GLN:HG3   | 1:J:148:ARG:HG3  | 1.73        | 0.70     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:J:300:SER:O    | 1:J:304:VAL:HG23  | 1.91        | 0.70     |
| 1:J:52:GLN:HE22  | 1:J:144:THR:HG21  | 1.56        | 0.70     |
| 1:D:414:VAL:O    | 1:D:418:MET:HG3   | 1.92        | 0.70     |
| 1:G:269:THR:CG2  | 1:G:345:VAL:HG21  | 2.22        | 0.70     |
| 3:C:152:GLN:NE2  | 3:C:153:THR:HG23  | 2.00        | 0.70     |
| 1:A:47:ALA:HB3   | 1:A:157:GLY:CA    | 2.22        | 0.70     |
| 2:K:58:ARG:HG2   | 2:K:58:ARG:O      | 1.89        | 0.70     |
| 3:I:4:GLU:HB3    | 3:I:15:PRO:HG2    | 1.73        | 0.70     |
| 3:I:189:ARG:HH11 | 3:I:189:ARG:HG3   | 1.57        | 0.70     |
| 1:A:414:VAL:O    | 1:A:418:MET:HG3   | 1.92        | 0.69     |
| 3:I:18:LYS:HE3   | 3:I:21:ARG:HH12   | 1.57        | 0.69     |
| 3:C:18:LYS:HE3   | 3:C:21:ARG:HH12   | 1.57        | 0.69     |
| 1:G:300:SER:O    | 1:G:304:VAL:HG23  | 1.91        | 0.69     |
| 1:A:469:ARG:O    | 1:A:473:VAL:HG23  | 1.90        | 0.69     |
| 2:E:1:MET:CE     | 2:E:31:ALA:HA     | 2.22        | 0.69     |
| 1:A:299:ALA:HB3  | 1:A:304:VAL:HG22  | 1.74        | 0.69     |
| 3:I:152:GLN:NE2  | 3:I:153:THR:HG23  | 2.00        | 0.69     |
| 3:F:175:LEU:HG   | 10:F:303:HEM:HMD3 | 1.75        | 0.69     |
| 3:I:142:VAL:CG2  | 3:I:143:HIS:H     | 2.04        | 0.69     |
| 1:G:562:ASN:H    | 1:G:562:ASN:HD22  | 1.39        | 0.69     |
| 2:B:1:MET:CE     | 2:B:31:ALA:HA     | 2.22        | 0.69     |
| 2:H:1:MET:CE     | 2:H:31:ALA:HA     | 2.22        | 0.69     |
| 1:G:141:PHE:HZ   | 5:G:702:MLA:HC22  | 1.58        | 0.69     |
| 1:G:47:ALA:HB3   | 1:G:157:GLY:CA    | 2.22        | 0.69     |
| 1:A:558:ILE:HA   | 1:A:606:ASN:HD22  | 1.56        | 0.69     |
| 1:G:558:ILE:HA   | 1:G:606:ASN:HD22  | 1.56        | 0.69     |
| 2:B:179:VAL:HG13 | 2:B:195:TYR:HD2   | 1.58        | 0.69     |
| 1:J:269:THR:CG2  | 1:J:345:VAL:HG21  | 2.22        | 0.69     |
| 1:G:299:ALA:HB1  | 1:G:303:VAL:HG11  | 1.72        | 0.69     |
| 1:D:299:ALA:HB1  | 1:D:303:VAL:HG11  | 1.72        | 0.69     |
| 3:C:175:LEU:HG   | 10:C:302:HEM:HMD3 | 1.75        | 0.69     |
| 3:C:142:VAL:HG21 | 3:C:171:LEU:CD1   | 2.20        | 0.69     |
| 1:A:52:GLN:HE22  | 1:A:144:THR:HG21  | 1.56        | 0.69     |
| 1:A:269:THR:CG2  | 1:A:345:VAL:HG21  | 2.21        | 0.69     |
| 3:F:142:VAL:CG2  | 3:F:143:HIS:H     | 2.04        | 0.69     |
| 1:G:52:GLN:NE2   | 1:G:144:THR:HG21  | 2.08        | 0.69     |
| 1:D:9:LEU:HD23   | 1:D:10:VAL:H      | 1.56        | 0.69     |
| 3:C:189:ARG:HH11 | 3:C:189:ARG:HG3   | 1.57        | 0.69     |
| 3:L:142:VAL:HG21 | 3:L:171:LEU:CD1   | 2.20        | 0.68     |
| 1:D:47:ALA:HB3   | 1:D:157:GLY:CA    | 2.22        | 0.68     |
| 2:K:179:VAL:HG13 | 2:K:195:TYR:HD2   | 1.58        | 0.68     |
| 1:D:52:GLN:NE2   | 1:D:144:THR:HG21  | 2.08        | 0.68     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:L:189:ARG:HG3  | 3:L:189:ARG:HH11 | 1.57        | 0.68     |
| 3:L:94:ALA:HB2   | 10:L:302:HEM:HAB | 1.75        | 0.68     |
| 3:I:156:PRO:HD2  | 3:I:254:HIS:NE2  | 2.08        | 0.68     |
| 3:L:18:LYS:HE3   | 3:L:21:ARG:HH12  | 1.57        | 0.68     |
| 1:G:9:LEU:HD23   | 1:G:10:VAL:H     | 1.56        | 0.68     |
| 1:G:535:LYS:HG3  | 1:G:578:LEU:HD11 | 1.75        | 0.68     |
| 1:D:299:ALA:HB3  | 1:D:304:VAL:HG22 | 1.74        | 0.68     |
| 1:D:325:HIS:HB2  | 1:D:364:VAL:O    | 1.93        | 0.68     |
| 1:A:288:MET:HB3  | 1:A:289:PRO:HD3  | 1.76        | 0.68     |
| 3:C:126:TRP:O    | 3:C:129:GLN:N    | 2.27        | 0.68     |
| 1:D:540:ARG:NH2  | 1:D:562:ASN:ND2  | 2.42        | 0.68     |
| 1:G:414:VAL:O    | 1:G:418:MET:HG3  | 1.92        | 0.68     |
| 2:K:1:MET:CE     | 2:K:31:ALA:HA    | 2.22        | 0.68     |
| 1:G:325:HIS:HB2  | 1:G:364:VAL:O    | 1.93        | 0.68     |
| 1:G:154:ASP:OD2  | 1:G:345:VAL:HG23 | 1.94        | 0.68     |
| 1:D:141:PHE:HZ   | 5:D:702:MLA:HC22 | 1.58        | 0.68     |
| 3:I:175:LEU:O    | 3:I:175:LEU:HD12 | 1.94        | 0.68     |
| 1:J:447:GLN:OE1  | 1:J:447:GLN:HA   | 1.94        | 0.68     |
| 2:E:68:MET:HB2   | 2:E:92:LEU:HB2   | 1.76        | 0.68     |
| 1:G:288:MET:HB3  | 1:G:289:PRO:HD3  | 1.76        | 0.68     |
| 3:I:126:TRP:O    | 3:I:129:GLN:N    | 2.27        | 0.68     |
| 3:L:126:TRP:O    | 3:L:129:GLN:N    | 2.27        | 0.68     |
| 1:A:314:LYS:HB2  | 1:A:314:LYS:NZ   | 2.09        | 0.68     |
| 1:D:360:LYS:HG3  | 1:D:361:TRP:H    | 1.58        | 0.68     |
| 1:A:52:GLN:NE2   | 1:A:144:THR:HG21 | 2.08        | 0.68     |
| 1:D:24:THR:OG1   | 1:D:31:THR:HG21  | 1.94        | 0.68     |
| 3:F:156:PRO:HD2  | 3:F:254:HIS:NE2  | 2.09        | 0.68     |
| 2:E:179:VAL:HG13 | 2:E:195:TYR:HD2  | 1.58        | 0.68     |
| 1:J:52:GLN:NE2   | 1:J:144:THR:HG21 | 2.08        | 0.68     |
| 1:J:325:HIS:HB2  | 1:J:364:VAL:O    | 1.93        | 0.68     |
| 1:A:360:LYS:HG3  | 1:A:361:TRP:H    | 1.58        | 0.68     |
| 1:D:447:GLN:HA   | 1:D:447:GLN:OE1  | 1.94        | 0.68     |
| 3:L:4:GLU:HB3    | 3:L:15:PRO:HG2   | 1.73        | 0.68     |
| 1:A:24:THR:OG1   | 1:A:31:THR:HG21  | 1.94        | 0.68     |
| 1:G:314:LYS:HB2  | 1:G:314:LYS:NZ   | 2.09        | 0.68     |
| 1:J:141:PHE:HZ   | 5:J:702:MLA:HC22 | 1.58        | 0.68     |
| 3:C:94:ALA:HB2   | 10:C:301:HEM:HAB | 1.75        | 0.68     |
| 3:F:94:ALA:HB2   | 10:F:302:HEM:HAB | 1.75        | 0.68     |
| 1:J:314:LYS:NZ   | 1:J:314:LYS:HB2  | 2.09        | 0.68     |
| 1:A:535:LYS:HG3  | 1:A:578:LEU:HD11 | 1.75        | 0.68     |
| 1:G:540:ARG:NH2  | 1:G:562:ASN:ND2  | 2.42        | 0.68     |
| 1:A:540:ARG:NH2  | 1:A:562:ASN:ND2  | 2.42        | 0.68     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:D:314:LYS:NZ   | 1:D:314:LYS:HB2   | 2.09        | 0.68     |
| 2:H:2:GLY:HA2    | 2:H:29:GLU:OE2    | 1.94        | 0.68     |
| 2:K:68:MET:HB2   | 2:K:92:LEU:HB2    | 1.76        | 0.68     |
| 1:J:303:VAL:HG12 | 1:J:304:VAL:N     | 2.09        | 0.67     |
| 1:J:154:ASP:OD2  | 1:J:345:VAL:HG23  | 1.94        | 0.67     |
| 1:D:269:THR:CG2  | 1:D:345:VAL:HG21  | 2.22        | 0.67     |
| 3:F:175:LEU:HD12 | 3:F:175:LEU:O     | 1.94        | 0.67     |
| 1:J:47:ALA:HB3   | 1:J:157:GLY:CA    | 2.22        | 0.67     |
| 3:C:156:PRO:HD2  | 3:C:254:HIS:NE2   | 2.08        | 0.67     |
| 2:H:179:VAL:HG13 | 2:H:195:TYR:HD2   | 1.58        | 0.67     |
| 1:A:562:ASN:HD22 | 1:A:562:ASN:H     | 1.39        | 0.67     |
| 2:H:68:MET:HB2   | 2:H:92:LEU:HB2    | 1.76        | 0.67     |
| 2:B:2:GLY:HA2    | 2:B:29:GLU:OE2    | 1.94        | 0.67     |
| 1:J:360:LYS:CG   | 1:J:361:TRP:N     | 2.57        | 0.67     |
| 1:A:303:VAL:HG12 | 1:A:304:VAL:N     | 2.09        | 0.67     |
| 3:I:94:ALA:HB2   | 10:I:301:HEM:HAB  | 1.75        | 0.67     |
| 3:L:175:LEU:HG   | 10:L:303:HEM:HMD3 | 1.75        | 0.67     |
| 3:L:156:PRO:HD2  | 3:L:254:HIS:NE2   | 2.08        | 0.67     |
| 2:H:179:VAL:HG13 | 2:H:195:TYR:CD2   | 2.30        | 0.67     |
| 2:B:179:VAL:HG13 | 2:B:195:TYR:CD2   | 2.30        | 0.67     |
| 2:E:179:VAL:HG13 | 2:E:195:TYR:CD2   | 2.30        | 0.67     |
| 1:D:574:THR:O    | 1:D:575:LEU:HD23  | 1.95        | 0.67     |
| 1:A:141:PHE:HZ   | 5:A:702:MLA:HC22  | 1.58        | 0.67     |
| 1:G:273:ARG:HA   | 1:G:277:GLY:O     | 1.95        | 0.67     |
| 1:D:535:LYS:HG3  | 1:D:578:LEU:HD11  | 1.75        | 0.67     |
| 3:C:175:LEU:HD12 | 3:C:175:LEU:O     | 1.94        | 0.67     |
| 1:D:562:ASN:H    | 1:D:562:ASN:HD22  | 1.40        | 0.67     |
| 1:G:314:LYS:HB2  | 1:G:314:LYS:HZ2   | 1.58        | 0.67     |
| 2:K:2:GLY:HA2    | 2:K:29:GLU:OE2    | 1.94        | 0.67     |
| 1:J:574:THR:O    | 1:J:575:LEU:HD23  | 1.95        | 0.67     |
| 1:J:216:THR:HG21 | 1:J:236:GLY:CA    | 2.19        | 0.67     |
| 1:A:496:GLU:O    | 1:A:500:LYS:HG3   | 1.95        | 0.67     |
| 1:G:303:VAL:HG12 | 1:G:304:VAL:N     | 2.09        | 0.67     |
| 1:A:325:HIS:HB2  | 1:A:364:VAL:O     | 1.93        | 0.67     |
| 1:J:24:THR:OG1   | 1:J:31:THR:HG21   | 1.94        | 0.67     |
| 1:A:154:ASP:OD2  | 1:A:345:VAL:HG23  | 1.94        | 0.67     |
| 3:L:175:LEU:HD12 | 3:L:175:LEU:O     | 1.94        | 0.67     |
| 1:J:540:ARG:NH2  | 1:J:562:ASN:ND2   | 2.42        | 0.67     |
| 1:G:447:GLN:OE1  | 1:G:447:GLN:HA    | 1.94        | 0.67     |
| 1:A:574:THR:O    | 1:A:575:LEU:HD23  | 1.95        | 0.67     |
| 2:E:2:GLY:HA2    | 2:E:29:GLU:OE2    | 1.94        | 0.67     |
| 1:G:24:THR:OG1   | 1:G:31:THR:HG21   | 1.94        | 0.67     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:D:154:ASP:OD2  | 1:D:345:VAL:HG23  | 1.94        | 0.67     |
| 3:F:157:VAL:HB   | 3:F:254:HIS:HE1   | 1.60        | 0.67     |
| 2:K:179:VAL:HG13 | 2:K:195:TYR:CD2   | 2.30        | 0.67     |
| 3:F:126:TRP:O    | 3:F:129:GLN:N     | 2.27        | 0.67     |
| 1:J:535:LYS:HG3  | 1:J:578:LEU:HD11  | 1.75        | 0.67     |
| 3:C:142:VAL:CG2  | 3:C:143:HIS:H     | 2.04        | 0.66     |
| 1:A:447:GLN:HA   | 1:A:447:GLN:OE1   | 1.94        | 0.66     |
| 1:G:289:PRO:HG3  | 1:G:295:LYS:HA    | 1.77        | 0.66     |
| 1:D:303:VAL:HG12 | 1:D:304:VAL:N     | 2.09        | 0.66     |
| 3:I:175:LEU:HG   | 10:I:302:HEM:HMD3 | 1.75        | 0.66     |
| 1:A:64:ASP:HA    | 1:A:68:LEU:HD12   | 1.78        | 0.66     |
| 1:J:288:MET:HB3  | 1:J:289:PRO:HD3   | 1.76        | 0.66     |
| 1:D:289:PRO:HG3  | 1:D:295:LYS:HA    | 1.77        | 0.66     |
| 1:A:360:LYS:CG   | 1:A:361:TRP:N     | 2.57        | 0.66     |
| 1:D:273:ARG:HA   | 1:D:277:GLY:O     | 1.95        | 0.66     |
| 2:B:68:MET:HB2   | 2:B:92:LEU:HB2    | 1.76        | 0.66     |
| 1:D:496:GLU:O    | 1:D:500:LYS:HG3   | 1.95        | 0.66     |
| 1:J:285:HIS:CD2  | 1:J:285:HIS:N     | 2.64        | 0.66     |
| 1:J:360:LYS:HG3  | 1:J:361:TRP:H     | 1.58        | 0.66     |
| 1:D:360:LYS:CG   | 1:D:361:TRP:N     | 2.58        | 0.66     |
| 1:A:279:LEU:N    | 1:A:288:MET:HE1   | 2.11        | 0.66     |
| 1:A:287:PHE:HB3  | 1:A:296:LYS:HZ2   | 1.56        | 0.66     |
| 3:L:157:VAL:HB   | 3:L:254:HIS:HE1   | 1.60        | 0.66     |
| 1:J:289:PRO:HG3  | 1:J:295:LYS:HA    | 1.77        | 0.66     |
| 1:G:360:LYS:CG   | 1:G:361:TRP:N     | 2.57        | 0.66     |
| 1:A:289:PRO:HG3  | 1:A:295:LYS:HA    | 1.77        | 0.66     |
| 1:J:496:GLU:O    | 1:J:500:LYS:HG3   | 1.95        | 0.66     |
| 1:G:216:THR:HG21 | 1:G:236:GLY:CA    | 2.19        | 0.66     |
| 3:C:157:VAL:HB   | 3:C:254:HIS:HE1   | 1.60        | 0.66     |
| 1:J:540:ARG:HH22 | 1:J:562:ASN:HD22  | 1.44        | 0.66     |
| 1:D:463:VAL:HB   | 1:D:504:VAL:HG11  | 1.78        | 0.66     |
| 1:G:285:HIS:N    | 1:G:285:HIS:CD2   | 2.64        | 0.66     |
| 1:D:286:ARG:C    | 1:D:288:MET:H     | 1.99        | 0.66     |
| 1:D:288:MET:HB3  | 1:D:289:PRO:HD3   | 1.76        | 0.66     |
| 1:G:64:ASP:HA    | 1:G:68:LEU:HD12   | 1.78        | 0.66     |
| 1:G:287:PHE:HB3  | 1:G:296:LYS:HZ2   | 1.59        | 0.66     |
| 1:G:360:LYS:HG3  | 1:G:361:TRP:H     | 1.58        | 0.66     |
| 1:A:289:PRO:HB3  | 1:A:293:PRO:HA    | 1.78        | 0.66     |
| 1:G:574:THR:O    | 1:G:575:LEU:HD23  | 1.95        | 0.66     |
| 1:G:496:GLU:O    | 1:G:500:LYS:HG3   | 1.95        | 0.66     |
| 1:J:273:ARG:HA   | 1:J:277:GLY:O     | 1.95        | 0.66     |
| 1:A:273:ARG:HA   | 1:A:277:GLY:O     | 1.95        | 0.66     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:H:125:GLN:HB2  | 2:H:189:GLU:OE1   | 1.96        | 0.66     |
| 2:B:125:GLN:HB2  | 2:B:189:GLU:OE1   | 1.96        | 0.66     |
| 1:G:289:PRO:HB3  | 1:G:293:PRO:HA    | 1.78        | 0.66     |
| 3:L:83:ALA:HA    | 10:L:303:HEM:HBB1 | 1.78        | 0.66     |
| 2:E:125:GLN:HB2  | 2:E:189:GLU:OE1   | 1.96        | 0.65     |
| 3:C:175:LEU:HG   | 10:C:302:HEM:CMD  | 2.26        | 0.65     |
| 1:J:463:VAL:HB   | 1:J:504:VAL:HG11  | 1.77        | 0.65     |
| 3:C:181:LEU:O    | 3:C:185:VAL:HG23  | 1.96        | 0.65     |
| 3:F:40:PHE:CE1   | 3:F:86:VAL:HG21   | 2.32        | 0.65     |
| 3:F:13:VAL:HG22  | 3:F:18:LYS:N      | 2.12        | 0.65     |
| 1:A:195:VAL:HG11 | 1:A:447:GLN:HG3   | 1.78        | 0.65     |
| 3:C:40:PHE:CE1   | 3:C:86:VAL:HG21   | 2.31        | 0.65     |
| 3:L:40:PHE:CE1   | 3:L:86:VAL:HG21   | 2.32        | 0.65     |
| 1:J:289:PRO:HB3  | 1:J:293:PRO:HA    | 1.78        | 0.65     |
| 1:J:64:ASP:HA    | 1:J:68:LEU:HD12   | 1.78        | 0.65     |
| 3:L:181:LEU:O    | 3:L:185:VAL:HG23  | 1.96        | 0.65     |
| 1:J:287:PHE:CD1  | 1:J:291:TYR:HB2   | 2.32        | 0.65     |
| 3:I:83:ALA:HA    | 10:I:302:HEM:HBB1 | 1.78        | 0.65     |
| 3:I:157:VAL:HB   | 3:I:254:HIS:HE1   | 1.60        | 0.65     |
| 1:J:286:ARG:C    | 1:J:288:MET:H     | 2.00        | 0.65     |
| 1:D:285:HIS:N    | 1:D:285:HIS:CD2   | 2.64        | 0.65     |
| 3:F:175:LEU:HG   | 10:F:303:HEM:CMD  | 2.27        | 0.65     |
| 1:G:330:ILE:O    | 1:G:338:ILE:HD11  | 1.97        | 0.65     |
| 1:D:64:ASP:HA    | 1:D:68:LEU:HD12   | 1.78        | 0.65     |
| 3:I:13:VAL:HG22  | 3:I:18:LYS:N      | 2.12        | 0.65     |
| 3:C:103:ILE:O    | 3:C:104:ASN:HB3   | 1.97        | 0.65     |
| 1:A:285:HIS:N    | 1:A:285:HIS:CD2   | 2.64        | 0.65     |
| 3:I:103:ILE:O    | 3:I:104:ASN:HB3   | 1.97        | 0.65     |
| 1:D:287:PHE:CD1  | 1:D:291:TYR:HB2   | 2.32        | 0.65     |
| 1:J:330:ILE:O    | 1:J:338:ILE:HD11  | 1.97        | 0.65     |
| 3:I:40:PHE:CE1   | 3:I:86:VAL:HG21   | 2.32        | 0.65     |
| 3:F:181:LEU:O    | 3:F:185:VAL:HG23  | 1.96        | 0.65     |
| 1:G:286:ARG:C    | 1:G:288:MET:H     | 2.00        | 0.64     |
| 3:I:142:VAL:CG2  | 3:I:171:LEU:HD11  | 2.25        | 0.64     |
| 1:G:241:LEU:HD12 | 1:G:248:LEU:CD2   | 2.28        | 0.64     |
| 1:A:241:LEU:HD12 | 1:A:248:LEU:CD2   | 2.27        | 0.64     |
| 3:F:103:ILE:O    | 3:F:104:ASN:HB3   | 1.97        | 0.64     |
| 1:J:279:LEU:N    | 1:J:288:MET:HE1   | 2.12        | 0.64     |
| 1:J:195:VAL:HG11 | 1:J:447:GLN:HG3   | 1.78        | 0.64     |
| 3:C:87:PHE:CD2   | 3:C:144:LEU:HD13  | 2.32        | 0.64     |
| 1:A:287:PHE:CD1  | 1:A:291:TYR:HB2   | 2.32        | 0.64     |
| 3:L:175:LEU:HG   | 10:L:303:HEM:CMD  | 2.26        | 0.64     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:G:287:PHE:CD1  | 1:G:291:TYR:HB2   | 2.32        | 0.64     |
| 1:D:289:PRO:HB3  | 1:D:293:PRO:HA    | 1.78        | 0.64     |
| 1:A:119:ILE:HG22 | 1:A:120:ASN:N     | 2.10        | 0.64     |
| 3:C:13:VAL:HG22  | 3:C:18:LYS:N      | 2.12        | 0.64     |
| 1:G:463:VAL:HB   | 1:G:504:VAL:HG11  | 1.78        | 0.64     |
| 1:A:463:VAL:HB   | 1:A:504:VAL:HG11  | 1.77        | 0.64     |
| 1:D:242:GLU:HG2  | 1:D:528:LYS:NZ    | 2.13        | 0.64     |
| 3:I:181:LEU:O    | 3:I:185:VAL:HG23  | 1.96        | 0.64     |
| 1:D:288:MET:C    | 1:D:290:ASP:H     | 2.01        | 0.64     |
| 3:I:145:TYR:CE2  | 3:I:149:THR:HG21  | 2.33        | 0.64     |
| 1:D:540:ARG:HH22 | 1:D:562:ASN:HD22  | 1.44        | 0.64     |
| 1:A:330:ILE:O    | 1:A:338:ILE:HD11  | 1.97        | 0.64     |
| 2:E:1:MET:HE3    | 2:E:31:ALA:HA     | 1.77        | 0.64     |
| 1:D:195:VAL:HG11 | 1:D:447:GLN:HG3   | 1.78        | 0.64     |
| 3:I:175:LEU:HG   | 10:I:302:HEM:CMD  | 2.26        | 0.64     |
| 3:L:103:ILE:O    | 3:L:103:ILE:HG12  | 1.98        | 0.64     |
| 3:C:83:ALA:HA    | 10:C:302:HEM:HBB1 | 1.78        | 0.64     |
| 1:D:330:ILE:O    | 1:D:338:ILE:HD11  | 1.97        | 0.64     |
| 3:C:145:TYR:CE2  | 3:C:149:THR:HG21  | 2.33        | 0.64     |
| 1:A:242:GLU:HG2  | 1:A:528:LYS:NZ    | 2.13        | 0.64     |
| 1:J:287:PHE:C    | 1:J:290:ASP:HB3   | 2.18        | 0.64     |
| 1:G:287:PHE:C    | 1:G:290:ASP:HB3   | 2.18        | 0.64     |
| 1:G:540:ARG:HH22 | 1:G:562:ASN:HD22  | 1.44        | 0.64     |
| 1:G:279:LEU:N    | 1:G:288:MET:HE1   | 2.12        | 0.64     |
| 1:D:287:PHE:C    | 1:D:290:ASP:HB3   | 2.18        | 0.64     |
| 1:A:288:MET:C    | 1:A:290:ASP:H     | 2.01        | 0.64     |
| 3:L:13:VAL:HG22  | 3:L:18:LYS:N      | 2.12        | 0.64     |
| 2:K:125:GLN:HB2  | 2:K:189:GLU:OE1   | 1.96        | 0.64     |
| 3:F:142:VAL:CG2  | 3:F:171:LEU:HD11  | 2.25        | 0.64     |
| 1:D:241:LEU:HD12 | 1:D:248:LEU:CD2   | 2.27        | 0.64     |
| 1:G:195:VAL:HG11 | 1:G:447:GLN:HG3   | 1.78        | 0.64     |
| 1:A:287:PHE:C    | 1:A:290:ASP:HB3   | 2.18        | 0.64     |
| 3:L:145:TYR:CE2  | 3:L:149:THR:HG21  | 2.33        | 0.64     |
| 1:J:241:LEU:HD12 | 1:J:248:LEU:CD2   | 2.28        | 0.64     |
| 1:G:242:GLU:HG2  | 1:G:528:LYS:NZ    | 2.13        | 0.64     |
| 1:A:286:ARG:C    | 1:A:288:MET:H     | 2.00        | 0.63     |
| 3:F:83:ALA:HA    | 10:F:303:HEM:HBB1 | 1.78        | 0.63     |
| 3:L:142:VAL:CG2  | 3:L:171:LEU:HD11  | 2.25        | 0.63     |
| 1:A:540:ARG:HH22 | 1:A:562:ASN:HD22  | 1.44        | 0.63     |
| 2:K:1:MET:HE2    | 2:K:30:GLU:O      | 1.98        | 0.63     |
| 3:F:145:TYR:CE2  | 3:F:149:THR:HG21  | 2.33        | 0.63     |
| 3:I:87:PHE:CD2   | 3:I:144:LEU:HD13  | 2.32        | 0.63     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:L:87:PHE:CD2   | 3:L:144:LEU:HD13 | 2.32        | 0.63     |
| 1:G:288:MET:C    | 1:G:290:ASP:H    | 2.01        | 0.63     |
| 3:L:103:ILE:O    | 3:L:104:ASN:HB3  | 1.97        | 0.63     |
| 1:J:288:MET:C    | 1:J:290:ASP:H    | 2.01        | 0.63     |
| 1:G:293:PRO:C    | 1:G:294:GLU:HG3  | 2.19        | 0.63     |
| 1:A:360:LYS:HG2  | 1:A:361:TRP:O    | 1.99        | 0.63     |
| 1:G:41:ARG:HH11  | 1:G:41:ARG:HG2   | 1.63        | 0.63     |
| 1:D:293:PRO:C    | 1:D:294:GLU:HG3  | 2.19        | 0.63     |
| 2:E:1:MET:HE2    | 2:E:30:GLU:O     | 1.99        | 0.63     |
| 2:H:1:MET:HE2    | 2:H:30:GLU:O     | 1.98        | 0.63     |
| 1:G:242:GLU:HG2  | 1:G:528:LYS:HZ1  | 1.64        | 0.63     |
| 1:G:15:LEU:HB2   | 1:G:44:SER:OG    | 1.98        | 0.63     |
| 1:D:41:ARG:HG2   | 1:D:41:ARG:HH11  | 1.63        | 0.63     |
| 1:J:293:PRO:C    | 1:J:294:GLU:HG3  | 2.19        | 0.63     |
| 1:D:15:LEU:HB2   | 1:D:44:SER:OG    | 1.98        | 0.63     |
| 1:A:15:LEU:HB2   | 1:A:44:SER:OG    | 1.98        | 0.63     |
| 1:A:216:THR:HG21 | 1:A:236:GLY:CA   | 2.19        | 0.63     |
| 1:A:41:ARG:HH11  | 1:A:41:ARG:HG2   | 1.63        | 0.63     |
| 3:F:87:PHE:CD2   | 3:F:144:LEU:HD13 | 2.32        | 0.63     |
| 1:J:41:ARG:HH11  | 1:J:41:ARG:HG2   | 1.63        | 0.63     |
| 1:J:570:ASN:ND2  | 1:J:571:PRO:HD2  | 2.14        | 0.63     |
| 1:D:288:MET:CB   | 1:D:289:PRO:CD   | 2.76        | 0.62     |
| 1:G:302:ASP:O    | 1:G:306:ARG:HD3  | 1.99        | 0.62     |
| 2:K:205:VAL:HG13 | 2:K:206:PHE:CD2  | 2.34        | 0.62     |
| 2:B:205:VAL:HG13 | 2:B:206:PHE:CD2  | 2.34        | 0.62     |
| 2:B:1:MET:HE2    | 2:B:30:GLU:O     | 1.98        | 0.62     |
| 1:D:463:VAL:HG21 | 1:D:519:GLU:O    | 1.99        | 0.62     |
| 1:J:288:MET:CB   | 1:J:289:PRO:CD   | 2.76        | 0.62     |
| 1:D:570:ASN:ND2  | 1:D:571:PRO:HD2  | 2.14        | 0.62     |
| 1:J:242:GLU:HG2  | 1:J:528:LYS:NZ   | 2.13        | 0.62     |
| 1:D:216:THR:HG21 | 1:D:236:GLY:CA   | 2.19        | 0.62     |
| 1:A:316:LYS:HA   | 1:A:316:LYS:HE2  | 1.82        | 0.62     |
| 1:D:279:LEU:N    | 1:D:288:MET:HE1  | 2.14        | 0.62     |
| 1:D:360:LYS:HG2  | 1:D:361:TRP:O    | 1.99        | 0.62     |
| 1:J:119:ILE:HG22 | 1:J:120:ASN:N    | 2.10        | 0.62     |
| 2:H:205:VAL:HG13 | 2:H:206:PHE:CD2  | 2.34        | 0.62     |
| 2:E:205:VAL:HG13 | 2:E:206:PHE:CD2  | 2.34        | 0.62     |
| 1:A:419:ILE:HG22 | 1:A:420:VAL:N    | 2.15        | 0.62     |
| 1:G:570:ASN:ND2  | 1:G:571:PRO:HD2  | 2.14        | 0.62     |
| 1:J:15:LEU:HB2   | 1:J:44:SER:OG    | 1.98        | 0.62     |
| 1:G:213:LEU:HD23 | 1:G:214:ILE:N    | 2.15        | 0.62     |
| 1:G:281:ASP:HB2  | 1:G:285:HIS:HD2  | 1.61        | 0.62     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:287:PHE:HB3  | 1:G:296:LYS:HZ3  | 1.64        | 0.62     |
| 1:D:316:LYS:HE2  | 1:D:316:LYS:HA   | 1.82        | 0.62     |
| 1:D:462:ASP:HB3  | 1:D:465:LYS:HG3  | 1.82        | 0.62     |
| 1:J:302:ASP:O    | 1:J:306:ARG:HD3  | 1.99        | 0.62     |
| 1:D:302:ASP:O    | 1:D:306:ARG:HD3  | 1.99        | 0.62     |
| 2:B:210:THR:HA   | 8:B:302:F3S:S1   | 2.40        | 0.62     |
| 1:D:411:SER:O    | 1:D:415:VAL:HG23 | 2.00        | 0.62     |
| 1:G:411:SER:O    | 1:G:415:VAL:HG23 | 2.00        | 0.62     |
| 1:G:463:VAL:HG21 | 1:G:519:GLU:O    | 1.99        | 0.62     |
| 1:J:360:LYS:HG2  | 1:J:361:TRP:O    | 1.99        | 0.62     |
| 1:G:272:CYS:HB3  | 1:G:328:LEU:HD21 | 1.82        | 0.62     |
| 1:D:272:CYS:HB3  | 1:D:328:LEU:HD21 | 1.82        | 0.62     |
| 3:C:103:ILE:HG12 | 3:C:103:ILE:O    | 1.98        | 0.62     |
| 3:F:103:ILE:O    | 3:F:103:ILE:HG12 | 1.98        | 0.62     |
| 1:J:462:ASP:HB3  | 1:J:465:LYS:HG3  | 1.82        | 0.62     |
| 1:G:462:ASP:HB3  | 1:G:465:LYS:HG3  | 1.82        | 0.62     |
| 2:E:210:THR:HG22 | 2:E:210:THR:O    | 2.00        | 0.62     |
| 1:A:302:ASP:O    | 1:A:306:ARG:HD3  | 1.99        | 0.62     |
| 2:H:1:MET:HE3    | 2:H:31:ALA:HA    | 1.82        | 0.62     |
| 1:A:463:VAL:HG21 | 1:A:519:GLU:O    | 1.99        | 0.62     |
| 2:H:210:THR:HA   | 8:H:302:F3S:S1   | 2.40        | 0.62     |
| 2:B:215:HIS:HA   | 2:B:224:LEU:HD12 | 1.82        | 0.62     |
| 1:G:360:LYS:HG2  | 1:G:361:TRP:O    | 1.99        | 0.61     |
| 3:L:146:ILE:O    | 3:L:148:MET:N    | 2.33        | 0.61     |
| 3:I:57:VAL:O     | 3:I:60:TRP:HB3   | 2.00        | 0.61     |
| 3:C:146:ILE:O    | 3:C:148:MET:N    | 2.33        | 0.61     |
| 1:A:462:ASP:HB3  | 1:A:465:LYS:HG3  | 1.82        | 0.61     |
| 1:J:271:GLY:O    | 1:J:275:ASP:HB2  | 2.00        | 0.61     |
| 1:A:213:LEU:HD23 | 1:A:214:ILE:N    | 2.15        | 0.61     |
| 3:C:142:VAL:CG2  | 3:C:171:LEU:HD11 | 2.25        | 0.61     |
| 3:L:57:VAL:O     | 3:L:60:TRP:HB3   | 2.00        | 0.61     |
| 1:A:411:SER:O    | 1:A:415:VAL:HG23 | 2.00        | 0.61     |
| 1:J:463:VAL:HG21 | 1:J:519:GLU:O    | 1.99        | 0.61     |
| 1:J:411:SER:O    | 1:J:415:VAL:HG23 | 2.00        | 0.61     |
| 1:D:145:LYS:O    | 1:D:146:LYS:HB2  | 2.00        | 0.61     |
| 1:A:570:ASN:ND2  | 1:A:571:PRO:HD2  | 2.14        | 0.61     |
| 1:D:271:GLY:O    | 1:D:275:ASP:HB2  | 2.01        | 0.61     |
| 1:J:272:CYS:HB3  | 1:J:328:LEU:HD21 | 1.82        | 0.61     |
| 1:J:288:MET:HG3  | 1:J:297:GLU:OE2  | 2.00        | 0.61     |
| 1:A:293:PRO:C    | 1:A:294:GLU:HG3  | 2.19        | 0.61     |
| 1:A:272:CYS:HB3  | 1:A:328:LEU:HD21 | 1.82        | 0.61     |
| 3:I:146:ILE:O    | 3:I:148:MET:N    | 2.33        | 0.61     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:E:210:THR:HA   | 8:E:302:F3S:S1   | 2.40        | 0.61     |
| 2:K:215:HIS:HA   | 2:K:224:LEU:HD12 | 1.82        | 0.61     |
| 2:E:215:HIS:HA   | 2:E:224:LEU:HD12 | 1.82        | 0.61     |
| 3:I:103:ILE:HG12 | 3:I:103:ILE:O    | 1.98        | 0.61     |
| 2:K:210:THR:HA   | 8:K:302:F3S:S1   | 2.40        | 0.61     |
| 1:G:119:ILE:HG22 | 1:G:120:ASN:N    | 2.10        | 0.61     |
| 1:G:316:LYS:HA   | 1:G:316:LYS:HE2  | 1.82        | 0.61     |
| 1:A:271:GLY:O    | 1:A:275:ASP:HB2  | 2.01        | 0.61     |
| 1:D:213:LEU:HD23 | 1:D:214:ILE:N    | 2.15        | 0.61     |
| 1:J:281:ASP:HB2  | 1:J:285:HIS:HD2  | 1.61        | 0.61     |
| 1:J:213:LEU:HD23 | 1:J:214:ILE:N    | 2.15        | 0.61     |
| 1:D:119:ILE:HG22 | 1:D:120:ASN:N    | 2.10        | 0.61     |
| 3:F:146:ILE:O    | 3:F:148:MET:N    | 2.33        | 0.61     |
| 1:J:570:ASN:OD1  | 1:J:572:GLU:N    | 2.34        | 0.61     |
| 1:J:565:LEU:HD11 | 1:J:581:GLU:OE2  | 2.01        | 0.61     |
| 1:D:565:LEU:HD11 | 1:D:581:GLU:OE2  | 2.01        | 0.61     |
| 1:G:271:GLY:O    | 1:G:275:ASP:HB2  | 2.01        | 0.61     |
| 1:J:285:HIS:O    | 1:J:286:ARG:HG2  | 2.01        | 0.61     |
| 1:J:289:PRO:O    | 1:J:293:PRO:HG3  | 2.01        | 0.61     |
| 1:G:285:HIS:O    | 1:G:286:ARG:HG2  | 2.01        | 0.61     |
| 1:A:288:MET:HG3  | 1:A:297:GLU:OE2  | 2.00        | 0.61     |
| 3:C:57:VAL:O     | 3:C:60:TRP:HB3   | 2.00        | 0.61     |
| 3:F:57:VAL:O     | 3:F:60:TRP:HB3   | 2.00        | 0.61     |
| 1:J:217:GLY:H    | 1:J:394:ALA:HB2  | 1.66        | 0.61     |
| 1:J:493:GLU:O    | 1:J:497:LEU:HD13 | 2.01        | 0.61     |
| 1:G:117:ALA:O    | 1:G:123:LYS:HA   | 2.01        | 0.61     |
| 1:J:288:MET:CB   | 1:J:289:PRO:HD3  | 2.31        | 0.61     |
| 1:J:288:MET:HA   | 1:J:296:LYS:CB   | 2.31        | 0.61     |
| 1:D:281:ASP:HB2  | 1:D:285:HIS:HD2  | 1.61        | 0.61     |
| 1:D:288:MET:HA   | 1:D:296:LYS:CB   | 2.31        | 0.61     |
| 1:A:404:ARG:HE   | 1:A:409:SER:CB   | 2.13        | 0.61     |
| 1:A:117:ALA:O    | 1:A:123:LYS:HA   | 2.01        | 0.61     |
| 1:G:208:VAL:CG1  | 1:G:440:LEU:HD11 | 2.31        | 0.61     |
| 1:J:208:VAL:CG1  | 1:J:440:LEU:HD11 | 2.31        | 0.61     |
| 2:E:213:ALA:O    | 2:E:217:VAL:HG22 | 2.01        | 0.61     |
| 1:G:145:LYS:O    | 1:G:146:LYS:HB2  | 2.00        | 0.61     |
| 1:D:288:MET:HG3  | 1:D:297:GLU:OE2  | 2.00        | 0.60     |
| 2:B:213:ALA:O    | 2:B:217:VAL:HG22 | 2.01        | 0.60     |
| 1:J:117:ALA:O    | 1:J:123:LYS:HA   | 2.01        | 0.60     |
| 2:E:28:ILE:HD12  | 2:E:42:MET:HE2   | 1.83        | 0.60     |
| 1:G:419:ILE:HG22 | 1:G:420:VAL:N    | 2.15        | 0.60     |
| 1:J:419:ILE:HG22 | 1:J:420:VAL:N    | 2.15        | 0.60     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:G:288:MET:HA    | 1:G:296:LYS:HB2  | 1.83        | 0.60     |
| 1:A:288:MET:CB    | 1:A:289:PRO:HD3  | 2.31        | 0.60     |
| 2:B:210:THR:HG22  | 2:B:210:THR:O    | 2.00        | 0.60     |
| 2:H:210:THR:HG22  | 2:H:210:THR:O    | 2.00        | 0.60     |
| 1:A:570:ASN:OD1   | 1:A:572:GLU:N    | 2.34        | 0.60     |
| 2:H:215:HIS:HA    | 2:H:224:LEU:HD12 | 1.82        | 0.60     |
| 1:A:145:LYS:O     | 1:A:146:LYS:HB2  | 2.00        | 0.60     |
| 1:D:493:GLU:O     | 1:D:497:LEU:HD13 | 2.01        | 0.60     |
| 1:A:217:GLY:H     | 1:A:394:ALA:HB2  | 1.66        | 0.60     |
| 1:G:493:GLU:O     | 1:G:497:LEU:HD13 | 2.01        | 0.60     |
| 1:A:565:LEU:HD11  | 1:A:581:GLU:OE2  | 2.01        | 0.60     |
| 1:A:288:MET:HA    | 1:A:296:LYS:HB2  | 1.83        | 0.60     |
| 1:J:87:ARG:HG3    | 1:J:638:MET:HE3  | 1.83        | 0.60     |
| 1:J:561:LEU:O     | 1:J:583:LEU:HD13 | 2.01        | 0.60     |
| 1:D:561:LEU:O     | 1:D:583:LEU:HD13 | 2.01        | 0.60     |
| 1:G:67:ASP:OD2    | 1:G:630:ARG:HD2  | 2.02        | 0.60     |
| 1:G:288:MET:CB    | 1:G:289:PRO:CD   | 2.76        | 0.60     |
| 1:G:288:MET:HA    | 1:G:296:LYS:CB   | 2.31        | 0.60     |
| 1:D:288:MET:HA    | 1:D:296:LYS:HB2  | 1.83        | 0.60     |
| 1:A:285:HIS:O     | 1:A:286:ARG:HG2  | 2.01        | 0.60     |
| 1:A:281:ASP:OD2   | 1:A:287:PHE:HB2  | 2.01        | 0.60     |
| 2:K:210:THR:HG22  | 2:K:210:THR:O    | 2.00        | 0.60     |
| 2:K:213:ALA:O     | 2:K:217:VAL:HG22 | 2.01        | 0.60     |
| 1:D:117:ALA:O     | 1:D:123:LYS:HA   | 2.01        | 0.60     |
| 1:D:510:ARG:HD2   | 1:D:512:HIS:O    | 2.02        | 0.60     |
| 1:G:565:LEU:HD11  | 1:G:581:GLU:OE2  | 2.01        | 0.60     |
| 1:G:652:ARG:HG3   | 1:G:652:ARG:HH11 | 1.67        | 0.60     |
| 1:D:281:ASP:OD2   | 1:D:287:PHE:HB2  | 2.01        | 0.60     |
| 1:A:288:MET:HA    | 1:A:296:LYS:CB   | 2.31        | 0.60     |
| 1:A:208:VAL:CG1   | 1:A:440:LEU:HD11 | 2.31        | 0.60     |
| 1:A:561:LEU:O     | 1:A:583:LEU:HD13 | 2.02        | 0.60     |
| 1:A:67:ASP:OD2    | 1:A:630:ARG:HD2  | 2.01        | 0.60     |
| 11:C:303:LMT:H101 | 11:C:303:LMT:H61 | 1.84        | 0.60     |
| 1:A:652:ARG:HH11  | 1:A:652:ARG:HG3  | 1.67        | 0.60     |
| 1:G:288:MET:HG3   | 1:G:297:GLU:OE2  | 2.00        | 0.60     |
| 1:J:316:LYS:HE2   | 1:J:316:LYS:HA   | 1.82        | 0.60     |
| 1:G:289:PRO:O     | 1:G:293:PRO:HG3  | 2.01        | 0.60     |
| 1:D:208:VAL:CG1   | 1:D:440:LEU:HD11 | 2.31        | 0.60     |
| 1:D:67:ASP:OD2    | 1:D:630:ARG:HD2  | 2.01        | 0.60     |
| 1:D:217:GLY:H     | 1:D:394:ALA:HB2  | 1.66        | 0.60     |
| 1:J:145:LYS:O     | 1:J:146:LYS:HB2  | 2.00        | 0.60     |
| 3:C:136:MET:HE1   | 3:C:179:VAL:HA   | 1.84        | 0.60     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:I:157:VAL:HB   | 3:I:254:HIS:CE1   | 2.37        | 0.60     |
| 2:B:166:MET:HE1  | 3:C:102:PRO:HA    | 1.84        | 0.60     |
| 2:E:166:MET:HE1  | 3:F:102:PRO:HA    | 1.84        | 0.60     |
| 1:D:570:ASN:OD1  | 1:D:572:GLU:N     | 2.34        | 0.60     |
| 1:J:186:HIS:HA   | 1:J:190:LYS:O     | 2.02        | 0.60     |
| 1:D:285:HIS:O    | 1:D:286:ARG:HG2   | 2.01        | 0.60     |
| 3:L:157:VAL:HB   | 3:L:254:HIS:CE1   | 2.37        | 0.60     |
| 1:A:87:ARG:HG3   | 1:A:638:MET:HE3   | 1.83        | 0.60     |
| 3:C:75:LYS:HA    | 3:C:75:LYS:HE2    | 1.84        | 0.60     |
| 1:G:561:LEU:O    | 1:G:583:LEU:HD13  | 2.02        | 0.60     |
| 1:J:67:ASP:OD2   | 1:J:630:ARG:HD2   | 2.01        | 0.60     |
| 1:D:419:ILE:HG22 | 1:D:420:VAL:N     | 2.15        | 0.60     |
| 2:H:28:ILE:HD12  | 2:H:42:MET:HE2    | 1.83        | 0.60     |
| 1:D:652:ARG:HG3  | 1:D:652:ARG:HH11  | 1.67        | 0.60     |
| 1:D:289:PRO:O    | 1:D:293:PRO:HG3   | 2.01        | 0.60     |
| 1:A:278:ILE:HD12 | 1:A:286:ARG:HH11  | 1.67        | 0.60     |
| 1:A:288:MET:CB   | 1:A:289:PRO:CD    | 2.76        | 0.60     |
| 3:I:75:LYS:HA    | 3:I:75:LYS:HE2    | 1.84        | 0.60     |
| 3:L:75:LYS:HA    | 3:L:75:LYS:HE2    | 1.84        | 0.60     |
| 11:F:301:LMT:H61 | 11:F:301:LMT:H101 | 1.84        | 0.60     |
| 1:J:288:MET:HA   | 1:J:296:LYS:HB2   | 1.83        | 0.59     |
| 1:A:289:PRO:O    | 1:A:293:PRO:HG3   | 2.01        | 0.59     |
| 1:G:314:LYS:CB   | 1:G:314:LYS:NZ    | 2.65        | 0.59     |
| 2:H:213:ALA:O    | 2:H:217:VAL:HG22  | 2.01        | 0.59     |
| 1:G:186:HIS:HA   | 1:G:190:LYS:O     | 2.02        | 0.59     |
| 1:J:652:ARG:HG3  | 1:J:652:ARG:HH11  | 1.67        | 0.59     |
| 1:J:281:ASP:OD2  | 1:J:287:PHE:HB2   | 2.01        | 0.59     |
| 1:G:281:ASP:OD2  | 1:G:287:PHE:HB2   | 2.01        | 0.59     |
| 1:G:288:MET:CB   | 1:G:289:PRO:HD3   | 2.31        | 0.59     |
| 1:D:288:MET:CB   | 1:D:289:PRO:HD3   | 2.31        | 0.59     |
| 3:L:249:ASP:CA   | 3:L:254:HIS:HB3   | 2.32        | 0.59     |
| 1:G:570:ASN:OD1  | 1:G:572:GLU:N     | 2.34        | 0.59     |
| 1:D:186:HIS:HA   | 1:D:190:LYS:O     | 2.02        | 0.59     |
| 2:E:46:THR:HG1   | 2:E:47:TYR:HD1    | 1.48        | 0.59     |
| 1:A:186:HIS:HA   | 1:A:190:LYS:O     | 2.02        | 0.59     |
| 1:J:214:ILE:HG23 | 1:J:216:THR:HG23  | 1.85        | 0.59     |
| 1:G:404:ARG:HE   | 1:G:409:SER:CB    | 2.13        | 0.59     |
| 1:G:87:ARG:HG3   | 1:G:638:MET:HE3   | 1.85        | 0.59     |
| 1:A:493:GLU:O    | 1:A:497:LEU:HD13  | 2.01        | 0.59     |
| 2:H:166:MET:HE1  | 3:I:102:PRO:HA    | 1.84        | 0.59     |
| 2:H:143:GLN:O    | 2:H:146:PHE:HB3   | 2.03        | 0.59     |
| 1:A:314:LYS:CB   | 1:A:314:LYS:NZ    | 2.65        | 0.59     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:D:70:PHE:O      | 1:D:74:VAL:HG23  | 2.03        | 0.59     |
| 1:A:539:ASP:O     | 1:A:541:THR:HG23 | 2.02        | 0.59     |
| 1:G:510:ARG:HD2   | 1:G:512:HIS:O    | 2.02        | 0.59     |
| 1:G:214:ILE:HG23  | 1:G:216:THR:HG23 | 1.85        | 0.59     |
| 1:J:404:ARG:HE    | 1:J:409:SER:CB   | 2.13        | 0.59     |
| 2:B:143:GLN:O     | 2:B:146:PHE:HB3  | 2.03        | 0.59     |
| 11:I:303:LMT:H101 | 11:I:303:LMT:H61 | 1.84        | 0.59     |
| 1:A:295:LYS:HD2   | 1:A:298:LEU:HD12 | 1.85        | 0.59     |
| 3:F:157:VAL:HB    | 3:F:254:HIS:CE1  | 2.37        | 0.59     |
| 3:F:75:LYS:HE2    | 3:F:75:LYS:HA    | 1.84        | 0.59     |
| 3:I:249:ASP:CA    | 3:I:254:HIS:HB3  | 2.32        | 0.59     |
| 2:K:1:MET:HE2     | 2:K:31:ALA:HA    | 1.84        | 0.59     |
| 2:B:145:VAL:O     | 2:B:145:VAL:HG12 | 2.03        | 0.59     |
| 1:D:214:ILE:HG23  | 1:D:216:THR:HG23 | 1.85        | 0.59     |
| 1:J:392:GLY:O     | 1:J:394:ALA:N    | 2.36        | 0.59     |
| 1:D:652:ARG:HG3   | 1:D:652:ARG:NH1  | 2.18        | 0.59     |
| 1:A:510:ARG:HD2   | 1:A:512:HIS:O    | 2.02        | 0.59     |
| 1:G:539:ASP:O     | 1:G:541:THR:HG23 | 2.03        | 0.59     |
| 3:L:208:ASN:HA    | 3:L:211:LYS:HG2  | 1.85        | 0.59     |
| 2:B:28:ILE:HD12   | 2:B:42:MET:HE2   | 1.85        | 0.59     |
| 1:D:539:ASP:O     | 1:D:541:THR:HG23 | 2.02        | 0.59     |
| 1:G:278:ILE:HD12  | 1:G:286:ARG:HH11 | 1.67        | 0.59     |
| 3:F:86:VAL:O      | 3:F:86:VAL:HG12  | 2.03        | 0.59     |
| 1:G:570:ASN:CG    | 1:G:571:PRO:HD2  | 2.24        | 0.59     |
| 1:J:70:PHE:O      | 1:J:74:VAL:HG23  | 2.03        | 0.59     |
| 1:G:217:GLY:H     | 1:G:394:ALA:HB2  | 1.66        | 0.59     |
| 2:K:166:MET:HE1   | 3:L:102:PRO:HA   | 1.84        | 0.59     |
| 1:D:461:GLU:O     | 1:D:504:VAL:HG13 | 2.03        | 0.59     |
| 1:J:570:ASN:CG    | 1:J:571:PRO:HD2  | 2.24        | 0.59     |
| 1:A:392:GLY:O     | 1:A:394:ALA:N    | 2.36        | 0.59     |
| 1:J:510:ARG:HD2   | 1:J:512:HIS:O    | 2.02        | 0.59     |
| 1:D:295:LYS:HD2   | 1:D:298:LEU:HD12 | 1.85        | 0.58     |
| 1:D:87:ARG:HG3    | 1:D:638:MET:HE3  | 1.84        | 0.58     |
| 1:J:461:GLU:O     | 1:J:504:VAL:HG13 | 2.03        | 0.58     |
| 3:C:86:VAL:HG12   | 3:C:86:VAL:O     | 2.03        | 0.58     |
| 2:E:171:VAL:HG12  | 2:E:175:GLY:HA3  | 1.85        | 0.58     |
| 1:D:93:ALA:HB3    | 1:D:94:PRO:HD3   | 1.85        | 0.58     |
| 1:J:98:ARG:NH2    | 2:K:133:LEU:HD12 | 2.18        | 0.58     |
| 1:A:346:GLN:CA    | 1:A:357:PRO:HG2  | 2.31        | 0.58     |
| 1:A:2:LYS:HB2     | 1:A:2:LYS:HZ2    | 1.68        | 0.58     |
| 2:B:1:MET:HE3     | 2:B:31:ALA:HA    | 1.84        | 0.58     |
| 1:D:98:ARG:NH2    | 2:E:133:LEU:HD12 | 2.18        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:392:GLY:O    | 1:G:394:ALA:N    | 2.36        | 0.58     |
| 1:J:179:LYS:HG3  | 1:J:196:VAL:HG11 | 1.85        | 0.58     |
| 1:A:98:ARG:NH2   | 2:B:133:LEU:HD12 | 2.18        | 0.58     |
| 2:E:143:GLN:O    | 2:E:146:PHE:HB3  | 2.03        | 0.58     |
| 3:C:208:ASN:HA   | 3:C:211:LYS:HG2  | 1.85        | 0.58     |
| 1:D:179:LYS:HG3  | 1:D:196:VAL:HG11 | 1.86        | 0.58     |
| 1:J:93:ALA:HB3   | 1:J:94:PRO:HD3   | 1.85        | 0.58     |
| 2:E:145:VAL:HG12 | 2:E:145:VAL:O    | 2.03        | 0.58     |
| 1:D:52:GLN:HE22  | 1:D:144:THR:CG2  | 2.17        | 0.58     |
| 1:A:570:ASN:CG   | 1:A:571:PRO:HD2  | 2.24        | 0.58     |
| 1:A:652:ARG:NH1  | 1:A:652:ARG:HG3  | 2.17        | 0.58     |
| 2:H:171:VAL:HG12 | 2:H:175:GLY:HA3  | 1.85        | 0.58     |
| 3:I:188:TYR:O    | 3:I:192:VAL:HG22 | 2.04        | 0.58     |
| 2:K:143:GLN:O    | 2:K:146:PHE:HB3  | 2.03        | 0.58     |
| 1:D:570:ASN:CG   | 1:D:571:PRO:HD2  | 2.24        | 0.58     |
| 1:D:122:GLN:O    | 1:D:124:THR:HG23 | 2.04        | 0.58     |
| 2:H:145:VAL:HG12 | 2:H:145:VAL:O    | 2.03        | 0.58     |
| 1:D:278:ILE:HD12 | 1:D:286:ARG:HH11 | 1.67        | 0.58     |
| 1:G:652:ARG:HG3  | 1:G:652:ARG:NH1  | 2.18        | 0.58     |
| 1:A:70:PHE:O     | 1:A:74:VAL:HG23  | 2.03        | 0.58     |
| 1:J:652:ARG:NH1  | 1:J:652:ARG:HG3  | 2.18        | 0.58     |
| 1:G:122:GLN:O    | 1:G:124:THR:HG23 | 2.04        | 0.58     |
| 2:K:145:VAL:O    | 2:K:145:VAL:HG12 | 2.03        | 0.58     |
| 1:A:93:ALA:HB3   | 1:A:94:PRO:HD3   | 1.84        | 0.58     |
| 1:G:98:ARG:NH2   | 2:H:133:LEU:HD12 | 2.18        | 0.58     |
| 2:H:46:THR:HG1   | 2:H:47:TYR:HD1   | 1.51        | 0.58     |
| 1:J:278:ILE:HD12 | 1:J:286:ARG:HH11 | 1.67        | 0.58     |
| 1:D:314:LYS:CB   | 1:D:314:LYS:NZ   | 2.65        | 0.58     |
| 3:C:145:TYR:O    | 3:C:148:MET:HB3  | 2.04        | 0.58     |
| 1:J:314:LYS:NZ   | 1:J:314:LYS:CB   | 2.65        | 0.58     |
| 1:D:392:GLY:O    | 1:D:394:ALA:N    | 2.36        | 0.58     |
| 2:B:171:VAL:HG12 | 2:B:175:GLY:HA3  | 1.85        | 0.58     |
| 2:H:193:GLU:CD   | 2:H:193:GLU:H    | 2.07        | 0.58     |
| 3:C:249:ASP:CA   | 3:C:254:HIS:HB3  | 2.32        | 0.58     |
| 3:C:157:VAL:HB   | 3:C:254:HIS:CE1  | 2.37        | 0.58     |
| 3:F:145:TYR:O    | 3:F:148:MET:HB3  | 2.04        | 0.58     |
| 1:G:93:ALA:HB3   | 1:G:94:PRO:HD3   | 1.85        | 0.58     |
| 3:C:188:TYR:O    | 3:C:192:VAL:HG22 | 2.04        | 0.58     |
| 1:A:78:ASP:OD2   | 1:A:544:ARG:HG3  | 2.04        | 0.58     |
| 1:G:78:ASP:OD2   | 1:G:544:ARG:HG3  | 2.04        | 0.58     |
| 1:A:179:LYS:HG3  | 1:A:196:VAL:HG11 | 1.86        | 0.58     |
| 1:A:410:VAL:HG22 | 4:A:701:FAD:O2   | 2.04        | 0.57     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 3:I:136:MET:HE1   | 3:I:179:VAL:HA   | 1.86        | 0.57     |
| 3:F:249:ASP:CA    | 3:F:254:HIS:HB3  | 2.32        | 0.57     |
| 11:L:301:LMT:H101 | 11:L:301:LMT:H61 | 1.84        | 0.57     |
| 2:E:108:GLY:O     | 2:E:110:TRP:N    | 2.37        | 0.57     |
| 2:K:193:GLU:H     | 2:K:193:GLU:CD   | 2.07        | 0.57     |
| 2:B:193:GLU:H     | 2:B:193:GLU:CD   | 2.07        | 0.57     |
| 1:A:287:PHE:HB3   | 1:A:296:LYS:HZ3  | 1.67        | 0.57     |
| 3:I:145:TYR:O     | 3:I:148:MET:HB3  | 2.04        | 0.57     |
| 3:C:58:MET:O      | 3:C:61:VAL:HG22  | 2.04        | 0.57     |
| 1:J:78:ASP:OD2    | 1:J:544:ARG:HG3  | 2.04        | 0.57     |
| 3:L:188:TYR:O     | 3:L:192:VAL:HG22 | 2.04        | 0.57     |
| 2:B:108:GLY:O     | 2:B:110:TRP:N    | 2.38        | 0.57     |
| 1:J:346:GLN:CA    | 1:J:357:PRO:HG2  | 2.31        | 0.57     |
| 1:G:52:GLN:HE22   | 1:G:144:THR:CG2  | 2.17        | 0.57     |
| 1:J:295:LYS:HD2   | 1:J:298:LEU:HD12 | 1.85        | 0.57     |
| 1:G:295:LYS:HD2   | 1:G:298:LEU:HD12 | 1.85        | 0.57     |
| 1:D:78:ASP:OD2    | 1:D:544:ARG:HG3  | 2.04        | 0.57     |
| 3:L:145:TYR:O     | 3:L:148:MET:HB3  | 2.04        | 0.57     |
| 2:H:138:GLU:HB2   | 2:H:141:VAL:CG2  | 2.33        | 0.57     |
| 1:J:52:GLN:HE22   | 1:J:144:THR:CG2  | 2.17        | 0.57     |
| 3:L:86:VAL:O      | 3:L:86:VAL:HG12  | 2.03        | 0.57     |
| 1:G:461:GLU:O     | 1:G:504:VAL:HG13 | 2.03        | 0.57     |
| 1:A:242:GLU:HG2   | 1:A:528:LYS:HZ1  | 1.69        | 0.57     |
| 1:J:462:ASP:OD2   | 1:J:465:LYS:HG3  | 2.05        | 0.57     |
| 1:J:539:ASP:O     | 1:J:541:THR:HG23 | 2.02        | 0.57     |
| 3:F:188:TYR:O     | 3:F:192:VAL:HG22 | 2.04        | 0.57     |
| 1:J:122:GLN:O     | 1:J:124:THR:HG23 | 2.04        | 0.57     |
| 1:A:461:GLU:O     | 1:A:504:VAL:HG13 | 2.03        | 0.57     |
| 1:G:70:PHE:O      | 1:G:74:VAL:HG23  | 2.03        | 0.57     |
| 2:K:28:ILE:HD12   | 2:K:42:MET:HE2   | 1.86        | 0.57     |
| 3:F:208:ASN:HA    | 3:F:211:LYS:HG2  | 1.85        | 0.57     |
| 1:D:93:ALA:O      | 1:D:96:ALA:HB3   | 2.05        | 0.57     |
| 1:A:214:ILE:HG23  | 1:A:216:THR:HG23 | 1.85        | 0.57     |
| 3:F:58:MET:O      | 3:F:61:VAL:HG22  | 2.04        | 0.57     |
| 3:I:86:VAL:HG12   | 3:I:86:VAL:O     | 2.03        | 0.57     |
| 3:I:208:ASN:HA    | 3:I:211:LYS:HG2  | 1.85        | 0.57     |
| 1:G:179:LYS:HG3   | 1:G:196:VAL:HG11 | 1.86        | 0.57     |
| 2:E:193:GLU:H     | 2:E:193:GLU:CD   | 2.07        | 0.57     |
| 2:K:171:VAL:HG12  | 2:K:175:GLY:HA3  | 1.85        | 0.57     |
| 1:J:410:VAL:HG22  | 4:J:701:FAD:O2   | 2.04        | 0.57     |
| 2:E:138:GLU:HB2   | 2:E:141:VAL:CG2  | 2.33        | 0.57     |
| 3:I:71:PHE:HB3    | 3:I:75:LYS:HG3   | 1.87        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:122:GLN:O    | 1:A:124:THR:HG23 | 2.04        | 0.57     |
| 1:J:296:LYS:O    | 1:J:304:VAL:HG22 | 2.05        | 0.57     |
| 1:G:410:VAL:HG22 | 4:G:701:FAD:O2   | 2.04        | 0.57     |
| 1:D:337:HIS:ND1  | 1:D:337:HIS:N    | 2.53        | 0.57     |
| 1:D:346:GLN:CA   | 1:D:357:PRO:HG2  | 2.31        | 0.56     |
| 1:D:462:ASP:OD2  | 1:D:465:LYS:HG3  | 2.05        | 0.56     |
| 1:A:93:ALA:O     | 1:A:96:ALA:HB3   | 2.05        | 0.56     |
| 1:D:410:VAL:HG22 | 4:D:701:FAD:O2   | 2.04        | 0.56     |
| 3:L:71:PHE:HB3   | 3:L:75:LYS:HG3   | 1.87        | 0.56     |
| 1:J:93:ALA:O     | 1:J:96:ALA:HB3   | 2.05        | 0.56     |
| 2:K:108:GLY:O    | 2:K:110:TRP:N    | 2.38        | 0.56     |
| 1:D:287:PHE:HB3  | 1:D:296:LYS:HZ3  | 1.71        | 0.56     |
| 1:A:296:LYS:O    | 1:A:304:VAL:HG22 | 2.05        | 0.56     |
| 3:I:103:ILE:HG21 | 3:L:103:ILE:HD13 | 1.86        | 0.56     |
| 3:I:58:MET:O     | 3:I:61:VAL:HG22  | 2.04        | 0.56     |
| 1:J:634:GLN:NE2  | 1:J:638:MET:O    | 2.37        | 0.56     |
| 2:K:147:GLU:HA   | 2:K:150:ARG:CD   | 2.36        | 0.56     |
| 1:D:296:LYS:O    | 1:D:304:VAL:HG22 | 2.05        | 0.56     |
| 2:H:123:HIS:CD2  | 2:H:190:ARG:CZ   | 2.89        | 0.56     |
| 2:H:108:GLY:O    | 2:H:110:TRP:N    | 2.37        | 0.56     |
| 1:J:281:ASP:HB2  | 1:J:285:HIS:NE2  | 2.21        | 0.56     |
| 2:E:123:HIS:CD2  | 2:E:190:ARG:CZ   | 2.89        | 0.56     |
| 1:A:52:GLN:HE22  | 1:A:144:THR:CG2  | 2.17        | 0.56     |
| 3:C:239:THR:O    | 3:C:241:PRO:HD3  | 2.06        | 0.56     |
| 1:A:229:ALA:HB1  | 2:B:56:VAL:O     | 2.06        | 0.56     |
| 3:L:58:MET:O     | 3:L:61:VAL:HG22  | 2.04        | 0.56     |
| 1:A:634:GLN:NE2  | 1:A:638:MET:O    | 2.37        | 0.56     |
| 2:K:123:HIS:CD2  | 2:K:190:ARG:CZ   | 2.89        | 0.56     |
| 2:B:123:HIS:CD2  | 2:B:190:ARG:CZ   | 2.89        | 0.56     |
| 1:A:462:ASP:OD2  | 1:A:465:LYS:HG3  | 2.05        | 0.56     |
| 1:G:93:ALA:O     | 1:G:96:ALA:HB3   | 2.05        | 0.56     |
| 1:D:221:ARG:O    | 1:D:471:LYS:HE3  | 2.05        | 0.56     |
| 3:L:239:THR:O    | 3:L:241:PRO:HD3  | 2.06        | 0.56     |
| 3:F:239:THR:O    | 3:F:241:PRO:HD3  | 2.06        | 0.56     |
| 1:G:296:LYS:O    | 1:G:304:VAL:HG22 | 2.05        | 0.56     |
| 3:F:89:VAL:HG12  | 3:F:89:VAL:O     | 2.06        | 0.56     |
| 1:A:179:LYS:HG3  | 1:A:196:VAL:CG1  | 2.36        | 0.56     |
| 1:G:32:ILE:HG22  | 1:G:33:VAL:N     | 2.21        | 0.56     |
| 1:J:337:HIS:N    | 1:J:337:HIS:ND1  | 2.53        | 0.56     |
| 1:G:221:ARG:O    | 1:G:471:LYS:HE3  | 2.05        | 0.56     |
| 1:J:380:ARG:HB2  | 1:J:423:TYR:CD1  | 2.41        | 0.56     |
| 1:G:462:ASP:OD2  | 1:G:465:LYS:HG3  | 2.05        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:147:GLU:HA   | 2:B:150:ARG:CD   | 2.36        | 0.56     |
| 1:D:404:ARG:HE   | 1:D:409:SER:CB   | 2.13        | 0.56     |
| 3:F:151:PRO:HA   | 3:F:154:ILE:HD11 | 1.88        | 0.56     |
| 1:J:179:LYS:HG3  | 1:J:196:VAL:CG1  | 2.36        | 0.56     |
| 1:D:179:LYS:HG3  | 1:D:196:VAL:CG1  | 2.36        | 0.56     |
| 2:H:147:GLU:HA   | 2:H:150:ARG:CD   | 2.36        | 0.56     |
| 3:I:103:ILE:HD13 | 3:L:103:ILE:HG21 | 1.88        | 0.56     |
| 3:I:103:ILE:HG13 | 3:L:99:ARG:HA    | 1.88        | 0.56     |
| 2:H:234:LYS:O    | 2:H:238:VAL:HG23 | 2.07        | 0.56     |
| 1:G:380:ARG:HB2  | 1:G:423:TYR:CD1  | 2.41        | 0.55     |
| 2:E:234:LYS:O    | 2:E:238:VAL:HG23 | 2.07        | 0.55     |
| 3:L:176:LEU:O    | 3:L:176:LEU:HD12 | 2.06        | 0.55     |
| 1:D:257:HIS:O    | 1:D:366:PRO:HA   | 2.07        | 0.55     |
| 1:A:482:ARG:HB3  | 1:A:487:LEU:CD1  | 2.34        | 0.55     |
| 3:F:71:PHE:HB3   | 3:F:75:LYS:HG3   | 1.87        | 0.55     |
| 1:G:179:LYS:HG3  | 1:G:196:VAL:CG1  | 2.36        | 0.55     |
| 1:J:221:ARG:O    | 1:J:471:LYS:HE3  | 2.06        | 0.55     |
| 3:I:49:SER:HA    | 3:I:227:THR:CG2  | 2.36        | 0.55     |
| 3:C:49:SER:HA    | 3:C:227:THR:CG2  | 2.36        | 0.55     |
| 1:A:32:ILE:HG22  | 1:A:33:VAL:N     | 2.21        | 0.55     |
| 1:A:337:HIS:ND1  | 1:A:337:HIS:N    | 2.53        | 0.55     |
| 1:D:32:ILE:HG22  | 1:D:33:VAL:N     | 2.21        | 0.55     |
| 3:C:176:LEU:HD12 | 3:C:176:LEU:O    | 2.06        | 0.55     |
| 1:A:221:ARG:O    | 1:A:471:LYS:HE3  | 2.05        | 0.55     |
| 1:J:270:GLU:N    | 5:J:702:MLA:O3B  | 2.40        | 0.55     |
| 1:G:270:GLU:N    | 5:G:702:MLA:O3B  | 2.40        | 0.55     |
| 3:F:136:MET:HE1  | 3:F:179:VAL:HA   | 1.88        | 0.55     |
| 1:J:344:ASP:C    | 1:J:346:GLN:H    | 2.10        | 0.55     |
| 3:C:71:PHE:HB3   | 3:C:75:LYS:HG3   | 1.87        | 0.55     |
| 3:C:89:VAL:HG12  | 3:C:89:VAL:O     | 2.06        | 0.55     |
| 3:L:89:VAL:HG12  | 3:L:89:VAL:O     | 2.06        | 0.55     |
| 3:I:151:PRO:HA   | 3:I:154:ILE:HD11 | 1.88        | 0.55     |
| 3:L:49:SER:HA    | 3:L:227:THR:CG2  | 2.37        | 0.55     |
| 1:J:229:ALA:HB1  | 2:K:56:VAL:O     | 2.06        | 0.55     |
| 1:D:344:ASP:C    | 1:D:346:GLN:H    | 2.10        | 0.55     |
| 3:I:89:VAL:HG12  | 3:I:89:VAL:O     | 2.06        | 0.55     |
| 2:K:234:LYS:O    | 2:K:238:VAL:HG23 | 2.07        | 0.55     |
| 3:F:49:SER:HA    | 3:F:227:THR:CG2  | 2.36        | 0.55     |
| 3:I:176:LEU:O    | 3:I:176:LEU:HD12 | 2.06        | 0.55     |
| 1:A:270:GLU:N    | 5:A:702:MLA:O3B  | 2.40        | 0.55     |
| 1:A:344:ASP:C    | 1:A:346:GLN:H    | 2.10        | 0.55     |
| 3:F:248:PHE:O    | 3:F:254:HIS:HB3  | 2.07        | 0.55     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:314:LYS:HB2  | 1:J:314:LYS:HZ2  | 1.71        | 0.55     |
| 1:G:337:HIS:ND1  | 1:G:337:HIS:N    | 2.53        | 0.55     |
| 1:G:229:ALA:HB1  | 2:H:56:VAL:O     | 2.06        | 0.55     |
| 2:E:147:GLU:HA   | 2:E:150:ARG:CD   | 2.36        | 0.55     |
| 1:G:281:ASP:HB2  | 1:G:285:HIS:NE2  | 2.21        | 0.55     |
| 1:D:270:GLU:N    | 5:D:702:MLA:O3B  | 2.40        | 0.55     |
| 1:A:278:ILE:HG21 | 1:A:286:ARG:NH1  | 2.22        | 0.55     |
| 1:A:241:LEU:HD12 | 1:A:248:LEU:HD21 | 1.88        | 0.55     |
| 2:B:234:LYS:O    | 2:B:238:VAL:HG23 | 2.07        | 0.55     |
| 1:J:32:ILE:HG22  | 1:J:33:VAL:N     | 2.21        | 0.55     |
| 1:D:229:ALA:HB1  | 2:E:56:VAL:O     | 2.06        | 0.55     |
| 2:H:8:ARG:HH12   | 3:L:3:ASN:HD21   | 1.54        | 0.55     |
| 1:A:281:ASP:HB2  | 1:A:285:HIS:NE2  | 2.21        | 0.55     |
| 3:L:248:PHE:O    | 3:L:254:HIS:HB3  | 2.07        | 0.55     |
| 1:D:380:ARG:HB2  | 1:D:423:TYR:CD1  | 2.41        | 0.55     |
| 1:A:380:ARG:HB2  | 1:A:423:TYR:CD1  | 2.41        | 0.55     |
| 3:C:191:ALA:O    | 3:C:195:GLY:HA2  | 2.07        | 0.55     |
| 1:J:302:ASP:HB2  | 1:J:546:ALA:HA   | 1.89        | 0.55     |
| 1:G:48:GLN:HG3   | 1:G:267:LEU:CD2  | 2.32        | 0.55     |
| 1:D:281:ASP:HB2  | 1:D:285:HIS:NE2  | 2.21        | 0.55     |
| 3:I:239:THR:O    | 3:I:241:PRO:HD3  | 2.06        | 0.55     |
| 3:F:176:LEU:HD12 | 3:F:176:LEU:O    | 2.06        | 0.55     |
| 2:K:138:GLU:HB2  | 2:K:141:VAL:CG2  | 2.33        | 0.55     |
| 1:D:88:MET:HA    | 1:D:642:LEU:HD21 | 1.88        | 0.55     |
| 1:G:88:MET:HA    | 1:G:642:LEU:HD21 | 1.89        | 0.55     |
| 1:G:241:LEU:HD12 | 1:G:248:LEU:HD21 | 1.88        | 0.55     |
| 3:C:223:LEU:O    | 3:C:223:LEU:HD23 | 2.07        | 0.55     |
| 1:J:106:PRO:O    | 1:J:152:THR:HG22 | 2.07        | 0.55     |
| 2:H:144:GLU:C    | 2:H:146:PHE:H    | 2.10        | 0.55     |
| 3:C:53:LEU:O     | 3:C:57:VAL:HB    | 2.07        | 0.55     |
| 3:L:53:LEU:O     | 3:L:57:VAL:HB    | 2.07        | 0.55     |
| 3:I:53:LEU:O     | 3:I:57:VAL:HB    | 2.07        | 0.55     |
| 1:G:53:ALA:O     | 1:G:55:LEU:N     | 2.38        | 0.55     |
| 1:J:278:ILE:HG21 | 1:J:286:ARG:NH1  | 2.22        | 0.54     |
| 1:J:303:VAL:O    | 1:J:307:ARG:CZ   | 2.56        | 0.54     |
| 1:D:278:ILE:HG21 | 1:D:286:ARG:NH1  | 2.22        | 0.54     |
| 1:D:303:VAL:O    | 1:D:307:ARG:CZ   | 2.55        | 0.54     |
| 1:D:106:PRO:O    | 1:D:152:THR:HG22 | 2.07        | 0.54     |
| 3:I:223:LEU:HD23 | 3:I:223:LEU:O    | 2.07        | 0.54     |
| 1:A:302:ASP:HB2  | 1:A:546:ALA:HA   | 1.89        | 0.54     |
| 1:G:344:ASP:C    | 1:G:346:GLN:H    | 2.10        | 0.54     |
| 1:A:257:HIS:O    | 1:A:366:PRO:HA   | 2.06        | 0.54     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:G:106:PRO:O    | 1:G:152:THR:HG22  | 2.07        | 0.54     |
| 3:C:248:PHE:O    | 3:C:254:HIS:HB3   | 2.07        | 0.54     |
| 1:J:88:MET:HA    | 1:J:642:LEU:HD21  | 1.89        | 0.54     |
| 1:D:241:LEU:HD12 | 1:D:248:LEU:HD21  | 1.88        | 0.54     |
| 3:L:246:LYS:HE3  | 3:L:247:TYR:CZ    | 2.43        | 0.54     |
| 1:G:278:ILE:HG21 | 1:G:286:ARG:NH1   | 2.22        | 0.54     |
| 1:A:288:MET:CG   | 1:A:297:GLU:OE2   | 2.56        | 0.54     |
| 1:G:257:HIS:O    | 1:G:366:PRO:HA    | 2.07        | 0.54     |
| 3:F:191:ALA:O    | 3:F:195:GLY:HA2   | 2.07        | 0.54     |
| 3:F:223:LEU:HD23 | 3:F:223:LEU:O     | 2.07        | 0.54     |
| 1:J:288:MET:CG   | 1:J:297:GLU:OE2   | 2.56        | 0.54     |
| 1:D:267:LEU:HD22 | 4:D:701:FAD:H6    | 1.90        | 0.54     |
| 1:A:281:ASP:HB2  | 1:A:285:HIS:HD2   | 1.61        | 0.54     |
| 3:L:136:MET:HE1  | 3:L:179:VAL:HA    | 1.88        | 0.54     |
| 3:L:191:ALA:O    | 3:L:195:GLY:HA2   | 2.07        | 0.54     |
| 2:B:8:ARG:HH12   | 3:F:3:ASN:HD21    | 1.55        | 0.54     |
| 1:J:257:HIS:O    | 1:J:366:PRO:HA    | 2.06        | 0.54     |
| 1:A:267:LEU:HD22 | 4:A:701:FAD:H6    | 1.90        | 0.54     |
| 1:A:423:TYR:CE2  | 1:A:643:PRO:HG3   | 2.43        | 0.54     |
| 3:L:151:PRO:HA   | 3:L:154:ILE:HD11  | 1.88        | 0.54     |
| 1:A:53:ALA:O     | 1:A:55:LEU:N      | 2.38        | 0.54     |
| 1:J:423:TYR:CE2  | 1:J:643:PRO:HG3   | 2.43        | 0.54     |
| 1:J:241:LEU:HD11 | 1:J:532:CYS:SG    | 2.48        | 0.54     |
| 2:E:57:CYS:O     | 2:E:58:ARG:HB3    | 2.08        | 0.54     |
| 3:C:103:ILE:HG21 | 3:F:103:ILE:HD13  | 1.89        | 0.54     |
| 3:I:191:ALA:O    | 3:I:195:GLY:HA2   | 2.07        | 0.54     |
| 1:J:53:ALA:O     | 1:J:55:LEU:N      | 2.38        | 0.54     |
| 1:J:272:CYS:CB   | 1:J:328:LEU:HD21  | 2.38        | 0.54     |
| 3:I:136:MET:HB2  | 10:I:301:HEM:HBB2 | 1.90        | 0.54     |
| 3:C:136:MET:HB2  | 10:C:301:HEM:HBB2 | 1.90        | 0.54     |
| 3:I:146:ILE:C    | 3:I:148:MET:N     | 2.61        | 0.54     |
| 3:L:146:ILE:C    | 3:L:148:MET:N     | 2.61        | 0.54     |
| 1:A:106:PRO:O    | 1:A:152:THR:HG22  | 2.07        | 0.54     |
| 3:C:249:ASP:OD1  | 3:C:253:THR:HA    | 2.08        | 0.54     |
| 3:F:53:LEU:O     | 3:F:57:VAL:HB     | 2.07        | 0.54     |
| 3:L:249:ASP:OD1  | 3:L:253:THR:HA    | 2.08        | 0.54     |
| 3:I:249:ASP:OD1  | 3:I:253:THR:HA    | 2.08        | 0.54     |
| 1:A:241:LEU:HD11 | 1:A:532:CYS:SG    | 2.48        | 0.54     |
| 3:C:146:ILE:C    | 3:C:148:MET:N     | 2.61        | 0.54     |
| 2:B:196:TYR:OH   | 3:C:21:ARG:HA     | 2.08        | 0.54     |
| 1:D:8:SER:OG     | 1:D:31:THR:HG22   | 2.08        | 0.54     |
| 1:D:32:ILE:CG2   | 1:D:33:VAL:N      | 2.71        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:L:223:LEU:HD23 | 3:L:223:LEU:O    | 2.07        | 0.54     |
| 1:G:302:ASP:HB2  | 1:G:546:ALA:HA   | 1.89        | 0.54     |
| 1:G:303:VAL:O    | 1:G:307:ARG:CZ   | 2.55        | 0.54     |
| 1:A:303:VAL:O    | 1:A:307:ARG:CZ   | 2.55        | 0.54     |
| 1:A:88:MET:HA    | 1:A:642:LEU:HD21 | 1.89        | 0.54     |
| 1:J:436:GLU:O    | 1:J:440:LEU:HD23 | 2.08        | 0.54     |
| 3:C:151:PRO:HA   | 3:C:154:ILE:HD11 | 1.88        | 0.54     |
| 1:A:259:THR:N    | 1:A:260:PRO:HD3  | 2.23        | 0.54     |
| 1:J:259:THR:N    | 1:J:260:PRO:HD3  | 2.23        | 0.54     |
| 3:I:248:PHE:O    | 3:I:254:HIS:HB3  | 2.07        | 0.54     |
| 1:D:634:GLN:NE2  | 1:D:638:MET:O    | 2.37        | 0.54     |
| 1:A:378:ASP:OD1  | 1:A:380:ARG:HG2  | 2.08        | 0.54     |
| 2:H:57:CYS:O     | 2:H:58:ARG:HB3   | 2.08        | 0.54     |
| 2:H:196:TYR:OH   | 3:I:21:ARG:HA    | 2.08        | 0.54     |
| 3:C:60:TRP:CE2   | 3:C:64:LYS:HD2   | 2.43        | 0.54     |
| 1:J:241:LEU:HD12 | 1:J:248:LEU:HD21 | 1.88        | 0.54     |
| 2:B:57:CYS:O     | 2:B:58:ARG:HB3   | 2.08        | 0.54     |
| 3:C:246:LYS:HE3  | 3:C:247:TYR:CZ   | 2.43        | 0.54     |
| 1:D:272:CYS:CB   | 1:D:328:LEU:HD21 | 2.38        | 0.53     |
| 1:D:288:MET:CG   | 1:D:297:GLU:OE2  | 2.56        | 0.53     |
| 1:A:349:CYS:HB2  | 1:A:357:PRO:HG3  | 1.90        | 0.53     |
| 2:B:144:GLU:C    | 2:B:146:PHE:H    | 2.10        | 0.53     |
| 3:I:60:TRP:CE2   | 3:I:64:LYS:HD2   | 2.44        | 0.53     |
| 1:G:32:ILE:CG2   | 1:G:33:VAL:N     | 2.71        | 0.53     |
| 1:G:288:MET:CG   | 1:G:297:GLU:OE2  | 2.56        | 0.53     |
| 1:D:302:ASP:HB2  | 1:D:546:ALA:HA   | 1.89        | 0.53     |
| 1:A:272:CYS:CB   | 1:A:328:LEU:HD21 | 2.38        | 0.53     |
| 1:D:436:GLU:O    | 1:D:440:LEU:HD23 | 2.08        | 0.53     |
| 1:G:8:SER:OG     | 1:G:31:THR:HG22  | 2.08        | 0.53     |
| 3:C:103:ILE:HG13 | 3:F:99:ARG:HA    | 1.89        | 0.53     |
| 1:G:259:THR:N    | 1:G:260:PRO:HD3  | 2.23        | 0.53     |
| 1:A:334:GLY:O    | 1:A:338:ILE:HG13 | 2.09        | 0.53     |
| 3:C:103:ILE:HD13 | 3:F:103:ILE:HG21 | 1.89        | 0.53     |
| 1:D:259:THR:N    | 1:D:260:PRO:HD3  | 2.23        | 0.53     |
| 1:G:272:CYS:CB   | 1:G:328:LEU:HD21 | 2.38        | 0.53     |
| 3:L:60:TRP:CE2   | 3:L:64:LYS:HD2   | 2.44        | 0.53     |
| 1:D:251:MET:CE   | 1:D:529:VAL:HG13 | 2.39        | 0.53     |
| 1:J:2:LYS:HB2    | 1:J:2:LYS:HZ2    | 1.71        | 0.53     |
| 3:F:223:LEU:HD23 | 3:F:223:LEU:C    | 2.29        | 0.53     |
| 1:J:267:LEU:HD21 | 5:J:702:MLA:O3A  | 2.09        | 0.53     |
| 3:F:249:ASP:OD1  | 3:F:253:THR:HA   | 2.08        | 0.53     |
| 1:J:378:ASP:OD1  | 1:J:380:ARG:HG2  | 2.08        | 0.53     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:G:3:VAL:HB     | 1:J:5:TYR:CD2     | 2.42        | 0.53     |
| 1:D:241:LEU:HD11 | 1:D:532:CYS:SG    | 2.48        | 0.53     |
| 1:A:32:ILE:CG2   | 1:A:33:VAL:N      | 2.71        | 0.53     |
| 3:L:136:MET:HB2  | 10:L:302:HEM:HBB2 | 1.90        | 0.53     |
| 2:E:167:ARG:HG3  | 2:E:167:ARG:NH1   | 2.23        | 0.53     |
| 2:E:196:TYR:OH   | 3:F:21:ARG:HA     | 2.08        | 0.53     |
| 3:C:223:LEU:C    | 3:C:223:LEU:HD23  | 2.29        | 0.53     |
| 3:I:246:LYS:HE3  | 3:I:247:TYR:CZ    | 2.43        | 0.53     |
| 1:J:349:CYS:HB2  | 1:J:357:PRO:HG3   | 1.91        | 0.53     |
| 1:G:423:TYR:CE2  | 1:G:643:PRO:HG3   | 2.43        | 0.53     |
| 1:J:8:SER:OG     | 1:J:31:THR:HG22   | 2.08        | 0.53     |
| 1:D:390:SER:OG   | 1:D:395:ALA:HB2   | 2.09        | 0.53     |
| 1:G:267:LEU:HD22 | 4:G:701:FAD:H6    | 1.90        | 0.53     |
| 1:D:423:TYR:CE2  | 1:D:643:PRO:HG3   | 2.43        | 0.53     |
| 1:G:251:MET:CE   | 1:G:529:VAL:HG13  | 2.39        | 0.53     |
| 1:A:436:GLU:O    | 1:A:440:LEU:HD23  | 2.08        | 0.53     |
| 3:L:36:PHE:CD2   | 3:L:37:LEU:HD23   | 2.44        | 0.53     |
| 2:K:167:ARG:NH1  | 2:K:167:ARG:HG3   | 2.23        | 0.53     |
| 2:K:196:TYR:OH   | 3:L:21:ARG:HA     | 2.08        | 0.53     |
| 2:H:10:PHE:HB2   | 2:H:92:LEU:HD23   | 1.91        | 0.53     |
| 3:I:223:LEU:C    | 3:I:223:LEU:HD23  | 2.29        | 0.53     |
| 3:L:246:LYS:HE3  | 3:L:247:TYR:CE2   | 2.44        | 0.53     |
| 1:G:319:GLN:HA   | 1:G:324:GLN:HA    | 1.91        | 0.53     |
| 1:A:390:SER:OG   | 1:A:395:ALA:HB2   | 2.09        | 0.53     |
| 3:F:246:LYS:HE3  | 3:F:247:TYR:CZ    | 2.43        | 0.53     |
| 2:E:144:GLU:C    | 2:E:146:PHE:H     | 2.10        | 0.53     |
| 1:G:634:GLN:NE2  | 1:G:638:MET:O     | 2.37        | 0.53     |
| 1:G:241:LEU:HD11 | 1:G:532:CYS:SG    | 2.48        | 0.53     |
| 1:G:461:GLU:HB2  | 1:G:504:VAL:HA    | 1.91        | 0.53     |
| 1:A:542:GLU:HA   | 1:A:552:TYR:HB3   | 1.91        | 0.53     |
| 1:J:267:LEU:HD22 | 4:J:701:FAD:H6    | 1.90        | 0.53     |
| 1:G:267:LEU:HD21 | 5:G:702:MLA:O3A   | 2.09        | 0.53     |
| 3:F:136:MET:HB2  | 10:F:302:HEM:HBB2 | 1.90        | 0.53     |
| 1:A:251:MET:CE   | 1:A:529:VAL:HG13  | 2.39        | 0.53     |
| 1:J:334:GLY:O    | 1:J:338:ILE:HG13  | 2.09        | 0.53     |
| 2:K:57:CYS:O     | 2:K:58:ARG:HB3    | 2.08        | 0.53     |
| 1:A:314:LYS:HB2  | 1:A:314:LYS:HZ2   | 1.72        | 0.53     |
| 1:J:242:GLU:HG2  | 1:J:528:LYS:HZ1   | 1.73        | 0.53     |
| 1:J:32:ILE:CG2   | 1:J:33:VAL:N      | 2.71        | 0.53     |
| 3:F:60:TRP:CE2   | 3:F:64:LYS:HD2    | 2.44        | 0.52     |
| 1:D:378:ASP:OD1  | 1:D:380:ARG:HG2   | 2.08        | 0.52     |
| 1:A:8:SER:OG     | 1:A:31:THR:HG22   | 2.08        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:214:ILE:CG2  | 1:J:216:THR:HG23 | 2.39        | 0.52     |
| 1:G:378:ASP:OD1  | 1:G:380:ARG:HG2  | 2.08        | 0.52     |
| 1:A:84:LYS:O     | 1:A:88:MET:HG3   | 2.10        | 0.52     |
| 1:D:562:ASN:HD22 | 1:D:562:ASN:N    | 2.03        | 0.52     |
| 3:L:223:LEU:HD23 | 3:L:223:LEU:C    | 2.29        | 0.52     |
| 1:D:319:GLN:HA   | 1:D:324:GLN:HA   | 1.91        | 0.52     |
| 1:A:267:LEU:HD21 | 5:A:702:MLA:O3A  | 2.09        | 0.52     |
| 1:D:349:CYS:HB2  | 1:D:357:PRO:HG3  | 1.90        | 0.52     |
| 2:K:144:GLU:C    | 2:K:146:PHE:H    | 2.10        | 0.52     |
| 1:G:436:GLU:O    | 1:G:440:LEU:HD23 | 2.08        | 0.52     |
| 1:G:390:SER:OG   | 1:G:395:ALA:HB2  | 2.09        | 0.52     |
| 1:D:214:ILE:CG2  | 1:D:216:THR:HG23 | 2.39        | 0.52     |
| 1:D:286:ARG:C    | 1:D:288:MET:N    | 2.62        | 0.52     |
| 1:A:279:LEU:H    | 1:A:288:MET:HE1  | 1.73        | 0.52     |
| 1:A:286:ARG:C    | 1:A:288:MET:N    | 2.62        | 0.52     |
| 3:F:53:LEU:O     | 3:F:54:GLY:O     | 2.27        | 0.52     |
| 1:J:586:ASN:HA   | 1:J:612:ARG:HD3  | 1.92        | 0.52     |
| 1:G:334:GLY:O    | 1:G:338:ILE:HG13 | 2.09        | 0.52     |
| 1:J:461:GLU:HB2  | 1:J:504:VAL:HA   | 1.91        | 0.52     |
| 3:I:197:PHE:N    | 3:I:197:PHE:CD2  | 2.78        | 0.52     |
| 1:J:286:ARG:C    | 1:J:288:MET:N    | 2.62        | 0.52     |
| 1:D:267:LEU:HD21 | 5:D:702:MLA:O3A  | 2.09        | 0.52     |
| 1:G:349:CYS:HB2  | 1:G:357:PRO:HG3  | 1.90        | 0.52     |
| 2:B:138:GLU:HB2  | 2:B:141:VAL:CG2  | 2.33        | 0.52     |
| 1:D:84:LYS:O     | 1:D:88:MET:HG3   | 2.10        | 0.52     |
| 1:A:3:VAL:HB     | 1:D:5:TYR:CD2    | 2.45        | 0.52     |
| 3:I:36:PHE:CD2   | 3:I:37:LEU:HD23  | 2.44        | 0.52     |
| 2:H:167:ARG:NH1  | 2:H:167:ARG:HG3  | 2.23        | 0.52     |
| 1:J:390:SER:OG   | 1:J:395:ALA:HB2  | 2.09        | 0.52     |
| 1:G:482:ARG:HB3  | 1:G:487:LEU:CD1  | 2.34        | 0.52     |
| 3:F:71:PHE:CB    | 3:F:75:LYS:HG3   | 2.39        | 0.52     |
| 3:I:249:ASP:HA   | 3:I:254:HIS:CB   | 2.39        | 0.52     |
| 3:I:53:LEU:O     | 3:I:54:GLY:O     | 2.27        | 0.52     |
| 3:C:71:PHE:CB    | 3:C:75:LYS:HG3   | 2.39        | 0.52     |
| 1:D:586:ASN:HA   | 1:D:612:ARG:HD3  | 1.92        | 0.52     |
| 2:E:111:PHE:C    | 2:E:113:GLY:N    | 2.63        | 0.52     |
| 1:J:295:LYS:CD   | 1:J:298:LEU:HD12 | 2.40        | 0.52     |
| 1:G:286:ARG:C    | 1:G:288:MET:N    | 2.62        | 0.52     |
| 3:F:249:ASP:HA   | 3:F:254:HIS:CB   | 2.40        | 0.52     |
| 3:L:53:LEU:O     | 3:L:54:GLY:O     | 2.27        | 0.52     |
| 1:J:84:LYS:O     | 1:J:88:MET:HG3   | 2.10        | 0.52     |
| 1:J:251:MET:CE   | 1:J:529:VAL:HG13 | 2.39        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:334:GLY:O    | 1:D:338:ILE:HG13 | 2.09        | 0.52     |
| 1:A:461:GLU:HB2  | 1:A:504:VAL:HA   | 1.91        | 0.52     |
| 3:I:246:LYS:HE3  | 3:I:247:TYR:CE2  | 2.44        | 0.52     |
| 1:J:285:HIS:N    | 1:J:285:HIS:HD2  | 2.08        | 0.52     |
| 1:G:214:ILE:CG2  | 1:G:216:THR:HG23 | 2.39        | 0.52     |
| 1:G:360:LYS:HG2  | 1:G:361:TRP:N    | 2.25        | 0.52     |
| 1:D:278:ILE:HB   | 1:D:288:MET:HE3  | 1.91        | 0.52     |
| 1:A:214:ILE:CG2  | 1:A:216:THR:HG23 | 2.39        | 0.52     |
| 1:G:84:LYS:O     | 1:G:88:MET:HG3   | 2.10        | 0.52     |
| 1:G:5:TYR:CD2    | 1:J:3:VAL:HB     | 2.45        | 0.52     |
| 1:G:346:GLN:CA   | 1:G:357:PRO:HG2  | 2.31        | 0.52     |
| 3:L:28:TRP:HE3   | 3:L:29:TRP:CD1   | 2.28        | 0.52     |
| 2:K:10:PHE:HB2   | 2:K:92:LEU:HD23  | 1.91        | 0.52     |
| 1:D:461:GLU:HB2  | 1:D:504:VAL:HA   | 1.91        | 0.52     |
| 1:J:303:VAL:HG13 | 1:J:307:ARG:NH2  | 2.25        | 0.52     |
| 1:G:295:LYS:CD   | 1:G:298:LEU:HD12 | 2.40        | 0.52     |
| 3:I:254:HIS:O    | 3:I:254:HIS:ND1  | 2.43        | 0.52     |
| 3:L:71:PHE:CB    | 3:L:75:LYS:HG3   | 2.39        | 0.52     |
| 1:A:217:GLY:N    | 1:A:394:ALA:HB2  | 2.25        | 0.52     |
| 1:G:542:GLU:HA   | 1:G:552:TYR:HB3  | 1.91        | 0.52     |
| 2:B:111:PHE:C    | 2:B:113:GLY:N    | 2.63        | 0.52     |
| 3:F:246:LYS:HE3  | 3:F:247:TYR:CE2  | 2.44        | 0.52     |
| 1:G:285:HIS:HD2  | 1:G:285:HIS:N    | 2.08        | 0.51     |
| 1:D:329:ASP:CG   | 1:D:361:TRP:HD1  | 2.14        | 0.51     |
| 3:L:249:ASP:HA   | 3:L:254:HIS:CB   | 2.40        | 0.51     |
| 3:C:36:PHE:CD2   | 3:C:37:LEU:HD23  | 2.44        | 0.51     |
| 3:C:28:TRP:HE3   | 3:C:29:TRP:CD1   | 2.28        | 0.51     |
| 2:E:85:GLU:HA    | 2:E:85:GLU:OE2   | 2.10        | 0.51     |
| 1:A:295:LYS:CD   | 1:A:298:LEU:HD12 | 2.40        | 0.51     |
| 3:C:53:LEU:O     | 3:C:54:GLY:O     | 2.28        | 0.51     |
| 1:J:643:PRO:O    | 1:J:647:LYS:HG2  | 2.11        | 0.51     |
| 3:F:28:TRP:HE3   | 3:F:29:TRP:CD1   | 2.28        | 0.51     |
| 2:B:167:ARG:NH1  | 2:B:167:ARG:HG3  | 2.23        | 0.51     |
| 3:F:18:LYS:HE3   | 3:F:21:ARG:NH1   | 2.23        | 0.51     |
| 3:I:18:LYS:HE3   | 3:I:21:ARG:NH1   | 2.23        | 0.51     |
| 2:B:10:PHE:HB2   | 2:B:92:LEU:HD23  | 1.91        | 0.51     |
| 3:I:87:PHE:HD2   | 3:I:144:LEU:HD13 | 1.76        | 0.51     |
| 3:L:197:PHE:HD2  | 3:L:197:PHE:N    | 2.08        | 0.51     |
| 1:D:90:VAL:HG23  | 1:D:91:ASN:N     | 2.25        | 0.51     |
| 1:G:132:ARG:HH11 | 1:G:132:ARG:HG2  | 1.76        | 0.51     |
| 1:A:132:ARG:HH11 | 1:A:132:ARG:HG2  | 1.76        | 0.51     |
| 1:A:319:GLN:HA   | 1:A:324:GLN:HA   | 1.91        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:360:LYS:HG2  | 1:J:361:TRP:N    | 2.25        | 0.51     |
| 1:A:303:VAL:HG13 | 1:A:307:ARG:NH2  | 2.25        | 0.51     |
| 1:J:319:GLN:HA   | 1:J:324:GLN:HA   | 1.91        | 0.51     |
| 2:K:85:GLU:HA    | 2:K:85:GLU:OE2   | 2.10        | 0.51     |
| 1:G:329:ASP:CG   | 1:G:361:TRP:HD1  | 2.14        | 0.51     |
| 1:D:295:LYS:HG3  | 1:D:298:LEU:HB2  | 1.93        | 0.51     |
| 1:A:360:LYS:HG2  | 1:A:361:TRP:N    | 2.25        | 0.51     |
| 1:G:344:ASP:C    | 1:G:348:ILE:HG12 | 2.31        | 0.51     |
| 3:F:254:HIS:O    | 3:F:254:HIS:ND1  | 2.43        | 0.51     |
| 3:I:71:PHE:CB    | 3:I:75:LYS:HG3   | 2.39        | 0.51     |
| 1:A:586:ASN:HA   | 1:A:612:ARG:HD3  | 1.92        | 0.51     |
| 3:F:36:PHE:CD2   | 3:F:37:LEU:HD23  | 2.44        | 0.51     |
| 1:G:217:GLY:N    | 1:G:394:ALA:HB2  | 2.25        | 0.51     |
| 1:A:543:SER:OG   | 1:A:553:PRO:HA   | 2.11        | 0.51     |
| 1:G:543:SER:OG   | 1:G:553:PRO:HA   | 2.11        | 0.51     |
| 1:J:552:TYR:N    | 1:J:553:PRO:CD   | 2.73        | 0.51     |
| 2:K:111:PHE:C    | 2:K:113:GLY:N    | 2.63        | 0.51     |
| 2:K:37:PHE:O     | 2:K:41:ASN:HB2   | 2.11        | 0.51     |
| 1:J:490:ALA:C    | 1:J:492:LYS:N    | 2.64        | 0.51     |
| 3:F:197:PHE:N    | 3:F:197:PHE:CD2  | 2.78        | 0.51     |
| 2:B:37:PHE:O     | 2:B:41:ASN:HB2   | 2.11        | 0.51     |
| 2:H:37:PHE:O     | 2:H:41:ASN:HB2   | 2.11        | 0.51     |
| 1:D:37:ILE:O     | 1:D:37:ILE:HD12  | 2.11        | 0.51     |
| 1:J:279:LEU:H    | 1:J:288:MET:HE1  | 1.76        | 0.51     |
| 1:G:643:PRO:O    | 1:G:647:LYS:HG2  | 2.11        | 0.51     |
| 1:J:318:VAL:HG13 | 1:J:318:VAL:O    | 2.11        | 0.51     |
| 3:C:99:ARG:HA    | 3:F:103:ILE:HG13 | 1.92        | 0.51     |
| 1:J:217:GLY:N    | 1:J:394:ALA:HB2  | 2.25        | 0.51     |
| 1:D:217:GLY:N    | 1:D:394:ALA:HB2  | 2.25        | 0.51     |
| 1:A:552:TYR:N    | 1:A:553:PRO:CD   | 2.73        | 0.51     |
| 1:D:542:GLU:HA   | 1:D:552:TYR:HB3  | 1.91        | 0.51     |
| 3:C:246:LYS:HE3  | 3:C:247:TYR:CE2  | 2.44        | 0.51     |
| 2:B:85:GLU:OE2   | 2:B:85:GLU:HA    | 2.10        | 0.51     |
| 1:G:318:VAL:HG13 | 1:G:318:VAL:O    | 2.11        | 0.51     |
| 1:A:325:HIS:HE1  | 1:A:327:TRP:CZ2  | 2.29        | 0.51     |
| 2:H:146:PHE:O    | 2:H:148:LEU:N    | 2.44        | 0.51     |
| 1:A:314:LYS:HZ3  | 1:A:314:LYS:CB   | 2.24        | 0.51     |
| 1:J:462:ASP:HB3  | 1:J:465:LYS:CG   | 2.40        | 0.51     |
| 1:A:462:ASP:HB3  | 1:A:465:LYS:CG   | 2.40        | 0.51     |
| 2:K:215:HIS:CG   | 2:K:225:GLN:HB2  | 2.46        | 0.51     |
| 1:G:392:GLY:C    | 1:G:394:ALA:N    | 2.64        | 0.51     |
| 1:J:542:GLU:HA   | 1:J:552:TYR:HB3  | 1.91        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:543:SER:OG   | 1:D:553:PRO:HA   | 2.11        | 0.51     |
| 3:F:197:PHE:N    | 3:F:197:PHE:HD2  | 2.08        | 0.51     |
| 1:A:594:TYR:CZ   | 1:A:600:LYS:HG2  | 2.46        | 0.51     |
| 1:D:53:ALA:O     | 1:D:55:LEU:N     | 2.38        | 0.51     |
| 1:G:594:TYR:CZ   | 1:G:600:LYS:HG2  | 2.46        | 0.51     |
| 1:J:132:ARG:HH11 | 1:J:132:ARG:HG2  | 1.76        | 0.51     |
| 1:A:37:ILE:HD12  | 1:A:37:ILE:O     | 2.11        | 0.51     |
| 1:J:482:ARG:HB3  | 1:J:487:LEU:CD1  | 2.34        | 0.51     |
| 2:E:146:PHE:O    | 2:E:148:LEU:N    | 2.44        | 0.51     |
| 1:D:643:PRO:O    | 1:D:647:LYS:HG2  | 2.11        | 0.51     |
| 3:I:28:TRP:HE3   | 3:I:29:TRP:CD1   | 2.28        | 0.51     |
| 1:A:318:VAL:HG13 | 1:A:318:VAL:O    | 2.11        | 0.51     |
| 2:E:10:PHE:HB2   | 2:E:92:LEU:HD23  | 1.91        | 0.51     |
| 1:J:392:GLY:C    | 1:J:394:ALA:N    | 2.64        | 0.51     |
| 2:H:215:HIS:CG   | 2:H:225:GLN:HB2  | 2.46        | 0.51     |
| 2:E:37:PHE:O     | 2:E:41:ASN:HB2   | 2.11        | 0.51     |
| 2:B:95:PRO:O     | 2:B:96:ALA:HB3   | 2.11        | 0.51     |
| 1:D:594:TYR:CZ   | 1:D:600:LYS:HG2  | 2.46        | 0.51     |
| 2:H:85:GLU:OE2   | 2:H:85:GLU:HA    | 2.10        | 0.51     |
| 1:G:295:LYS:HG3  | 1:G:298:LEU:HB2  | 1.93        | 0.51     |
| 1:D:267:LEU:HG   | 1:D:268:LEU:N    | 2.26        | 0.51     |
| 3:C:254:HIS:O    | 3:C:254:HIS:ND1  | 2.43        | 0.51     |
| 1:G:462:ASP:HB3  | 1:G:465:LYS:CG   | 2.41        | 0.51     |
| 1:D:392:GLY:C    | 1:D:394:ALA:N    | 2.64        | 0.51     |
| 1:J:543:SER:OG   | 1:J:553:PRO:HA   | 2.11        | 0.51     |
| 1:D:86:ALA:O     | 1:D:90:VAL:HG13  | 2.11        | 0.51     |
| 1:G:441:GLU:OE2  | 1:J:210:LYS:NZ   | 2.43        | 0.51     |
| 1:D:295:LYS:CD   | 1:D:298:LEU:HD12 | 2.40        | 0.51     |
| 1:A:295:LYS:HG3  | 1:A:298:LEU:HB2  | 1.93        | 0.51     |
| 3:I:75:LYS:HA    | 3:I:75:LYS:CE    | 2.41        | 0.51     |
| 1:A:643:PRO:O    | 1:A:647:LYS:HG2  | 2.11        | 0.51     |
| 3:L:63:LYS:O     | 3:L:66:GLN:HB2   | 2.11        | 0.51     |
| 3:L:227:THR:HG22 | 3:L:231:TYR:HE1  | 1.76        | 0.51     |
| 1:J:90:VAL:HG23  | 1:J:91:ASN:N     | 2.25        | 0.51     |
| 1:G:60:MET:HB3   | 1:G:147:TRP:CG   | 2.46        | 0.51     |
| 1:A:60:MET:HB3   | 1:A:147:TRP:CG   | 2.46        | 0.51     |
| 1:G:303:VAL:HG13 | 1:G:307:ARG:NH2  | 2.25        | 0.51     |
| 1:G:325:HIS:HE1  | 1:G:327:TRP:CZ2  | 2.29        | 0.51     |
| 1:D:303:VAL:HG13 | 1:D:307:ARG:NH2  | 2.25        | 0.51     |
| 1:D:325:HIS:HE1  | 1:D:327:TRP:CZ2  | 2.29        | 0.51     |
| 1:A:329:ASP:CG   | 1:A:361:TRP:HD1  | 2.14        | 0.51     |
| 1:G:586:ASN:HA   | 1:G:612:ARG:HD3  | 1.92        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:562:ASN:HD22 | 1:A:562:ASN:N    | 2.03        | 0.51     |
| 1:G:495:GLU:HG3  | 1:G:574:THR:HB   | 1.93        | 0.51     |
| 2:B:215:HIS:CG   | 2:B:225:GLN:HB2  | 2.46        | 0.51     |
| 1:G:552:TYR:N    | 1:G:553:PRO:CD   | 2.73        | 0.51     |
| 3:C:197:PHE:N    | 3:C:197:PHE:HD2  | 2.08        | 0.51     |
| 1:G:37:ILE:HD12  | 1:G:37:ILE:O     | 2.11        | 0.51     |
| 1:J:295:LYS:HG3  | 1:J:298:LEU:HB2  | 1.93        | 0.50     |
| 1:D:48:GLN:HG3   | 1:D:267:LEU:CD2  | 2.32        | 0.50     |
| 3:F:63:LYS:O     | 3:F:66:GLN:HB2   | 2.11        | 0.50     |
| 3:L:75:LYS:CE    | 3:L:75:LYS:HA    | 2.41        | 0.50     |
| 1:A:5:TYR:CD2    | 1:D:3:VAL:HB     | 2.46        | 0.50     |
| 3:C:18:LYS:HE3   | 3:C:21:ARG:NH1   | 2.23        | 0.50     |
| 1:D:462:ASP:HB3  | 1:D:465:LYS:CG   | 2.41        | 0.50     |
| 2:E:111:PHE:C    | 2:E:113:GLY:H    | 2.15        | 0.50     |
| 1:D:552:TYR:N    | 1:D:553:PRO:CD   | 2.73        | 0.50     |
| 2:H:111:PHE:C    | 2:H:113:GLY:N    | 2.63        | 0.50     |
| 3:F:227:THR:HG22 | 3:F:231:TYR:HE1  | 1.76        | 0.50     |
| 1:G:90:VAL:HG23  | 1:G:91:ASN:N     | 2.25        | 0.50     |
| 3:I:169:TRP:CD1  | 3:I:170:PRO:HD3  | 2.46        | 0.50     |
| 1:J:37:ILE:HD12  | 1:J:37:ILE:O     | 2.11        | 0.50     |
| 1:G:267:LEU:HG   | 1:G:268:LEU:N    | 2.26        | 0.50     |
| 1:D:360:LYS:HG2  | 1:D:361:TRP:N    | 2.25        | 0.50     |
| 1:A:214:ILE:HG23 | 1:A:216:THR:CG2  | 2.42        | 0.50     |
| 3:I:99:ARG:HA    | 3:L:103:ILE:HG13 | 1.92        | 0.50     |
| 2:B:146:PHE:O    | 2:B:148:LEU:N    | 2.44        | 0.50     |
| 3:L:87:PHE:HD2   | 3:L:144:LEU:HD13 | 1.76        | 0.50     |
| 3:C:169:TRP:CD1  | 3:C:170:PRO:HD3  | 2.47        | 0.50     |
| 2:E:95:PRO:O     | 2:E:96:ALA:HB3   | 2.11        | 0.50     |
| 1:J:329:ASP:CG   | 1:J:361:TRP:HD1  | 2.14        | 0.50     |
| 1:G:270:GLU:HB2  | 5:G:702:MLA:O3B  | 2.12        | 0.50     |
| 2:K:146:PHE:O    | 2:K:148:LEU:N    | 2.44        | 0.50     |
| 2:E:215:HIS:CG   | 2:E:225:GLN:HB2  | 2.46        | 0.50     |
| 3:F:14:THR:O     | 3:F:17:ARG:N     | 2.43        | 0.50     |
| 1:D:132:ARG:HH11 | 1:D:132:ARG:HG2  | 1.76        | 0.50     |
| 1:G:490:ALA:C    | 1:G:492:LYS:N    | 2.64        | 0.50     |
| 1:A:628:LYS:HE3  | 1:A:628:LYS:HA   | 1.94        | 0.50     |
| 1:J:270:GLU:HB2  | 5:J:702:MLA:O3B  | 2.12        | 0.50     |
| 1:A:101:ALA:HB2  | 1:A:107:TRP:CD1  | 2.47        | 0.50     |
| 3:C:249:ASP:HA   | 3:C:254:HIS:CB   | 2.40        | 0.50     |
| 3:F:249:ASP:HA   | 3:F:254:HIS:N    | 2.27        | 0.50     |
| 3:L:254:HIS:O    | 3:L:254:HIS:ND1  | 2.43        | 0.50     |
| 3:F:75:LYS:CE    | 3:F:75:LYS:HA    | 2.41        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:K:1:MET:HE3    | 2:K:31:ALA:HA    | 1.93        | 0.50     |
| 1:J:495:GLU:HG3  | 1:J:574:THR:HB   | 1.93        | 0.50     |
| 1:A:392:GLY:C    | 1:A:394:ALA:N    | 2.64        | 0.50     |
| 3:L:197:PHE:CD2  | 3:L:197:PHE:N    | 2.78        | 0.50     |
| 1:A:90:VAL:HG23  | 1:A:91:ASN:N     | 2.25        | 0.50     |
| 3:L:31:SER:HB3   | 3:L:190:LEU:HD11 | 1.94        | 0.50     |
| 1:D:270:GLU:HB2  | 5:D:702:MLA:O3B  | 2.12        | 0.50     |
| 1:A:107:TRP:O    | 1:A:109:ARG:HD2  | 2.12        | 0.50     |
| 3:C:249:ASP:HA   | 3:C:254:HIS:N    | 2.27        | 0.50     |
| 2:B:1:MET:HE2    | 2:B:31:ALA:HA    | 1.93        | 0.50     |
| 2:H:111:PHE:C    | 2:H:113:GLY:H    | 2.15        | 0.50     |
| 3:C:227:THR:HG22 | 3:C:231:TYR:HE1  | 1.76        | 0.50     |
| 3:C:31:SER:HB3   | 3:C:190:LEU:HD11 | 1.94        | 0.50     |
| 1:D:60:MET:HB3   | 1:D:147:TRP:CG   | 2.46        | 0.50     |
| 1:D:288:MET:CG   | 1:D:289:PRO:HD3  | 2.42        | 0.50     |
| 1:J:101:ALA:HB2  | 1:J:107:TRP:CD1  | 2.47        | 0.50     |
| 1:G:107:TRP:O    | 1:G:109:ARG:HD2  | 2.12        | 0.50     |
| 3:C:63:LYS:O     | 3:C:66:GLN:HB2   | 2.11        | 0.50     |
| 1:J:616:ILE:HG23 | 1:J:637:LEU:HD22 | 1.94        | 0.50     |
| 1:D:242:GLU:HG2  | 1:D:528:LYS:HZ1  | 1.74        | 0.50     |
| 2:H:46:THR:OG1   | 2:H:47:TYR:HD1   | 1.95        | 0.50     |
| 1:G:86:ALA:O     | 1:G:90:VAL:HG13  | 2.11        | 0.50     |
| 1:D:628:LYS:HE3  | 1:D:628:LYS:HA   | 1.94        | 0.50     |
| 1:J:325:HIS:HE1  | 1:J:327:TRP:CZ2  | 2.29        | 0.50     |
| 1:G:288:MET:CG   | 1:G:289:PRO:HD3  | 2.42        | 0.50     |
| 1:A:48:GLN:HG3   | 1:A:267:LEU:CD2  | 2.32        | 0.50     |
| 3:C:75:LYS:HA    | 3:C:75:LYS:CE    | 2.41        | 0.50     |
| 2:E:199:ILE:HD12 | 2:E:231:LEU:HD21 | 1.94        | 0.50     |
| 1:D:318:VAL:O    | 1:D:318:VAL:HG13 | 2.11        | 0.50     |
| 1:G:461:GLU:HB3  | 1:G:466:ILE:HD11 | 1.94        | 0.50     |
| 1:D:40:LYS:HD3   | 2:E:153:GLU:OE1  | 2.12        | 0.50     |
| 3:L:95:PHE:CE1   | 11:L:301:LMT:H82 | 2.47        | 0.50     |
| 3:I:227:THR:HG22 | 3:I:231:TYR:HE1  | 1.76        | 0.50     |
| 3:F:197:PHE:O    | 3:F:198:ASP:C    | 2.50        | 0.50     |
| 3:F:169:TRP:CD1  | 3:F:170:PRO:HD3  | 2.47        | 0.50     |
| 1:J:60:MET:HB3   | 1:J:147:TRP:CG   | 2.46        | 0.50     |
| 1:J:48:GLN:HG3   | 1:J:267:LEU:CD2  | 2.32        | 0.50     |
| 1:A:288:MET:CG   | 1:A:289:PRO:HD3  | 2.42        | 0.50     |
| 1:A:344:ASP:C    | 1:A:348:ILE:HG12 | 2.31        | 0.50     |
| 1:D:251:MET:HE1  | 1:D:529:VAL:HG13 | 1.93        | 0.50     |
| 1:J:241:LEU:HD12 | 1:J:248:LEU:HD23 | 1.94        | 0.50     |
| 3:L:40:PHE:C     | 3:L:40:PHE:CD2   | 2.85        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:40:LYS:HD3   | 2:H:153:GLU:OE1  | 2.12        | 0.50     |
| 1:J:40:LYS:HD3   | 2:K:153:GLU:OE1  | 2.12        | 0.50     |
| 3:C:197:PHE:N    | 3:C:197:PHE:CD2  | 2.78        | 0.50     |
| 3:F:31:SER:HB3   | 3:F:190:LEU:HD11 | 1.94        | 0.50     |
| 1:D:303:VAL:O    | 1:D:307:ARG:NH1  | 2.45        | 0.50     |
| 1:A:267:LEU:HG   | 1:A:268:LEU:N    | 2.26        | 0.50     |
| 1:A:285:HIS:HD2  | 1:A:285:HIS:N    | 2.08        | 0.50     |
| 3:I:63:LYS:O     | 3:I:66:GLN:HB2   | 2.11        | 0.50     |
| 2:B:199:ILE:HD12 | 2:B:231:LEU:HD21 | 1.94        | 0.50     |
| 3:C:40:PHE:CD2   | 3:C:40:PHE:C     | 2.85        | 0.50     |
| 3:I:197:PHE:O    | 3:I:198:ASP:C    | 2.50        | 0.50     |
| 1:J:86:ALA:O     | 1:J:90:VAL:HG13  | 2.11        | 0.50     |
| 2:H:95:PRO:O     | 2:H:96:ALA:HB3   | 2.11        | 0.50     |
| 1:D:523:VAL:HB   | 1:D:524:PRO:HD3  | 1.94        | 0.50     |
| 1:G:214:ILE:HG23 | 1:G:216:THR:CG2  | 2.42        | 0.49     |
| 1:G:141:PHE:O    | 1:G:298:LEU:HD22 | 2.12        | 0.49     |
| 1:D:141:PHE:O    | 1:D:298:LEU:HD22 | 2.12        | 0.49     |
| 1:A:278:ILE:HG21 | 1:A:286:ARG:HH11 | 1.77        | 0.49     |
| 1:G:101:ALA:HB2  | 1:G:107:TRP:CD1  | 2.47        | 0.49     |
| 3:L:248:PHE:HB3  | 3:L:254:HIS:HD1  | 1.77        | 0.49     |
| 1:A:642:LEU:HB2  | 1:A:647:LYS:HE3  | 1.94        | 0.49     |
| 1:A:616:ILE:HG23 | 1:A:637:LEU:HD22 | 1.93        | 0.49     |
| 2:E:191:THR:O    | 2:E:195:TYR:HD1  | 1.95        | 0.49     |
| 1:A:52:GLN:CG    | 1:A:148:ARG:HG3  | 2.42        | 0.49     |
| 3:I:40:PHE:CD2   | 3:I:40:PHE:C     | 2.85        | 0.49     |
| 2:B:111:PHE:C    | 2:B:113:GLY:H    | 2.15        | 0.49     |
| 1:A:86:ALA:O     | 1:A:90:VAL:HG13  | 2.11        | 0.49     |
| 1:J:104:GLY:O    | 1:J:105:VAL:C    | 2.50        | 0.49     |
| 1:J:594:TYR:CZ   | 1:J:600:LYS:HG2  | 2.46        | 0.49     |
| 1:J:307:ARG:HA   | 1:J:310:GLU:HB2  | 1.94        | 0.49     |
| 1:G:303:VAL:O    | 1:G:307:ARG:NH1  | 2.45        | 0.49     |
| 1:D:101:ALA:HB2  | 1:D:107:TRP:CD1  | 2.47        | 0.49     |
| 3:L:58:MET:HE3   | 3:L:156:PRO:HA   | 1.94        | 0.49     |
| 1:A:40:LYS:HD3   | 2:B:153:GLU:OE1  | 2.12        | 0.49     |
| 3:I:197:PHE:N    | 3:I:197:PHE:HD2  | 2.08        | 0.49     |
| 3:L:169:TRP:CD1  | 3:L:170:PRO:HD3  | 2.46        | 0.49     |
| 1:J:628:LYS:HE3  | 1:J:628:LYS:HA   | 1.94        | 0.49     |
| 1:D:214:ILE:HG23 | 1:D:216:THR:CG2  | 2.42        | 0.49     |
| 1:J:214:ILE:HG23 | 1:J:216:THR:CG2  | 2.42        | 0.49     |
| 1:A:303:VAL:O    | 1:A:307:ARG:NH1  | 2.45        | 0.49     |
| 3:C:248:PHE:HB3  | 3:C:254:HIS:HD1  | 1.77        | 0.49     |
| 1:J:642:LEU:HB2  | 1:J:647:LYS:HE3  | 1.94        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:F:40:PHE:CD2    | 3:F:40:PHE:C      | 2.85        | 0.49     |
| 3:I:31:SER:HB3    | 3:I:190:LEU:HD11  | 1.94        | 0.49     |
| 1:J:211:GLY:HA3   | 1:J:428:CYS:SG    | 2.53        | 0.49     |
| 1:J:303:VAL:O     | 1:J:307:ARG:NH1   | 2.45        | 0.49     |
| 3:L:249:ASP:HA    | 3:L:254:HIS:N     | 2.27        | 0.49     |
| 1:G:523:VAL:HB    | 1:G:524:PRO:HD3   | 1.94        | 0.49     |
| 2:K:95:PRO:O      | 2:K:96:ALA:HB3    | 2.11        | 0.49     |
| 3:I:249:ASP:HA    | 3:I:254:HIS:N     | 2.27        | 0.49     |
| 1:G:585:VAL:HA    | 1:G:588:MET:HG3   | 1.95        | 0.49     |
| 1:G:616:ILE:HG23  | 1:G:637:LEU:HD22  | 1.93        | 0.49     |
| 3:I:189:ARG:NH1   | 3:I:189:ARG:HG3   | 2.26        | 0.49     |
| 1:A:490:ALA:C     | 1:A:492:LYS:N     | 2.64        | 0.49     |
| 1:D:285:HIS:N     | 1:D:285:HIS:HD2   | 2.08        | 0.49     |
| 1:D:482:ARG:HB3   | 1:D:487:LEU:CD1   | 2.34        | 0.49     |
| 3:I:58:MET:HE3    | 3:I:156:PRO:HA    | 1.94        | 0.49     |
| 1:J:111:HIS:CD2   | 2:K:139:PRO:HG3   | 2.48        | 0.49     |
| 2:B:48:ASP:OD1    | 2:B:50:ASP:HB3    | 2.13        | 0.49     |
| 1:J:267:LEU:HG    | 1:J:268:LEU:N     | 2.26        | 0.49     |
| 1:J:410:VAL:HG13  | 4:J:701:FAD:N1    | 2.28        | 0.49     |
| 1:A:306:ARG:HB2   | 1:A:307:ARG:HH12  | 1.78        | 0.49     |
| 2:H:191:THR:O     | 2:H:195:TYR:HD1   | 1.95        | 0.49     |
| 1:D:495:GLU:HG3   | 1:D:574:THR:HB    | 1.93        | 0.49     |
| 1:A:461:GLU:HB3   | 1:A:466:ILE:HD11  | 1.94        | 0.49     |
| 2:H:215:HIS:CD2   | 2:H:225:GLN:HB2   | 2.48        | 0.49     |
| 3:C:197:PHE:O     | 3:C:198:ASP:C     | 2.50        | 0.49     |
| 3:C:169:TRP:N     | 3:C:170:PRO:CD    | 2.76        | 0.49     |
| 1:D:211:GLY:HA3   | 1:D:428:CYS:SG    | 2.53        | 0.49     |
| 1:G:111:HIS:CD2   | 2:H:139:PRO:HG3   | 2.48        | 0.49     |
| 2:H:36:ILE:HG22   | 2:H:76:ALA:HB1    | 1.95        | 0.49     |
| 1:G:278:ILE:HG21  | 1:G:286:ARG:HH11  | 1.77        | 0.49     |
| 1:D:307:ARG:HA    | 1:D:310:GLU:HB2   | 1.94        | 0.49     |
| 3:F:126:TRP:O     | 3:F:127:TRP:C     | 2.51        | 0.49     |
| 1:J:107:TRP:O     | 1:J:109:ARG:HD2   | 2.12        | 0.49     |
| 1:A:585:VAL:HA    | 1:A:588:MET:HG3   | 1.95        | 0.49     |
| 1:G:241:LEU:HD12  | 1:G:248:LEU:HD23  | 1.93        | 0.49     |
| 2:K:191:THR:O     | 2:K:195:TYR:HD1   | 1.95        | 0.49     |
| 1:G:2:LYS:HB2     | 1:G:2:LYS:HZ2     | 1.74        | 0.49     |
| 3:L:189:ARG:HG3   | 3:L:189:ARG:NH1   | 2.26        | 0.49     |
| 11:F:301:LMT:C6   | 11:F:301:LMT:H101 | 2.43        | 0.49     |
| 11:L:301:LMT:H101 | 11:L:301:LMT:C6   | 2.43        | 0.49     |
| 1:G:57:ASN:OD1    | 1:G:135:LEU:HB3   | 2.13        | 0.49     |
| 2:B:36:ILE:HG22   | 2:B:76:ALA:HB1    | 1.95        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:K:46:THR:OG1   | 2:K:47:TYR:HD1   | 1.95        | 0.49     |
| 1:A:523:VAL:HB   | 1:A:524:PRO:HD3  | 1.94        | 0.49     |
| 2:K:48:ASP:OD1   | 2:K:50:ASP:HB3   | 2.13        | 0.49     |
| 1:J:141:PHE:O    | 1:J:298:LEU:HD22 | 2.13        | 0.49     |
| 1:G:306:ARG:HB2  | 1:G:307:ARG:HH12 | 1.78        | 0.49     |
| 1:G:307:ARG:HA   | 1:G:310:GLU:HB2  | 1.94        | 0.49     |
| 1:A:307:ARG:HA   | 1:A:310:GLU:HB2  | 1.94        | 0.49     |
| 1:D:642:LEU:HB2  | 1:D:647:LYS:HE3  | 1.94        | 0.49     |
| 3:L:161:PHE:CE2  | 3:L:246:LYS:HB2  | 2.48        | 0.49     |
| 3:L:197:PHE:O    | 3:L:198:ASP:C    | 2.50        | 0.49     |
| 3:L:169:TRP:N    | 3:L:170:PRO:CD   | 2.76        | 0.49     |
| 1:A:51:MET:SD    | 1:A:97:ILE:HG13  | 2.53        | 0.49     |
| 1:G:405:LEU:O    | 1:G:408:ASN:HB2  | 2.13        | 0.49     |
| 1:G:628:LYS:HA   | 1:G:628:LYS:HE3  | 1.94        | 0.49     |
| 1:J:288:MET:CG   | 1:J:289:PRO:HD3  | 2.42        | 0.49     |
| 1:G:278:ILE:HB   | 1:G:288:MET:HE3  | 1.95        | 0.49     |
| 1:G:410:VAL:HG13 | 4:G:701:FAD:N1   | 2.28        | 0.49     |
| 1:G:48:GLN:HA    | 1:G:154:ASP:O    | 2.13        | 0.49     |
| 1:G:118:ILE:CD1  | 1:G:123:LYS:HE3  | 2.41        | 0.49     |
| 3:L:18:LYS:HE3   | 3:L:21:ARG:NH1   | 2.23        | 0.49     |
| 2:E:46:THR:OG1   | 2:E:47:TYR:HD1   | 1.95        | 0.49     |
| 2:K:111:PHE:C    | 2:K:113:GLY:H    | 2.15        | 0.49     |
| 1:G:211:GLY:HA3  | 1:G:428:CYS:SG   | 2.53        | 0.49     |
| 1:D:104:GLY:O    | 1:D:105:VAL:C    | 2.50        | 0.49     |
| 2:E:48:ASP:OD1   | 2:E:50:ASP:HB3   | 2.13        | 0.49     |
| 1:D:111:HIS:CD2  | 2:E:139:PRO:HG3  | 2.48        | 0.49     |
| 2:E:36:ILE:HG22  | 2:E:76:ALA:HB1   | 1.95        | 0.49     |
| 3:I:14:THR:O     | 3:I:17:ARG:N     | 2.42        | 0.49     |
| 1:A:104:GLY:O    | 1:A:105:VAL:C    | 2.50        | 0.49     |
| 2:H:48:ASP:OD1   | 2:H:50:ASP:HB3   | 2.13        | 0.49     |
| 1:J:306:ARG:HB2  | 1:J:307:ARG:HH12 | 1.78        | 0.48     |
| 1:A:141:PHE:O    | 1:A:298:LEU:HD22 | 2.12        | 0.48     |
| 3:L:126:TRP:O    | 3:L:127:TRP:C    | 2.51        | 0.48     |
| 2:H:199:ILE:HD12 | 2:H:231:LEU:HD21 | 1.94        | 0.48     |
| 1:D:241:LEU:HD12 | 1:D:248:LEU:HD23 | 1.94        | 0.48     |
| 2:K:215:HIS:CD2  | 2:K:225:GLN:HB2  | 2.48        | 0.48     |
| 2:E:215:HIS:CD2  | 2:E:225:GLN:HB2  | 2.48        | 0.48     |
| 1:J:57:ASN:OD1   | 1:J:135:LEU:HB3  | 2.13        | 0.48     |
| 1:D:57:ASN:OD1   | 1:D:135:LEU:HB3  | 2.13        | 0.48     |
| 3:F:169:TRP:N    | 3:F:170:PRO:CD   | 2.76        | 0.48     |
| 1:J:48:GLN:NE2   | 1:J:345:VAL:HG22 | 2.28        | 0.48     |
| 1:D:303:VAL:O    | 1:D:305:SER:N    | 2.46        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:270:GLU:HB2   | 5:A:702:MLA:O3B   | 2.12        | 0.48     |
| 1:A:241:LEU:HD12  | 1:A:248:LEU:HD23  | 1.94        | 0.48     |
| 1:A:495:GLU:HG3   | 1:A:574:THR:HB    | 1.93        | 0.48     |
| 1:D:461:GLU:HB3   | 1:D:466:ILE:HD11  | 1.94        | 0.48     |
| 1:D:111:HIS:HD2   | 2:E:139:PRO:HG3   | 1.78        | 0.48     |
| 1:D:112:LYS:HG3   | 1:D:133:HIS:HB2   | 1.95        | 0.48     |
| 1:G:247:GLN:HG2   | 1:G:567:SER:HB3   | 1.95        | 0.48     |
| 1:J:48:GLN:HA     | 1:J:154:ASP:O     | 2.13        | 0.48     |
| 2:H:209:MET:SD    | 3:I:100:LYS:HG3   | 2.53        | 0.48     |
| 2:B:209:MET:SD    | 3:C:100:LYS:HG3   | 2.53        | 0.48     |
| 1:D:344:ASP:C     | 1:D:348:ILE:HG12  | 2.31        | 0.48     |
| 1:D:107:TRP:O     | 1:D:109:ARG:HD2   | 2.12        | 0.48     |
| 1:J:464:PHE:CD1   | 2:K:45:GLU:HA     | 2.48        | 0.48     |
| 3:I:161:PHE:CE2   | 3:I:246:LYS:HB2   | 2.48        | 0.48     |
| 3:I:169:TRP:N     | 3:I:170:PRO:CD    | 2.76        | 0.48     |
| 1:D:490:ALA:C     | 1:D:492:LYS:N     | 2.64        | 0.48     |
| 1:G:104:GLY:O     | 1:G:105:VAL:C     | 2.50        | 0.48     |
| 1:J:523:VAL:HB    | 1:J:524:PRO:HD3   | 1.94        | 0.48     |
| 1:A:111:HIS:CD2   | 2:B:139:PRO:HG3   | 2.48        | 0.48     |
| 1:A:405:LEU:O     | 1:A:408:ASN:HB2   | 2.13        | 0.48     |
| 1:D:306:ARG:HB2   | 1:D:307:ARG:HH12  | 1.78        | 0.48     |
| 3:L:83:ALA:CA     | 10:L:303:HEM:HBB1 | 2.42        | 0.48     |
| 3:C:126:TRP:O     | 3:C:127:TRP:C     | 2.51        | 0.48     |
| 2:B:57:CYS:SG     | 2:B:61:ILE:HD12   | 2.53        | 0.48     |
| 2:B:215:HIS:CD2   | 2:B:225:GLN:HB2   | 2.48        | 0.48     |
| 11:C:303:LMT:H101 | 11:C:303:LMT:C6   | 2.43        | 0.48     |
| 1:J:74:VAL:O      | 1:J:77:SER:OG     | 2.28        | 0.48     |
| 3:F:161:PHE:CE2   | 3:F:246:LYS:HB2   | 2.48        | 0.48     |
| 1:G:112:LYS:HG3   | 1:G:133:HIS:HB2   | 1.95        | 0.48     |
| 2:H:157:CYS:SG    | 2:H:174:ALA:HB2   | 2.54        | 0.48     |
| 2:K:36:ILE:HG22   | 2:K:76:ALA:HB1    | 1.95        | 0.48     |
| 1:D:278:ILE:HG21  | 1:D:286:ARG:HH11  | 1.78        | 0.48     |
| 1:D:410:VAL:HG13  | 4:D:701:FAD:N1    | 2.28        | 0.48     |
| 2:E:209:MET:SD    | 3:F:100:LYS:HG3   | 2.53        | 0.48     |
| 3:I:248:PHE:HB3   | 3:I:254:HIS:HD1   | 1.77        | 0.48     |
| 1:D:616:ILE:HG23  | 1:D:637:LEU:HD22  | 1.94        | 0.48     |
| 1:J:314:LYS:CB    | 1:J:314:LYS:HZ3   | 2.25        | 0.48     |
| 1:D:464:PHE:CD1   | 2:E:45:GLU:HA     | 2.48        | 0.48     |
| 3:F:87:PHE:HD2    | 3:F:144:LEU:HD13  | 1.76        | 0.48     |
| 11:I:303:LMT:C6   | 11:I:303:LMT:H101 | 2.43        | 0.48     |
| 1:J:539:ASP:HB3   | 1:J:580:TYR:OH    | 2.14        | 0.48     |
| 1:G:108:THR:HG21  | 1:G:151:TYR:HE1   | 1.79        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:157:CYS:SG   | 2:B:174:ALA:HB2  | 2.54        | 0.48     |
| 1:J:247:GLN:HG2  | 1:J:567:SER:HB3  | 1.95        | 0.48     |
| 1:A:410:VAL:HG13 | 4:A:701:FAD:N1   | 2.28        | 0.48     |
| 2:K:199:ILE:HD12 | 2:K:231:LEU:HD21 | 1.94        | 0.48     |
| 1:J:461:GLU:HB3  | 1:J:466:ILE:HD11 | 1.94        | 0.48     |
| 1:G:464:PHE:CD1  | 2:H:45:GLU:HA    | 2.48        | 0.48     |
| 3:C:161:PHE:CE2  | 3:C:246:LYS:HB2  | 2.48        | 0.48     |
| 1:G:51:MET:SD    | 1:G:97:ILE:HG13  | 2.53        | 0.48     |
| 1:D:115:ARG:HG2  | 1:D:115:ARG:HH11 | 1.79        | 0.48     |
| 1:J:303:VAL:O    | 1:J:305:SER:N    | 2.46        | 0.48     |
| 1:G:303:VAL:O    | 1:G:305:SER:N    | 2.46        | 0.48     |
| 1:A:48:GLN:HA    | 1:A:154:ASP:O    | 2.13        | 0.48     |
| 1:A:303:VAL:O    | 1:A:305:SER:N    | 2.46        | 0.48     |
| 1:A:48:GLN:NE2   | 1:A:345:VAL:HG22 | 2.28        | 0.48     |
| 2:E:57:CYS:SG    | 2:E:61:ILE:HD12  | 2.53        | 0.48     |
| 2:K:57:CYS:SG    | 2:K:61:ILE:HD12  | 2.53        | 0.48     |
| 3:C:87:PHE:HD2   | 3:C:144:LEU:HD13 | 1.76        | 0.48     |
| 1:A:57:ASN:OD1   | 1:A:135:LEU:HB3  | 2.13        | 0.48     |
| 1:D:51:MET:SD    | 1:D:97:ILE:HG13  | 2.53        | 0.48     |
| 1:A:211:GLY:HA3  | 1:A:428:CYS:SG   | 2.53        | 0.48     |
| 2:B:46:THR:OG1   | 2:B:47:TYR:HD1   | 1.95        | 0.48     |
| 1:J:115:ARG:HG2  | 1:J:115:ARG:HH11 | 1.79        | 0.48     |
| 1:D:213:LEU:HD23 | 1:D:213:LEU:C    | 2.34        | 0.48     |
| 1:G:279:LEU:H    | 1:G:288:MET:HE1  | 1.76        | 0.48     |
| 1:D:48:GLN:HA    | 1:D:154:ASP:O    | 2.13        | 0.48     |
| 1:D:48:GLN:NE2   | 1:D:345:VAL:HG22 | 2.28        | 0.48     |
| 1:J:344:ASP:C    | 1:J:348:ILE:HG12 | 2.31        | 0.48     |
| 3:F:248:PHE:HB3  | 3:F:254:HIS:HD1  | 1.77        | 0.48     |
| 1:J:585:VAL:HA   | 1:J:588:MET:HG3  | 1.95        | 0.48     |
| 1:D:52:GLN:CG    | 1:D:148:ARG:HG3  | 2.42        | 0.48     |
| 3:F:95:PHE:CE1   | 11:F:301:LMT:H82 | 2.49        | 0.48     |
| 1:G:111:HIS:HD2  | 2:H:139:PRO:HG3  | 1.78        | 0.48     |
| 1:A:247:GLN:HG2  | 1:A:567:SER:HB3  | 1.95        | 0.48     |
| 1:D:518:GLU:O    | 1:D:522:ARG:HG3  | 2.14        | 0.48     |
| 4:G:701:FAD:H9   | 4:G:701:FAD:H1'1 | 1.63        | 0.48     |
| 3:I:126:TRP:O    | 3:I:127:TRP:C    | 2.51        | 0.48     |
| 2:E:144:GLU:C    | 2:E:146:PHE:N    | 2.68        | 0.48     |
| 1:D:585:VAL:HA   | 1:D:588:MET:HG3  | 1.95        | 0.48     |
| 2:B:191:THR:O    | 2:B:195:TYR:HD1  | 1.95        | 0.48     |
| 3:F:13:VAL:HG22  | 3:F:18:LYS:H     | 1.79        | 0.48     |
| 1:D:539:ASP:HB3  | 1:D:580:TYR:OH   | 2.14        | 0.48     |
| 1:J:111:HIS:HD2  | 2:K:139:PRO:HG3  | 1.78        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:E:157:CYS:SG   | 2:E:174:ALA:HB2  | 2.54        | 0.48     |
| 1:J:51:MET:SD    | 1:J:97:ILE:HG13  | 2.53        | 0.48     |
| 1:J:278:ILE:HB   | 1:J:288:MET:HE3  | 1.95        | 0.48     |
| 1:A:288:MET:HB3  | 1:A:289:PRO:HD2  | 1.89        | 0.48     |
| 2:K:209:MET:SD   | 3:L:100:LYS:HG3  | 2.53        | 0.48     |
| 3:C:248:PHE:HB3  | 3:C:254:HIS:ND1  | 2.29        | 0.48     |
| 3:F:69:PHE:CD1   | 3:F:70:ILE:HG13  | 2.40        | 0.48     |
| 1:A:112:LYS:HG3  | 1:A:133:HIS:HB2  | 1.95        | 0.48     |
| 1:D:405:LEU:O    | 1:D:408:ASN:HB2  | 2.13        | 0.48     |
| 1:J:518:GLU:O    | 1:J:522:ARG:HG3  | 2.14        | 0.48     |
| 1:G:115:ARG:HG2  | 1:G:115:ARG:HH11 | 1.79        | 0.48     |
| 1:A:213:LEU:C    | 1:A:213:LEU:HD23 | 2.34        | 0.47     |
| 3:F:58:MET:HE3   | 3:F:156:PRO:HA   | 1.95        | 0.47     |
| 1:G:642:LEU:HB2  | 1:G:647:LYS:HE3  | 1.94        | 0.47     |
| 1:A:5:TYR:HD1    | 1:A:208:VAL:HG23 | 1.79        | 0.47     |
| 3:F:36:PHE:HD2   | 3:F:89:VAL:CG1   | 2.25        | 0.47     |
| 1:A:115:ARG:HG2  | 1:A:115:ARG:HH11 | 1.79        | 0.47     |
| 1:G:48:GLN:NE2   | 1:G:345:VAL:HG22 | 2.28        | 0.47     |
| 1:A:349:CYS:O    | 1:A:353:ALA:HB3  | 2.14        | 0.47     |
| 3:I:248:PHE:HB3  | 3:I:254:HIS:ND1  | 2.29        | 0.47     |
| 1:G:52:GLN:CG    | 1:G:148:ARG:HG3  | 2.42        | 0.47     |
| 2:H:57:CYS:SG    | 2:H:61:ILE:HD12  | 2.53        | 0.47     |
| 1:J:112:LYS:HG3  | 1:J:133:HIS:HB2  | 1.95        | 0.47     |
| 2:K:34:MET:SD    | 2:K:39:VAL:HG22  | 2.55        | 0.47     |
| 1:J:405:LEU:O    | 1:J:408:ASN:HB2  | 2.13        | 0.47     |
| 2:K:157:CYS:SG   | 2:K:174:ALA:HB2  | 2.54        | 0.47     |
| 1:J:278:ILE:CD1  | 1:J:286:ARG:HH11 | 2.28        | 0.47     |
| 1:G:278:ILE:HD12 | 1:G:286:ARG:NH1  | 2.29        | 0.47     |
| 2:K:144:GLU:C    | 2:K:146:PHE:N    | 2.67        | 0.47     |
| 1:J:233:GLU:HB3  | 1:J:526:MET:HE3  | 1.96        | 0.47     |
| 1:J:451:MET:O    | 1:J:455:VAL:HG23 | 2.15        | 0.47     |
| 3:I:136:MET:CE   | 3:I:179:VAL:HA   | 2.45        | 0.47     |
| 1:D:349:CYS:O    | 1:D:353:ALA:HB3  | 2.14        | 0.47     |
| 2:H:144:GLU:C    | 2:H:146:PHE:N    | 2.68        | 0.47     |
| 3:I:69:PHE:CD1   | 3:I:70:ILE:HG13  | 2.40        | 0.47     |
| 2:E:166:MET:HE2  | 3:F:107:GLN:HB3  | 1.95        | 0.47     |
| 1:A:464:PHE:CD1  | 2:B:45:GLU:HA    | 2.48        | 0.47     |
| 1:D:319:GLN:CA   | 1:D:324:GLN:HA   | 2.45        | 0.47     |
| 3:L:168:MET:HB3  | 3:L:172:TYR:CE1  | 2.50        | 0.47     |
| 1:A:518:GLU:O    | 1:A:522:ARG:HG3  | 2.14        | 0.47     |
| 1:D:255:GLN:HE21 | 1:D:403:ASN:ND2  | 2.12        | 0.47     |
| 3:F:204:LYS:O    | 3:F:207:ALA:HB3  | 2.15        | 0.47     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:D:247:GLN:HG2  | 1:D:567:SER:HB3   | 1.95        | 0.47     |
| 3:F:218:ALA:O    | 3:F:222:VAL:HG23  | 2.15        | 0.47     |
| 1:A:255:GLN:HE21 | 1:A:403:ASN:ND2   | 2.12        | 0.47     |
| 1:J:278:ILE:HG21 | 1:J:286:ARG:HH11  | 1.77        | 0.47     |
| 3:F:136:MET:CE   | 3:F:179:VAL:HA    | 2.45        | 0.47     |
| 1:A:357:PRO:C    | 1:A:359:GLU:H     | 2.18        | 0.47     |
| 1:J:356:ASP:HA   | 1:J:357:PRO:HD3   | 1.71        | 0.47     |
| 1:A:152:THR:O    | 1:A:153:ALA:HB3   | 2.15        | 0.47     |
| 1:J:152:THR:O    | 1:J:153:ALA:HB3   | 2.15        | 0.47     |
| 1:G:349:CYS:O    | 1:G:353:ALA:HB3   | 2.14        | 0.47     |
| 1:A:251:MET:HE1  | 1:A:529:VAL:HG13  | 1.97        | 0.47     |
| 1:A:540:ARG:NH2  | 1:A:562:ASN:HD22  | 2.08        | 0.47     |
| 1:G:186:HIS:CD2  | 1:G:243:THR:HB    | 2.50        | 0.47     |
| 1:D:186:HIS:CD2  | 1:D:243:THR:HB    | 2.50        | 0.47     |
| 1:A:319:GLN:CA   | 1:A:324:GLN:HA    | 2.45        | 0.47     |
| 3:I:204:LYS:O    | 3:I:207:ALA:HB3   | 2.15        | 0.47     |
| 3:F:168:MET:HB3  | 3:F:172:TYR:CE1   | 2.50        | 0.47     |
| 1:G:219:TYR:O    | 1:G:222:ILE:HG12  | 2.15        | 0.47     |
| 3:L:218:ALA:O    | 3:L:222:VAL:HG23  | 2.15        | 0.47     |
| 1:G:368:GLN:NE2  | 1:G:368:GLN:C     | 2.68        | 0.47     |
| 3:L:136:MET:CE   | 3:L:179:VAL:HA    | 2.44        | 0.47     |
| 1:J:349:CYS:O    | 1:J:353:ALA:HB3   | 2.15        | 0.47     |
| 1:D:5:TYR:HD1    | 1:D:208:VAL:HG23  | 1.79        | 0.47     |
| 3:C:36:PHE:HD2   | 3:C:89:VAL:CG1    | 2.25        | 0.47     |
| 1:D:540:ARG:NH2  | 1:D:562:ASN:HD22  | 2.08        | 0.47     |
| 1:J:41:ARG:NH2   | 2:K:153:GLU:O     | 2.42        | 0.47     |
| 1:A:539:ASP:HB3  | 1:A:580:TYR:OH    | 2.14        | 0.47     |
| 1:A:32:ILE:HD13  | 1:A:207:TYR:HE2   | 1.80        | 0.47     |
| 1:A:351:TYR:CD2  | 2:B:78:ARG:HD3    | 2.50        | 0.47     |
| 3:L:14:THR:O     | 3:L:17:ARG:N      | 2.42        | 0.47     |
| 1:G:518:GLU:O    | 1:G:522:ARG:HG3   | 2.14        | 0.47     |
| 3:C:14:THR:O     | 3:C:17:ARG:N      | 2.43        | 0.47     |
| 2:H:34:MET:SD    | 2:H:39:VAL:HG22   | 2.55        | 0.47     |
| 1:J:108:THR:HG21 | 1:J:151:TYR:HE1   | 1.79        | 0.47     |
| 1:G:71:MET:O     | 1:G:75:LYS:HG3    | 2.15        | 0.47     |
| 1:G:213:LEU:C    | 1:G:213:LEU:HD23  | 2.34        | 0.47     |
| 1:J:213:LEU:HD23 | 1:J:213:LEU:C     | 2.34        | 0.47     |
| 1:D:278:ILE:CD1  | 1:D:286:ARG:HH11  | 2.28        | 0.47     |
| 3:I:83:ALA:CA    | 10:I:302:HEM:HBB1 | 2.42        | 0.47     |
| 1:G:152:THR:O    | 1:G:153:ALA:HB3   | 2.15        | 0.47     |
| 1:A:487:LEU:O    | 1:A:538:LEU:HD22  | 2.15        | 0.47     |
| 3:C:58:MET:HE3   | 3:C:156:PRO:HA    | 1.96        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:5:TYR:HD1    | 1:J:208:VAL:HG23 | 1.79        | 0.47     |
| 1:G:32:ILE:HD13  | 1:G:207:TYR:HE2  | 1.80        | 0.47     |
| 1:G:319:GLN:CA   | 1:G:324:GLN:HA   | 2.45        | 0.47     |
| 1:J:319:GLN:CA   | 1:J:324:GLN:HA   | 2.45        | 0.47     |
| 1:D:37:ILE:O     | 1:D:38:PRO:C     | 2.53        | 0.47     |
| 1:G:492:LYS:O    | 1:G:492:LYS:HD3  | 2.15        | 0.47     |
| 1:A:111:HIS:HD2  | 2:B:139:PRO:HG3  | 1.78        | 0.47     |
| 1:A:71:MET:O     | 1:A:75:LYS:HG3   | 2.15        | 0.47     |
| 2:E:34:MET:SD    | 2:E:39:VAL:HG22  | 2.55        | 0.47     |
| 3:I:218:ALA:O    | 3:I:222:VAL:HG23 | 2.15        | 0.47     |
| 1:J:58:SER:HA    | 1:J:110:ILE:CD1  | 2.45        | 0.47     |
| 1:A:368:GLN:NE2  | 1:A:368:GLN:C    | 2.68        | 0.47     |
| 3:I:168:MET:HB3  | 3:I:172:TYR:CE1  | 2.50        | 0.47     |
| 1:G:255:GLN:HE21 | 1:G:403:ASN:ND2  | 2.12        | 0.47     |
| 3:I:171:LEU:HD12 | 3:L:145:TYR:CE1  | 2.49        | 0.47     |
| 1:J:487:LEU:O    | 1:J:538:LEU:HD22 | 2.15        | 0.47     |
| 2:B:144:GLU:C    | 2:B:146:PHE:N    | 2.68        | 0.47     |
| 1:G:539:ASP:HB3  | 1:G:580:TYR:OH   | 2.14        | 0.47     |
| 2:B:147:GLU:HA   | 2:B:150:ARG:HD3  | 1.97        | 0.47     |
| 1:J:219:TYR:O    | 1:J:222:ILE:HG12 | 2.15        | 0.47     |
| 1:A:451:MET:O    | 1:A:455:VAL:HG23 | 2.15        | 0.47     |
| 1:J:255:GLN:HE21 | 1:J:403:ASN:ND2  | 2.12        | 0.47     |
| 1:G:355:ILE:C    | 1:G:355:ILE:HD12 | 2.35        | 0.47     |
| 1:J:288:MET:HB3  | 1:J:289:PRO:HD2  | 1.89        | 0.47     |
| 3:I:103:ILE:H    | 3:I:107:GLN:HE21 | 1.62        | 0.47     |
| 1:D:2:LYS:HB2    | 1:D:2:LYS:HZ3    | 1.76        | 0.47     |
| 1:J:10:VAL:O     | 1:J:10:VAL:HG12  | 2.15        | 0.47     |
| 1:J:32:ILE:HD13  | 1:J:207:TYR:HE2  | 1.80        | 0.47     |
| 3:C:72:GLU:HB3   | 3:C:73:GLY:H     | 1.47        | 0.47     |
| 1:G:617:ASP:HA   | 1:G:620:GLN:HB2  | 1.97        | 0.47     |
| 2:B:34:MET:SD    | 2:B:39:VAL:HG22  | 2.55        | 0.47     |
| 2:E:232:ARG:HG2  | 3:F:194:TRP:CZ3  | 2.50        | 0.47     |
| 1:D:351:TYR:CD2  | 2:E:78:ARG:HD3   | 2.50        | 0.47     |
| 1:D:278:ILE:HD12 | 1:D:286:ARG:NH1  | 2.29        | 0.47     |
| 3:L:103:ILE:H    | 3:L:107:GLN:HE21 | 1.62        | 0.47     |
| 3:F:248:PHE:HB3  | 3:F:254:HIS:ND1  | 2.29        | 0.47     |
| 3:L:248:PHE:HB3  | 3:L:254:HIS:ND1  | 2.29        | 0.47     |
| 1:G:5:TYR:HD1    | 1:G:208:VAL:HG23 | 1.79        | 0.47     |
| 1:A:10:VAL:O     | 1:A:10:VAL:HG12  | 2.15        | 0.47     |
| 1:D:10:VAL:HG12  | 1:D:10:VAL:O     | 2.15        | 0.47     |
| 3:C:85:PHE:C     | 3:C:87:PHE:H     | 2.19        | 0.47     |
| 1:A:186:HIS:CD2  | 1:A:243:THR:HB   | 2.50        | 0.47     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:D:32:ILE:HD13  | 1:D:207:TYR:HE2   | 1.80        | 0.47     |
| 1:G:37:ILE:O     | 1:G:38:PRO:C      | 2.53        | 0.47     |
| 1:J:71:MET:O     | 1:J:75:LYS:HG3    | 2.15        | 0.47     |
| 2:K:114:MET:O    | 2:K:118:VAL:HG22  | 2.15        | 0.47     |
| 1:D:108:THR:HG21 | 1:D:151:TYR:HE1   | 1.79        | 0.47     |
| 1:A:108:THR:HG21 | 1:A:151:TYR:HE1   | 1.79        | 0.47     |
| 1:J:278:ILE:HD12 | 1:J:286:ARG:NH1   | 2.29        | 0.46     |
| 1:D:487:LEU:O    | 1:D:538:LEU:HD22  | 2.15        | 0.46     |
| 1:J:52:GLN:CG    | 1:J:148:ARG:HG3   | 2.42        | 0.46     |
| 2:H:147:GLU:HA   | 2:H:150:ARG:HD3   | 1.97        | 0.46     |
| 1:G:57:ASN:O     | 1:G:132:ARG:NH1   | 2.48        | 0.46     |
| 3:C:204:LYS:O    | 3:C:207:ALA:HB3   | 2.15        | 0.46     |
| 1:J:368:GLN:NE2  | 1:J:368:GLN:C     | 2.68        | 0.46     |
| 2:H:114:MET:O    | 2:H:118:VAL:HG22  | 2.15        | 0.46     |
| 1:A:281:ASP:CG   | 1:A:287:PHE:HB2   | 2.36        | 0.46     |
| 3:L:13:VAL:HG22  | 3:L:18:LYS:H      | 1.79        | 0.46     |
| 2:K:147:GLU:HA   | 2:K:150:ARG:HD3   | 1.97        | 0.46     |
| 2:H:230:TYR:CE1  | 2:H:234:LYS:HD2   | 2.50        | 0.46     |
| 1:J:57:ASN:O     | 1:J:132:ARG:NH1   | 2.48        | 0.46     |
| 3:L:186:GLY:O    | 3:L:190:LEU:HB2   | 2.15        | 0.46     |
| 3:F:186:GLY:O    | 3:F:190:LEU:HB2   | 2.15        | 0.46     |
| 2:H:222:LEU:HB3  | 2:H:223:PRO:HD2   | 1.97        | 0.46     |
| 2:H:232:ARG:HG2  | 3:I:194:TRP:CZ3   | 2.50        | 0.46     |
| 1:G:18:LEU:O     | 1:G:22:VAL:HG23   | 2.15        | 0.46     |
| 1:G:451:MET:O    | 1:G:455:VAL:HG23  | 2.15        | 0.46     |
| 3:L:204:LYS:O    | 3:L:207:ALA:HB3   | 2.15        | 0.46     |
| 1:D:368:GLN:NE2  | 1:D:368:GLN:C     | 2.68        | 0.46     |
| 1:J:281:ASP:CG   | 1:J:287:PHE:HB2   | 2.36        | 0.46     |
| 1:J:296:LYS:HG3  | 1:J:307:ARG:HE    | 1.81        | 0.46     |
| 1:G:278:ILE:CD1  | 1:G:286:ARG:HH11  | 2.28        | 0.46     |
| 1:G:288:MET:HB3  | 1:G:289:PRO:HD2   | 1.89        | 0.46     |
| 3:C:83:ALA:CA    | 10:C:302:HEM:HBB1 | 2.42        | 0.46     |
| 3:C:253:THR:HG22 | 3:C:254:HIS:N     | 2.21        | 0.46     |
| 1:D:225:ASN:HB3  | 1:D:367:MET:CE    | 2.41        | 0.46     |
| 1:G:225:ASN:HB3  | 1:G:367:MET:CE    | 2.41        | 0.46     |
| 3:C:13:VAL:HG22  | 3:C:18:LYS:H      | 1.79        | 0.46     |
| 1:J:37:ILE:O     | 1:J:38:PRO:C      | 2.53        | 0.46     |
| 1:D:110:ILE:HA   | 1:D:137:HIS:HD2   | 1.80        | 0.46     |
| 1:D:58:SER:HA    | 1:D:110:ILE:CD1   | 2.45        | 0.46     |
| 1:G:351:TYR:CD2  | 2:H:78:ARG:HD3    | 2.50        | 0.46     |
| 1:D:219:TYR:O    | 1:D:222:ILE:HG12  | 2.15        | 0.46     |
| 2:K:222:LEU:HB3  | 2:K:223:PRO:HD2   | 1.97        | 0.46     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:C:168:MET:HB3  | 3:C:172:TYR:CE1   | 2.50        | 0.46     |
| 1:G:58:SER:HA    | 1:G:110:ILE:CD1   | 2.45        | 0.46     |
| 1:J:351:TYR:CD2  | 2:K:78:ARG:HD3    | 2.50        | 0.46     |
| 1:A:355:ILE:HD12 | 1:A:355:ILE:C     | 2.35        | 0.46     |
| 3:L:36:PHE:HD2   | 3:L:89:VAL:CG1    | 2.25        | 0.46     |
| 1:J:186:HIS:CD2  | 1:J:243:THR:HB    | 2.50        | 0.46     |
| 2:E:145:VAL:CG1  | 2:E:145:VAL:O     | 2.64        | 0.46     |
| 2:E:230:TYR:CE1  | 2:E:234:LYS:HD2   | 2.51        | 0.46     |
| 1:J:492:LYS:O    | 1:J:492:LYS:HD3   | 2.15        | 0.46     |
| 2:B:222:LEU:HB3  | 2:B:223:PRO:HD2   | 1.97        | 0.46     |
| 1:G:233:GLU:HB3  | 1:G:526:MET:HE3   | 1.98        | 0.46     |
| 2:B:232:ARG:HG2  | 3:C:194:TRP:CZ3   | 2.50        | 0.46     |
| 2:B:114:MET:O    | 2:B:118:VAL:HG22  | 2.15        | 0.46     |
| 3:F:83:ALA:CA    | 10:F:303:HEM:HBB1 | 2.42        | 0.46     |
| 1:D:119:ILE:CG2  | 1:D:120:ASN:H     | 2.15        | 0.46     |
| 1:G:487:LEU:O    | 1:G:538:LEU:HD22  | 2.15        | 0.46     |
| 2:B:206:PHE:CE1  | 3:C:24:ALA:HB2    | 2.51        | 0.46     |
| 2:E:206:PHE:CE1  | 3:F:24:ALA:HB2    | 2.51        | 0.46     |
| 2:H:1:MET:HE2    | 2:H:31:ALA:HA     | 1.95        | 0.46     |
| 2:H:145:VAL:O    | 2:H:145:VAL:CG1   | 2.64        | 0.46     |
| 1:A:542:GLU:HG2  | 1:A:560:TRP:CD1   | 2.51        | 0.46     |
| 3:I:98:MET:O     | 3:I:101:PHE:HB2   | 2.16        | 0.46     |
| 2:E:222:LEU:HB3  | 2:E:223:PRO:HD2   | 1.97        | 0.46     |
| 1:D:617:ASP:HA   | 1:D:620:GLN:HB2   | 1.97        | 0.46     |
| 1:D:18:LEU:O     | 1:D:22:VAL:HG23   | 2.15        | 0.46     |
| 1:G:296:LYS:HG3  | 1:G:307:ARG:HE    | 1.81        | 0.46     |
| 1:D:152:THR:O    | 1:D:153:ALA:HB3   | 2.15        | 0.46     |
| 1:J:41:ARG:HH11  | 1:J:41:ARG:CG     | 2.29        | 0.46     |
| 1:D:57:ASN:O     | 1:D:132:ARG:NH1   | 2.48        | 0.46     |
| 3:I:186:GLY:O    | 3:I:190:LEU:HB2   | 2.15        | 0.46     |
| 1:G:173:VAL:HG12 | 1:G:174:SER:N     | 2.31        | 0.46     |
| 1:J:18:LEU:O     | 1:J:22:VAL:HG23   | 2.15        | 0.46     |
| 1:A:296:LYS:HG3  | 1:A:307:ARG:HE    | 1.81        | 0.46     |
| 1:J:478:VAL:O    | 1:J:478:VAL:HG12  | 2.16        | 0.46     |
| 3:I:253:THR:HG22 | 3:I:254:HIS:N     | 2.21        | 0.46     |
| 1:J:84:LYS:HE3   | 1:J:638:MET:HG3   | 1.97        | 0.46     |
| 1:G:10:VAL:O     | 1:G:10:VAL:HG12   | 2.15        | 0.46     |
| 3:C:103:ILE:H    | 3:C:107:GLN:HE21  | 1.62        | 0.46     |
| 1:J:93:ALA:N     | 1:J:94:PRO:CD     | 2.79        | 0.46     |
| 1:A:226:THR:OG1  | 1:A:368:GLN:NE2   | 2.49        | 0.46     |
| 2:E:114:MET:O    | 2:E:118:VAL:HG22  | 2.15        | 0.46     |
| 1:D:451:MET:O    | 1:D:455:VAL:HG23  | 2.15        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:288:MET:O    | 1:G:290:ASP:N    | 2.48        | 0.46     |
| 1:G:295:LYS:HG3  | 1:G:297:GLU:O    | 2.16        | 0.46     |
| 1:D:295:LYS:HG3  | 1:D:297:GLU:O    | 2.16        | 0.46     |
| 1:A:281:ASP:CB   | 1:A:285:HIS:NE2  | 2.79        | 0.46     |
| 4:A:701:FAD:H1'1 | 4:A:701:FAD:H9   | 1.63        | 0.46     |
| 3:C:136:MET:CE   | 3:C:179:VAL:HA   | 2.45        | 0.46     |
| 1:D:478:VAL:HG12 | 1:D:478:VAL:O    | 2.16        | 0.46     |
| 3:F:146:ILE:C    | 3:F:148:MET:N    | 2.61        | 0.46     |
| 3:L:49:SER:HA    | 3:L:227:THR:HG21 | 1.98        | 0.46     |
| 1:J:617:ASP:HA   | 1:J:620:GLN:HB2  | 1.97        | 0.46     |
| 1:A:219:TYR:O    | 1:A:222:ILE:HG12 | 2.15        | 0.46     |
| 1:J:288:MET:O    | 1:J:290:ASP:N    | 2.48        | 0.46     |
| 1:G:281:ASP:CB   | 1:G:285:HIS:NE2  | 2.79        | 0.46     |
| 1:D:281:ASP:CB   | 1:D:285:HIS:NE2  | 2.79        | 0.46     |
| 1:D:288:MET:HB3  | 1:D:289:PRO:HD2  | 1.89        | 0.46     |
| 1:D:296:LYS:HG3  | 1:D:307:ARG:HE   | 1.81        | 0.46     |
| 1:A:295:LYS:HG3  | 1:A:297:GLU:O    | 2.16        | 0.46     |
| 2:K:166:MET:HE2  | 3:L:107:GLN:HB3  | 1.97        | 0.46     |
| 3:C:61:VAL:HA    | 3:C:64:LYS:HG3   | 1.98        | 0.46     |
| 3:F:64:LYS:HB3   | 3:F:64:LYS:HE2   | 1.79        | 0.46     |
| 3:I:248:PHE:O    | 3:I:254:HIS:ND1  | 2.49        | 0.46     |
| 1:D:84:LYS:HE3   | 1:D:638:MET:HG3  | 1.97        | 0.46     |
| 1:J:118:ILE:CD1  | 1:J:123:LYS:HE3  | 2.41        | 0.46     |
| 3:L:69:PHE:CD1   | 3:L:70:ILE:HG13  | 2.40        | 0.46     |
| 3:F:85:PHE:C     | 3:F:87:PHE:H     | 2.19        | 0.46     |
| 2:K:230:TYR:CE1  | 2:K:234:LYS:HD2  | 2.50        | 0.46     |
| 1:G:110:ILE:HA   | 1:G:137:HIS:HD2  | 1.80        | 0.46     |
| 2:B:82:LYS:HE3   | 2:B:83:ASP:OD2   | 2.16        | 0.46     |
| 3:C:218:ALA:O    | 3:C:222:VAL:HG23 | 2.15        | 0.46     |
| 1:D:281:ASP:CG   | 1:D:287:PHE:HB2  | 2.36        | 0.46     |
| 1:D:357:PRO:C    | 1:D:359:GLU:H    | 2.18        | 0.46     |
| 3:I:151:PRO:O    | 3:I:154:ILE:HG13 | 2.16        | 0.46     |
| 3:F:103:ILE:H    | 3:F:107:GLN:HE21 | 1.62        | 0.46     |
| 1:D:93:ALA:N     | 1:D:94:PRO:CD    | 2.79        | 0.46     |
| 2:B:230:TYR:CE1  | 2:B:234:LYS:HD2  | 2.51        | 0.46     |
| 1:A:57:ASN:O     | 1:A:132:ARG:NH1  | 2.48        | 0.46     |
| 1:A:37:ILE:O     | 1:A:38:PRO:C     | 2.53        | 0.46     |
| 2:B:46:THR:OG1   | 2:B:47:TYR:N     | 2.49        | 0.46     |
| 1:J:226:THR:OG1  | 1:J:368:GLN:NE2  | 2.49        | 0.46     |
| 1:G:110:ILE:HA   | 1:G:137:HIS:CD2  | 2.51        | 0.46     |
| 1:G:238:ALA:CB   | 1:G:525:MET:HB3  | 2.46        | 0.46     |
| 1:A:173:VAL:HG12 | 1:A:174:SER:N    | 2.31        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:I:1:MET:HB3    | 3:L:112:LYS:NZ   | 2.31        | 0.46     |
| 1:A:110:ILE:HA   | 1:A:137:HIS:HD2  | 1.80        | 0.46     |
| 1:J:355:ILE:C    | 1:J:355:ILE:HD12 | 2.35        | 0.46     |
| 1:A:84:LYS:HE3   | 1:A:638:MET:HG3  | 1.97        | 0.45     |
| 3:L:151:PRO:O    | 3:L:154:ILE:HG13 | 2.16        | 0.45     |
| 1:J:542:GLU:HG2  | 1:J:560:TRP:CD1  | 2.51        | 0.45     |
| 1:G:112:LYS:NZ   | 1:G:130:ASP:HB3  | 2.32        | 0.45     |
| 1:A:238:ALA:CB   | 1:A:525:MET:HB3  | 2.46        | 0.45     |
| 1:A:18:LEU:O     | 1:A:22:VAL:HG23  | 2.15        | 0.45     |
| 1:D:71:MET:O     | 1:D:75:LYS:HG3   | 2.15        | 0.45     |
| 1:J:295:LYS:HG3  | 1:J:297:GLU:O    | 2.16        | 0.45     |
| 2:H:190:ARG:HB3  | 2:H:195:TYR:CE1  | 2.51        | 0.45     |
| 1:G:540:ARG:NH2  | 1:G:562:ASN:HD22 | 2.08        | 0.45     |
| 1:G:562:ASN:HD22 | 1:G:562:ASN:N    | 2.03        | 0.45     |
| 1:D:613:GLN:O    | 1:D:616:ILE:HB   | 2.17        | 0.45     |
| 1:G:9:LEU:CD2    | 1:G:10:VAL:H     | 2.28        | 0.45     |
| 1:J:311:HIS:HA   | 1:J:314:LYS:HD3  | 1.99        | 0.45     |
| 2:B:145:VAL:O    | 2:B:145:VAL:CG1  | 2.64        | 0.45     |
| 3:C:49:SER:HA    | 3:C:227:THR:HG21 | 1.98        | 0.45     |
| 1:A:112:LYS:NZ   | 1:A:130:ASP:HB3  | 2.31        | 0.45     |
| 1:J:238:ALA:CB   | 1:J:525:MET:HB3  | 2.46        | 0.45     |
| 1:D:238:ALA:CB   | 1:D:525:MET:HB3  | 2.46        | 0.45     |
| 1:J:173:VAL:HG12 | 1:J:174:SER:N    | 2.31        | 0.45     |
| 1:D:355:ILE:C    | 1:D:355:ILE:HD12 | 2.35        | 0.45     |
| 3:C:109:LEU:O    | 3:C:109:LEU:HD12 | 2.16        | 0.45     |
| 1:D:288:MET:O    | 1:D:290:ASP:N    | 2.48        | 0.45     |
| 1:D:345:VAL:HG12 | 1:D:345:VAL:O    | 2.17        | 0.45     |
| 1:A:345:VAL:HG12 | 1:A:345:VAL:O    | 2.17        | 0.45     |
| 3:F:248:PHE:O    | 3:F:254:HIS:ND1  | 2.49        | 0.45     |
| 3:L:248:PHE:O    | 3:L:254:HIS:ND1  | 2.49        | 0.45     |
| 1:A:380:ARG:CB   | 1:A:423:TYR:CD1  | 3.00        | 0.45     |
| 3:L:63:LYS:O     | 3:L:66:GLN:N     | 2.45        | 0.45     |
| 2:B:122:ILE:HD13 | 2:B:188:ASP:HB2  | 1.99        | 0.45     |
| 3:L:13:VAL:CG2   | 3:L:18:LYS:N     | 2.79        | 0.45     |
| 1:D:112:LYS:HZ2  | 1:D:130:ASP:HB3  | 1.82        | 0.45     |
| 1:D:226:THR:OG1  | 1:D:368:GLN:NE2  | 2.49        | 0.45     |
| 3:F:98:MET:O     | 3:F:101:PHE:HB2  | 2.16        | 0.45     |
| 1:J:129:GLU:HG2  | 1:J:131:PHE:HE2  | 1.82        | 0.45     |
| 1:D:129:GLU:HG2  | 1:D:131:PHE:HE2  | 1.82        | 0.45     |
| 2:E:82:LYS:HE3   | 2:E:83:ASP:OD2   | 2.16        | 0.45     |
| 1:J:357:PRO:C    | 1:J:359:GLU:H    | 2.18        | 0.45     |
| 1:A:478:VAL:O    | 1:A:478:VAL:HG12 | 2.16        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:478:VAL:O    | 1:G:478:VAL:HG12 | 2.16        | 0.45     |
| 1:D:380:ARG:CB   | 1:D:423:TYR:CD1  | 3.00        | 0.45     |
| 2:H:206:PHE:CE1  | 3:I:24:ALA:HB2   | 2.51        | 0.45     |
| 3:F:13:VAL:CG2   | 3:F:18:LYS:N     | 2.79        | 0.45     |
| 1:A:93:ALA:N     | 1:A:94:PRO:CD    | 2.79        | 0.45     |
| 2:H:46:THR:OG1   | 2:H:47:TYR:N     | 2.49        | 0.45     |
| 1:D:173:VAL:HG12 | 1:D:174:SER:N    | 2.31        | 0.45     |
| 1:D:427:HIS:O    | 1:D:431:THR:HG22 | 2.17        | 0.45     |
| 1:J:427:HIS:O    | 1:J:431:THR:HG22 | 2.17        | 0.45     |
| 1:D:279:LEU:H    | 1:D:288:MET:HE1  | 1.78        | 0.45     |
| 1:G:84:LYS:HE3   | 1:G:638:MET:HG3  | 1.97        | 0.45     |
| 1:A:613:GLN:O    | 1:A:616:ILE:HB   | 2.16        | 0.45     |
| 1:A:311:HIS:HA   | 1:A:314:LYS:HD3  | 1.99        | 0.45     |
| 3:L:85:PHE:C     | 3:L:87:PHE:H     | 2.19        | 0.45     |
| 1:D:41:ARG:NH2   | 2:E:153:GLU:O    | 2.42        | 0.45     |
| 2:K:145:VAL:O    | 2:K:145:VAL:CG1  | 2.64        | 0.45     |
| 3:I:49:SER:HA    | 3:I:227:THR:HG21 | 1.98        | 0.45     |
| 3:F:49:SER:HA    | 3:F:227:THR:HG21 | 1.98        | 0.45     |
| 3:L:161:PHE:CD1  | 3:L:245:TYR:HB2  | 2.52        | 0.45     |
| 3:I:161:PHE:CD1  | 3:I:245:TYR:HB2  | 2.52        | 0.45     |
| 1:J:60:MET:HB2   | 1:J:147:TRP:HB2  | 1.99        | 0.45     |
| 1:A:492:LYS:O    | 1:A:492:LYS:HD3  | 2.15        | 0.45     |
| 1:J:110:ILE:HA   | 1:J:137:HIS:CD2  | 2.51        | 0.45     |
| 1:J:22:VAL:O     | 1:J:26:GLN:HG2   | 2.17        | 0.45     |
| 1:A:58:SER:HA    | 1:A:110:ILE:CD1  | 2.45        | 0.45     |
| 2:E:7:ILE:HG22   | 2:E:9:VAL:HG23   | 1.99        | 0.45     |
| 3:L:98:MET:O     | 3:L:101:PHE:HB2  | 2.16        | 0.45     |
| 3:C:160:SER:O    | 3:C:163:MET:HB3  | 2.17        | 0.45     |
| 2:H:7:ILE:HG22   | 2:H:9:VAL:HG23   | 1.99        | 0.45     |
| 1:J:281:ASP:CB   | 1:J:285:HIS:NE2  | 2.79        | 0.45     |
| 1:G:345:VAL:HG12 | 1:G:345:VAL:O    | 2.17        | 0.45     |
| 3:I:61:VAL:HA    | 3:I:64:LYS:HG3   | 1.98        | 0.45     |
| 1:G:380:ARG:CB   | 1:G:423:TYR:CD1  | 3.00        | 0.45     |
| 1:D:123:LYS:HG2  | 1:D:123:LYS:H    | 1.59        | 0.45     |
| 2:K:190:ARG:HB3  | 2:K:195:TYR:CE1  | 2.51        | 0.45     |
| 2:K:206:PHE:CE1  | 3:L:24:ALA:HB2   | 2.51        | 0.45     |
| 1:J:613:GLN:O    | 1:J:616:ILE:HB   | 2.17        | 0.45     |
| 1:J:562:ASN:HA   | 1:J:583:LEU:CD1  | 2.47        | 0.45     |
| 1:J:562:ASN:HD22 | 1:J:562:ASN:N    | 2.03        | 0.45     |
| 3:C:40:PHE:HE1   | 3:C:86:VAL:HG21  | 1.81        | 0.45     |
| 1:A:467:LYS:HG3  | 1:A:468:ASN:N    | 2.31        | 0.45     |
| 3:I:95:PHE:CE1   | 11:I:303:LMT:H82 | 2.52        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:512:HIS:O    | 1:A:513:ALA:C    | 2.55        | 0.45     |
| 3:C:51:ILE:HG21  | 3:C:231:TYR:CE1  | 2.52        | 0.45     |
| 3:C:186:GLY:O    | 3:C:190:LEU:HB2  | 2.15        | 0.45     |
| 1:J:112:LYS:NZ   | 1:J:130:ASP:HB3  | 2.32        | 0.45     |
| 2:H:82:LYS:HE3   | 2:H:83:ASP:OD2   | 2.16        | 0.45     |
| 1:D:470:MET:SD   | 1:D:527:LEU:HD23 | 2.57        | 0.45     |
| 1:J:281:ASP:OD1  | 1:J:287:PHE:HB2  | 2.17        | 0.45     |
| 1:G:281:ASP:CG   | 1:G:287:PHE:HB2  | 2.36        | 0.45     |
| 1:A:278:ILE:HD12 | 1:A:286:ARG:NH1  | 2.29        | 0.45     |
| 1:J:251:MET:HE1  | 1:J:529:VAL:HG13 | 1.98        | 0.45     |
| 2:K:122:ILE:HD13 | 2:K:188:ASP:HB2  | 1.99        | 0.45     |
| 2:B:190:ARG:HB3  | 2:B:195:TYR:CE1  | 2.51        | 0.45     |
| 1:G:613:GLN:O    | 1:G:616:ILE:HB   | 2.17        | 0.45     |
| 1:A:562:ASN:H    | 1:A:562:ASN:ND2  | 2.12        | 0.45     |
| 2:E:190:ARG:HB3  | 2:E:195:TYR:CE1  | 2.51        | 0.45     |
| 3:F:151:PRO:O    | 3:F:154:ILE:HG13 | 2.16        | 0.45     |
| 3:C:151:PRO:O    | 3:C:154:ILE:HG13 | 2.16        | 0.45     |
| 2:B:166:MET:HE2  | 3:C:107:GLN:HB3  | 1.98        | 0.45     |
| 2:E:213:ALA:HA   | 3:F:120:HIS:CE1  | 2.52        | 0.45     |
| 1:G:93:ALA:N     | 1:G:94:PRO:CD    | 2.79        | 0.45     |
| 1:A:60:MET:HB2   | 1:A:147:TRP:HB2  | 1.99        | 0.45     |
| 1:D:492:LYS:HD3  | 1:D:492:LYS:O    | 2.15        | 0.45     |
| 1:G:226:THR:OG1  | 1:G:368:GLN:NE2  | 2.49        | 0.45     |
| 1:D:110:ILE:HA   | 1:D:137:HIS:CD2  | 2.51        | 0.45     |
| 2:B:226:SER:O    | 2:B:229:ALA:HB3  | 2.17        | 0.45     |
| 1:A:617:ASP:HA   | 1:A:620:GLN:HB2  | 1.97        | 0.45     |
| 2:K:232:ARG:HG2  | 3:L:194:TRP:CZ3  | 2.50        | 0.45     |
| 2:K:82:LYS:HE3   | 2:K:83:ASP:OD2   | 2.16        | 0.45     |
| 2:K:65:CYS:SG    | 2:K:65:CYS:O     | 2.75        | 0.45     |
| 1:J:345:VAL:O    | 1:J:345:VAL:HG12 | 2.17        | 0.45     |
| 1:G:288:MET:HA   | 1:G:296:LYS:HB3  | 1.99        | 0.45     |
| 1:A:278:ILE:CD1  | 1:A:286:ARG:HH11 | 2.28        | 0.45     |
| 2:H:166:MET:HE2  | 3:I:107:GLN:HB3  | 1.99        | 0.45     |
| 2:K:213:ALA:HA   | 3:L:120:HIS:CE1  | 2.52        | 0.45     |
| 2:B:209:MET:O    | 2:B:211:LEU:HD23 | 2.17        | 0.45     |
| 1:G:348:ILE:O    | 1:G:352:PHE:HD1  | 2.00        | 0.45     |
| 1:A:562:ASN:HA   | 1:A:583:LEU:CD1  | 2.47        | 0.45     |
| 1:J:467:LYS:HG3  | 1:J:468:ASN:N    | 2.31        | 0.45     |
| 1:D:512:HIS:O    | 1:D:513:ALA:C    | 2.55        | 0.45     |
| 1:A:67:ASP:O     | 1:A:70:PHE:HB3   | 2.17        | 0.45     |
| 3:C:95:PHE:CE1   | 11:C:303:LMT:H82 | 2.52        | 0.45     |
| 1:G:512:HIS:O    | 1:G:513:ALA:C    | 2.55        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:L:51:ILE:HG21  | 3:L:231:TYR:CE1  | 2.52        | 0.45     |
| 2:H:67:MET:CE    | 2:H:76:ALA:HB2   | 2.47        | 0.45     |
| 1:A:110:ILE:HA   | 1:A:137:HIS:CD2  | 2.51        | 0.45     |
| 1:G:427:HIS:O    | 1:G:431:THR:HG22 | 2.17        | 0.45     |
| 1:A:233:GLU:HB3  | 1:A:526:MET:HE3  | 1.98        | 0.45     |
| 2:E:226:SER:O    | 2:E:229:ALA:HB3  | 2.17        | 0.45     |
| 3:L:109:LEU:HD12 | 3:L:109:LEU:O    | 2.16        | 0.45     |
| 2:E:209:MET:O    | 2:E:211:LEU:HD23 | 2.17        | 0.45     |
| 3:I:142:VAL:CG2  | 3:I:143:HIS:N    | 2.66        | 0.45     |
| 1:A:348:ILE:O    | 1:A:352:PHE:HD1  | 2.00        | 0.45     |
| 3:C:248:PHE:O    | 3:C:254:HIS:ND1  | 2.49        | 0.45     |
| 3:F:61:VAL:HA    | 3:F:64:LYS:HG3   | 1.98        | 0.45     |
| 3:I:36:PHE:HD2   | 3:I:89:VAL:CG1   | 2.25        | 0.45     |
| 2:E:122:ILE:HD13 | 2:E:188:ASP:HB2  | 1.99        | 0.45     |
| 1:J:9:LEU:CD2    | 1:J:10:VAL:H     | 2.28        | 0.45     |
| 3:C:87:PHE:HA    | 3:C:144:LEU:HD13 | 1.99        | 0.45     |
| 2:H:213:ALA:HA   | 3:I:120:HIS:CE1  | 2.52        | 0.45     |
| 1:J:512:HIS:O    | 1:J:513:ALA:C    | 2.55        | 0.45     |
| 1:G:542:GLU:HG2  | 1:G:560:TRP:CD1  | 2.51        | 0.45     |
| 1:D:542:GLU:HG2  | 1:D:560:TRP:CD1  | 2.51        | 0.45     |
| 3:C:161:PHE:CD1  | 3:C:245:TYR:HB2  | 2.52        | 0.45     |
| 1:D:60:MET:HB2   | 1:D:147:TRP:HB2  | 1.99        | 0.45     |
| 2:B:67:MET:CE    | 2:B:76:ALA:HB2   | 2.47        | 0.45     |
| 1:D:22:VAL:O     | 1:D:26:GLN:HG2   | 2.17        | 0.45     |
| 3:C:98:MET:O     | 3:C:101:PHE:HB2  | 2.16        | 0.45     |
| 3:I:160:SER:O    | 3:I:163:MET:HB3  | 2.17        | 0.45     |
| 2:K:158:ILE:CD1  | 2:K:172:GLY:HA3  | 2.47        | 0.45     |
| 2:H:126:LYS:HE3  | 2:H:126:LYS:HB3  | 1.88        | 0.45     |
| 2:E:65:CYS:O     | 2:E:65:CYS:SG    | 2.75        | 0.45     |
| 1:G:306:ARG:HB2  | 1:G:307:ARG:NH1  | 2.32        | 0.45     |
| 2:B:213:ALA:HA   | 3:C:120:HIS:CE1  | 2.52        | 0.45     |
| 1:D:348:ILE:O    | 1:D:352:PHE:HD1  | 2.00        | 0.45     |
| 1:A:356:ASP:HA   | 1:A:357:PRO:HD3  | 1.71        | 0.45     |
| 1:G:357:PRO:C    | 1:G:359:GLU:H    | 2.18        | 0.45     |
| 3:F:158:SER:H    | 3:F:254:HIS:CE1  | 2.35        | 0.45     |
| 1:G:84:LYS:HE2   | 1:G:639:PRO:O    | 2.17        | 0.45     |
| 1:G:118:ILE:HB   | 1:G:276:GLY:HA3  | 1.99        | 0.45     |
| 1:G:562:ASN:HA   | 1:G:583:LEU:CD1  | 2.47        | 0.45     |
| 3:I:25:LYS:O     | 3:I:29:TRP:HD1   | 2.00        | 0.45     |
| 1:J:67:ASP:O     | 1:J:70:PHE:HB3   | 2.17        | 0.45     |
| 3:I:51:ILE:HG21  | 3:I:231:TYR:CE1  | 2.52        | 0.45     |
| 3:F:161:PHE:CD1  | 3:F:245:TYR:HB2  | 2.52        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:111:HIS:CD2  | 1:A:133:HIS:HE1  | 2.35        | 0.45     |
| 1:J:110:ILE:HA   | 1:J:137:HIS:HD2  | 1.80        | 0.45     |
| 2:B:65:CYS:O     | 2:B:65:CYS:SG    | 2.75        | 0.45     |
| 1:J:297:GLU:O    | 1:J:298:LEU:HB2  | 2.17        | 0.44     |
| 1:D:288:MET:HA   | 1:D:296:LYS:HB3  | 1.99        | 0.44     |
| 1:A:281:ASP:OD1  | 1:A:287:PHE:HB2  | 2.17        | 0.44     |
| 2:H:209:MET:O    | 2:H:211:LEU:HD23 | 2.16        | 0.44     |
| 3:L:61:VAL:HA    | 3:L:64:LYS:HG3   | 1.98        | 0.44     |
| 1:J:118:ILE:HB   | 1:J:276:GLY:HA3  | 1.99        | 0.44     |
| 3:L:25:LYS:O     | 3:L:29:TRP:HD1   | 2.00        | 0.44     |
| 1:D:311:HIS:HA   | 1:D:314:LYS:HD3  | 1.99        | 0.44     |
| 1:G:41:ARG:NH2   | 2:H:153:GLU:O    | 2.42        | 0.44     |
| 1:G:512:HIS:O    | 1:G:514:ASN:N    | 2.50        | 0.44     |
| 1:J:98:ARG:NH2   | 2:K:133:LEU:CD1  | 2.80        | 0.44     |
| 1:D:98:ARG:NH2   | 2:E:133:LEU:CD1  | 2.81        | 0.44     |
| 1:D:542:GLU:OE1  | 1:D:544:ARG:NH1  | 2.50        | 0.44     |
| 3:F:51:ILE:HG21  | 3:F:231:TYR:CE1  | 2.52        | 0.44     |
| 2:E:147:GLU:HA   | 2:E:150:ARG:HD3  | 1.97        | 0.44     |
| 1:D:112:LYS:NZ   | 1:D:130:ASP:HB3  | 2.32        | 0.44     |
| 1:D:111:HIS:CD2  | 1:D:133:HIS:HE1  | 2.35        | 0.44     |
| 2:K:67:MET:CE    | 2:K:76:ALA:HB2   | 2.47        | 0.44     |
| 1:A:22:VAL:O     | 1:A:26:GLN:HG2   | 2.17        | 0.44     |
| 3:F:160:SER:O    | 3:F:163:MET:HB3  | 2.17        | 0.44     |
| 3:I:72:GLU:HB3   | 3:I:73:GLY:H     | 1.47        | 0.44     |
| 2:K:226:SER:O    | 2:K:229:ALA:HB3  | 2.17        | 0.44     |
| 3:F:109:LEU:O    | 3:F:109:LEU:HD12 | 2.16        | 0.44     |
| 1:D:281:ASP:OD1  | 1:D:287:PHE:HB2  | 2.17        | 0.44     |
| 3:C:158:SER:H    | 3:C:254:HIS:CE1  | 2.35        | 0.44     |
| 1:J:540:ARG:NH2  | 1:J:562:ASN:HD22 | 2.08        | 0.44     |
| 1:D:512:HIS:O    | 1:D:514:ASN:N    | 2.50        | 0.44     |
| 2:B:133:LEU:HD12 | 2:B:133:LEU:HA   | 1.84        | 0.44     |
| 2:B:7:ILE:HG22   | 2:B:9:VAL:HG23   | 1.99        | 0.44     |
| 3:I:109:LEU:O    | 3:I:109:LEU:HD12 | 2.16        | 0.44     |
| 1:J:306:ARG:HB2  | 1:J:307:ARG:NH1  | 2.32        | 0.44     |
| 1:D:297:GLU:O    | 1:D:298:LEU:HB2  | 2.17        | 0.44     |
| 2:K:209:MET:O    | 2:K:211:LEU:HD23 | 2.17        | 0.44     |
| 3:I:158:SER:H    | 3:I:254:HIS:CE1  | 2.35        | 0.44     |
| 1:J:84:LYS:HE2   | 1:J:639:PRO:O    | 2.18        | 0.44     |
| 2:H:122:ILE:HD13 | 2:H:188:ASP:HB2  | 1.99        | 0.44     |
| 3:F:25:LYS:O     | 3:F:29:TRP:HD1   | 2.00        | 0.44     |
| 3:I:85:PHE:C     | 3:I:87:PHE:H     | 2.19        | 0.44     |
| 2:E:46:THR:OG1   | 2:E:47:TYR:N     | 2.49        | 0.44     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:J:512:HIS:O    | 1:J:514:ASN:N     | 2.50        | 0.44     |
| 2:H:226:SER:O    | 2:H:229:ALA:HB3   | 2.17        | 0.44     |
| 2:K:7:ILE:HG22   | 2:K:9:VAL:HG23    | 1.99        | 0.44     |
| 1:G:129:GLU:HG2  | 1:G:131:PHE:HE2   | 1.82        | 0.44     |
| 2:E:181:ARG:HD3  | 2:E:181:ARG:C     | 2.38        | 0.44     |
| 1:G:287:PHE:CA   | 1:G:290:ASP:HB3   | 2.48        | 0.44     |
| 1:A:288:MET:HA   | 1:A:296:LYS:HB3   | 1.99        | 0.44     |
| 1:D:84:LYS:HE2   | 1:D:639:PRO:O     | 2.17        | 0.44     |
| 1:D:118:ILE:HB   | 1:D:276:GLY:HA3   | 1.99        | 0.44     |
| 1:G:67:ASP:O     | 1:G:70:PHE:HB3    | 2.17        | 0.44     |
| 1:J:147:TRP:N    | 1:J:147:TRP:CD1   | 2.86        | 0.44     |
| 1:A:490:ALA:C    | 1:A:492:LYS:H     | 2.21        | 0.44     |
| 1:J:111:HIS:CD2  | 1:J:133:HIS:HE1   | 2.35        | 0.44     |
| 1:J:112:LYS:HZ2  | 1:J:130:ASP:HB3   | 1.83        | 0.44     |
| 2:E:67:MET:CE    | 2:E:76:ALA:HB2    | 2.47        | 0.44     |
| 3:L:160:SER:O    | 3:L:163:MET:HB3   | 2.17        | 0.44     |
| 3:I:232:VAL:O    | 3:I:236:LEU:HG    | 2.18        | 0.44     |
| 2:H:158:ILE:CD1  | 2:H:172:GLY:HA3   | 2.47        | 0.44     |
| 1:A:470:MET:SD   | 1:A:527:LEU:HD23  | 2.57        | 0.44     |
| 1:G:281:ASP:OD1  | 1:G:287:PHE:HB2   | 2.17        | 0.44     |
| 1:A:297:GLU:O    | 1:A:298:LEU:HB2   | 2.17        | 0.44     |
| 1:A:84:LYS:HE2   | 1:A:639:PRO:O     | 2.17        | 0.44     |
| 1:A:118:ILE:HB   | 1:A:276:GLY:HA3   | 1.99        | 0.44     |
| 3:C:63:LYS:O     | 3:C:66:GLN:N      | 2.45        | 0.44     |
| 1:D:562:ASN:HA   | 1:D:583:LEU:CD1   | 2.47        | 0.44     |
| 1:G:311:HIS:HA   | 1:G:314:LYS:HD3   | 1.99        | 0.44     |
| 1:G:467:LYS:HG3  | 1:G:468:ASN:N     | 2.31        | 0.44     |
| 1:J:542:GLU:OE1  | 1:J:544:ARG:NH1   | 2.50        | 0.44     |
| 1:G:111:HIS:CD2  | 1:G:133:HIS:HE1   | 2.35        | 0.44     |
| 2:E:158:ILE:CD1  | 2:E:172:GLY:HA3   | 2.47        | 0.44     |
| 1:G:470:MET:SD   | 1:G:527:LEU:HD23  | 2.57        | 0.44     |
| 2:K:181:ARG:C    | 2:K:181:ARG:HD3   | 2.38        | 0.44     |
| 1:J:287:PHE:CA   | 1:J:290:ASP:HB3   | 2.48        | 0.44     |
| 1:D:278:ILE:HD12 | 1:D:286:ARG:HD3   | 2.00        | 0.44     |
| 3:L:126:TRP:HE1  | 10:L:302:HEM:HBA1 | 1.83        | 0.44     |
| 3:L:158:SER:H    | 3:L:254:HIS:CE1   | 2.35        | 0.44     |
| 3:C:25:LYS:O     | 3:C:29:TRP:HD1    | 2.00        | 0.44     |
| 3:F:40:PHE:HE1   | 3:F:86:VAL:HG21   | 1.81        | 0.44     |
| 1:A:542:GLU:OE1  | 1:A:544:ARG:NH1   | 2.50        | 0.44     |
| 1:G:542:GLU:OE1  | 1:G:544:ARG:NH1   | 2.50        | 0.44     |
| 1:A:287:PHE:CA   | 1:A:290:ASP:HB3   | 2.48        | 0.44     |
| 1:J:380:ARG:CB   | 1:J:423:TYR:CD1   | 3.00        | 0.44     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:D:467:LYS:HG3  | 1:D:468:ASN:N     | 2.31        | 0.44     |
| 1:G:98:ARG:NH2   | 2:H:133:LEU:CD1   | 2.81        | 0.44     |
| 1:G:60:MET:HB2   | 1:G:147:TRP:HB2   | 1.99        | 0.44     |
| 1:D:490:ALA:C    | 1:D:492:LYS:H     | 2.20        | 0.44     |
| 1:A:427:HIS:O    | 1:A:431:THR:HG22  | 2.17        | 0.44     |
| 3:C:232:VAL:O    | 3:C:236:LEU:HG    | 2.18        | 0.44     |
| 1:J:348:ILE:O    | 1:J:352:PHE:HD1   | 2.00        | 0.44     |
| 1:J:606:ASN:HB3  | 1:J:609:SER:OG    | 2.18        | 0.44     |
| 1:A:606:ASN:HB3  | 1:A:609:SER:OG    | 2.18        | 0.44     |
| 3:I:40:PHE:HE1   | 3:I:86:VAL:HG21   | 1.81        | 0.44     |
| 3:I:87:PHE:HA    | 3:I:144:LEU:HD13  | 1.99        | 0.44     |
| 2:K:46:THR:OG1   | 2:K:47:TYR:N      | 2.49        | 0.44     |
| 1:G:22:VAL:O     | 1:G:26:GLN:HG2    | 2.17        | 0.44     |
| 1:J:470:MET:SD   | 1:J:527:LEU:HD23  | 2.57        | 0.44     |
| 2:B:158:ILE:CD1  | 2:B:172:GLY:HA3   | 2.47        | 0.44     |
| 2:B:181:ARG:HD3  | 2:B:181:ARG:C     | 2.38        | 0.44     |
| 3:F:126:TRP:HE1  | 10:F:302:HEM:HBA1 | 1.83        | 0.44     |
| 1:J:562:ASN:N    | 1:J:562:ASN:ND2   | 2.66        | 0.44     |
| 2:B:110:TRP:HZ3  | 2:B:111:PHE:CE2   | 2.36        | 0.44     |
| 1:G:238:ALA:HB1  | 1:G:525:MET:HB3   | 2.00        | 0.44     |
| 1:J:376:ARG:NH2  | 1:J:563:ARG:NH1   | 2.66        | 0.44     |
| 2:E:40:LEU:HD22  | 2:E:53:PHE:CD2    | 2.53        | 0.44     |
| 1:A:129:GLU:HG2  | 1:A:131:PHE:HE2   | 1.82        | 0.44     |
| 2:H:65:CYS:SG    | 2:H:65:CYS:O      | 2.75        | 0.44     |
| 1:G:297:GLU:O    | 1:G:298:LEU:HB2   | 2.17        | 0.43     |
| 1:A:278:ILE:HD12 | 1:A:286:ARG:HD3   | 2.00        | 0.43     |
| 1:A:278:ILE:HB   | 1:A:288:MET:HE3   | 2.00        | 0.43     |
| 1:A:306:ARG:HB2  | 1:A:307:ARG:NH1   | 2.32        | 0.43     |
| 3:I:75:LYS:CA    | 3:I:75:LYS:HE2    | 2.48        | 0.43     |
| 3:I:64:LYS:HE2   | 3:I:64:LYS:HB3    | 1.79        | 0.43     |
| 1:A:512:HIS:O    | 1:A:514:ASN:N     | 2.50        | 0.43     |
| 2:K:110:TRP:HZ3  | 2:K:111:PHE:CE2   | 2.36        | 0.43     |
| 1:A:374:GLY:O    | 1:A:375:ILE:C     | 2.57        | 0.43     |
| 1:D:238:ALA:HB1  | 1:D:525:MET:HB3   | 2.00        | 0.43     |
| 1:G:376:ARG:NH2  | 1:G:563:ARG:NH1   | 2.66        | 0.43     |
| 3:F:112:LYS:O    | 3:F:113:THR:C     | 2.56        | 0.43     |
| 1:G:551:ASP:N    | 1:G:551:ASP:OD1   | 2.51        | 0.43     |
| 1:D:306:ARG:HB2  | 1:D:307:ARG:NH1   | 2.32        | 0.43     |
| 1:A:562:ASN:ND2  | 1:A:562:ASN:N     | 2.66        | 0.43     |
| 3:I:13:VAL:CG2   | 3:I:18:LYS:N      | 2.79        | 0.43     |
| 1:G:606:ASN:HB3  | 1:G:609:SER:OG    | 2.18        | 0.43     |
| 3:F:87:PHE:HA    | 3:F:144:LEU:HD13  | 1.99        | 0.43     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:D:67:ASP:O     | 1:D:70:PHE:HB3    | 2.17        | 0.43     |
| 1:G:147:TRP:CD1  | 1:G:147:TRP:N     | 2.86        | 0.43     |
| 1:G:490:ALA:C    | 1:G:492:LYS:H     | 2.20        | 0.43     |
| 3:L:232:VAL:O    | 3:L:236:LEU:HG    | 2.18        | 0.43     |
| 1:G:484:GLY:HA2  | 1:G:549:ARG:HH12  | 1.83        | 0.43     |
| 2:K:179:VAL:HG11 | 2:K:199:ILE:HD11  | 2.01        | 0.43     |
| 3:L:40:PHE:HE1   | 3:L:86:VAL:HG21   | 1.81        | 0.43     |
| 1:J:490:ALA:C    | 1:J:492:LYS:H     | 2.20        | 0.43     |
| 3:F:221:ILE:HA   | 3:F:221:ILE:HD13  | 1.90        | 0.43     |
| 1:J:278:ILE:HD12 | 1:J:286:ARG:HD3   | 2.00        | 0.43     |
| 1:G:356:ASP:HA   | 1:G:357:PRO:HD3   | 1.71        | 0.43     |
| 2:B:179:VAL:HG11 | 2:B:199:ILE:HD11  | 2.01        | 0.43     |
| 3:L:87:PHE:HA    | 3:L:144:LEU:HD13  | 1.99        | 0.43     |
| 1:J:188:ASP:O    | 1:J:190:LYS:HG3   | 2.19        | 0.43     |
| 1:D:147:TRP:N    | 1:D:147:TRP:CD1   | 2.86        | 0.43     |
| 1:D:250:ASN:OD1  | 1:D:563:ARG:HG3   | 2.19        | 0.43     |
| 2:K:40:LEU:HD22  | 2:K:53:PHE:CD2    | 2.53        | 0.43     |
| 1:A:250:ASN:OD1  | 1:A:563:ARG:HG3   | 2.18        | 0.43     |
| 3:F:118:MET:O    | 3:F:119:ARG:HB2   | 2.18        | 0.43     |
| 2:H:40:LEU:HD22  | 2:H:53:PHE:CD2    | 2.53        | 0.43     |
| 2:B:40:LEU:HD22  | 2:B:53:PHE:CD2    | 2.53        | 0.43     |
| 1:D:164:VAL:O    | 1:D:167:GLU:HB2   | 2.19        | 0.43     |
| 3:I:221:ILE:HA   | 3:I:221:ILE:HD13  | 1.90        | 0.43     |
| 3:I:126:TRP:HE1  | 10:I:301:HEM:HBA1 | 1.83        | 0.43     |
| 1:D:356:ASP:HA   | 1:D:357:PRO:HD3   | 1.71        | 0.43     |
| 1:G:562:ASN:H    | 1:G:562:ASN:ND2   | 2.12        | 0.43     |
| 1:G:2:LYS:HB2    | 1:G:2:LYS:HZ3     | 1.82        | 0.43     |
| 1:A:9:LEU:CD2    | 1:A:10:VAL:H      | 2.28        | 0.43     |
| 1:A:99:GLU:OE1   | 1:A:418:MET:HE3   | 2.18        | 0.43     |
| 1:A:41:ARG:HH11  | 1:A:41:ARG:CG     | 2.29        | 0.43     |
| 3:L:112:LYS:O    | 3:L:113:THR:C     | 2.56        | 0.43     |
| 1:J:288:MET:HA   | 1:J:296:LYS:HB3   | 1.99        | 0.43     |
| 1:G:278:ILE:HD12 | 1:G:286:ARG:HD3   | 2.00        | 0.43     |
| 1:D:288:MET:C    | 1:D:290:ASP:N     | 2.72        | 0.43     |
| 2:K:213:ALA:N    | 8:K:302:F3S:S4    | 2.91        | 0.43     |
| 2:H:179:VAL:HG11 | 2:H:199:ILE:HD11  | 2.01        | 0.43     |
| 3:C:189:ARG:NH1  | 3:C:189:ARG:HG3   | 2.26        | 0.43     |
| 1:G:415:VAL:O    | 1:G:418:MET:N     | 2.52        | 0.43     |
| 1:J:464:PHE:HE2  | 1:J:519:GLU:HG3   | 1.84        | 0.43     |
| 1:G:188:ASP:O    | 1:G:190:LYS:HG3   | 2.19        | 0.43     |
| 2:E:110:TRP:HZ3  | 2:E:111:PHE:CE2   | 2.36        | 0.43     |
| 1:G:594:TYR:CE1  | 1:G:600:LYS:HG2   | 2.54        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:594:TYR:CE1  | 1:D:600:LYS:HG2  | 2.54        | 0.43     |
| 1:D:376:ARG:NH2  | 1:D:563:ARG:NH1  | 2.66        | 0.43     |
| 2:H:181:ARG:HD3  | 2:H:181:ARG:C    | 2.38        | 0.43     |
| 1:D:286:ARG:HD2  | 1:D:288:MET:HE2  | 1.99        | 0.43     |
| 1:J:562:ASN:H    | 1:J:562:ASN:ND2  | 2.12        | 0.43     |
| 1:D:562:ASN:ND2  | 1:D:562:ASN:N    | 2.66        | 0.43     |
| 1:A:464:PHE:HE2  | 1:A:519:GLU:HG3  | 1.84        | 0.43     |
| 1:A:41:ARG:NH2   | 2:B:153:GLU:O    | 2.42        | 0.43     |
| 1:A:419:ILE:C    | 1:A:421:GLY:N    | 2.72        | 0.43     |
| 1:G:419:ILE:C    | 1:G:421:GLY:N    | 2.72        | 0.43     |
| 1:J:515:PRO:O    | 1:J:518:GLU:HB2  | 2.19        | 0.43     |
| 1:A:515:PRO:O    | 1:A:518:GLU:HB2  | 2.19        | 0.43     |
| 1:A:238:ALA:HB1  | 1:A:525:MET:HB3  | 2.00        | 0.43     |
| 1:G:164:VAL:O    | 1:G:167:GLU:HB2  | 2.19        | 0.43     |
| 1:A:164:VAL:O    | 1:A:167:GLU:HB2  | 2.19        | 0.43     |
| 3:L:118:MET:O    | 3:L:119:ARG:HB2  | 2.18        | 0.43     |
| 2:K:176:LEU:HD13 | 2:K:228:ILE:HG23 | 2.01        | 0.43     |
| 1:J:287:PHE:O    | 1:J:290:ASP:HB3  | 2.19        | 0.43     |
| 1:J:531:LEU:O    | 1:J:535:LYS:HB3  | 2.19        | 0.43     |
| 2:H:110:TRP:HZ3  | 2:H:111:PHE:CE2  | 2.36        | 0.43     |
| 1:G:374:GLY:O    | 1:G:375:ILE:C    | 2.57        | 0.43     |
| 1:D:515:PRO:O    | 1:D:518:GLU:HB2  | 2.19        | 0.43     |
| 1:A:376:ARG:NH2  | 1:A:563:ARG:NH1  | 2.66        | 0.43     |
| 3:I:112:LYS:O    | 3:I:113:THR:C    | 2.56        | 0.43     |
| 3:I:118:MET:O    | 3:I:119:ARG:HB2  | 2.18        | 0.43     |
| 1:D:484:GLY:HA2  | 1:D:549:ARG:HH12 | 1.83        | 0.43     |
| 1:A:288:MET:O    | 1:A:290:ASP:N    | 2.48        | 0.43     |
| 3:C:69:PHE:CD1   | 3:C:70:ILE:HG13  | 2.40        | 0.43     |
| 2:E:179:VAL:HG11 | 2:E:199:ILE:HD11 | 2.01        | 0.43     |
| 2:B:167:ARG:NH1  | 2:B:167:ARG:CG   | 2.82        | 0.43     |
| 2:E:1:MET:HE2    | 2:E:31:ALA:HA    | 1.99        | 0.43     |
| 1:A:29:LEU:O     | 1:A:31:THR:HG23  | 2.19        | 0.43     |
| 1:D:531:LEU:O    | 1:D:535:LYS:HB3  | 2.19        | 0.43     |
| 1:A:98:ARG:NH2   | 2:B:133:LEU:CD1  | 2.81        | 0.43     |
| 1:D:374:GLY:O    | 1:D:375:ILE:C    | 2.57        | 0.43     |
| 1:A:594:TYR:CE1  | 1:A:600:LYS:HG2  | 2.54        | 0.43     |
| 1:D:591:ALA:HA   | 1:D:592:PRO:HD3  | 1.83        | 0.43     |
| 1:D:551:ASP:OD1  | 1:D:551:ASP:N    | 2.51        | 0.43     |
| 1:J:611:LYS:HE2  | 1:J:611:LYS:HB3  | 1.84        | 0.43     |
| 3:I:104:ASN:OD1  | 3:I:107:GLN:HB2  | 2.19        | 0.43     |
| 3:I:171:LEU:HB2  | 3:L:145:TYR:OH   | 2.18        | 0.43     |
| 1:G:251:MET:HE1  | 1:G:529:VAL:HG13 | 2.00        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:464:PHE:HE2  | 1:D:519:GLU:HG3  | 1.84        | 0.43     |
| 1:G:250:ASN:OD1  | 1:G:563:ARG:HG3  | 2.18        | 0.43     |
| 3:C:112:LYS:O    | 3:C:113:THR:C    | 2.56        | 0.43     |
| 1:G:611:LYS:HB3  | 1:G:611:LYS:HE2  | 1.84        | 0.43     |
| 3:C:253:THR:CG2  | 3:C:254:HIS:H    | 2.20        | 0.42     |
| 3:F:253:THR:CG2  | 3:F:254:HIS:H    | 2.20        | 0.42     |
| 3:I:63:LYS:O     | 3:I:66:GLN:N     | 2.45        | 0.42     |
| 2:E:191:THR:O    | 2:E:195:TYR:CD1  | 2.72        | 0.42     |
| 1:J:328:LEU:O    | 1:J:361:TRP:HA   | 2.20        | 0.42     |
| 1:G:562:ASN:ND2  | 1:G:562:ASN:N    | 2.66        | 0.42     |
| 3:I:13:VAL:HG22  | 3:I:18:LYS:H     | 1.79        | 0.42     |
| 1:G:531:LEU:O    | 1:G:535:LYS:HB3  | 2.19        | 0.42     |
| 2:E:176:LEU:HD13 | 2:E:228:ILE:HG23 | 2.01        | 0.42     |
| 1:A:484:GLY:HA2  | 1:A:549:ARG:HH12 | 1.83        | 0.42     |
| 3:L:104:ASN:OD1  | 3:L:107:GLN:HB2  | 2.19        | 0.42     |
| 3:F:75:LYS:HE2   | 3:F:75:LYS:CA    | 2.48        | 0.42     |
| 1:D:6:CYS:O      | 1:D:209:ALA:CB   | 2.68        | 0.42     |
| 2:K:191:THR:O    | 2:K:195:TYR:CD1  | 2.72        | 0.42     |
| 1:J:338:ILE:HD13 | 1:J:358:ALA:HA   | 2.02        | 0.42     |
| 3:F:104:ASN:OD1  | 3:F:107:GLN:HB2  | 2.19        | 0.42     |
| 1:A:147:TRP:CD1  | 1:A:147:TRP:N    | 2.86        | 0.42     |
| 1:J:250:ASN:OD1  | 1:J:563:ARG:HG3  | 2.18        | 0.42     |
| 2:E:20:LYS:HA    | 2:E:21:PRO:HD3   | 1.93        | 0.42     |
| 2:H:176:LEU:HD13 | 2:H:228:ILE:HG23 | 2.01        | 0.42     |
| 1:G:270:GLU:C    | 1:G:272:CYS:N    | 2.73        | 0.42     |
| 1:J:478:VAL:CG1  | 1:J:482:ARG:HE   | 2.33        | 0.42     |
| 1:J:225:ASN:HB3  | 1:J:367:MET:HG2  | 2.01        | 0.42     |
| 1:G:338:ILE:HD13 | 1:G:358:ALA:HA   | 2.01        | 0.42     |
| 3:F:189:ARG:NH1  | 3:F:189:ARG:HG3  | 2.26        | 0.42     |
| 1:J:238:ALA:HB1  | 1:J:525:MET:HB3  | 2.00        | 0.42     |
| 3:C:118:MET:O    | 3:C:119:ARG:HB2  | 2.18        | 0.42     |
| 3:F:232:VAL:O    | 3:F:236:LEU:HG   | 2.18        | 0.42     |
| 1:J:164:VAL:O    | 1:J:167:GLU:HB2  | 2.19        | 0.42     |
| 1:A:551:ASP:OD1  | 1:A:551:ASP:N    | 2.51        | 0.42     |
| 1:D:287:PHE:CA   | 1:D:290:ASP:HB3  | 2.48        | 0.42     |
| 3:L:75:LYS:CA    | 3:L:75:LYS:HE2   | 2.48        | 0.42     |
| 2:H:199:ILE:O    | 2:H:205:VAL:HG12 | 2.20        | 0.42     |
| 2:E:199:ILE:O    | 2:E:205:VAL:HG12 | 2.20        | 0.42     |
| 3:I:29:TRP:HA    | 3:I:32:ALA:CB    | 2.45        | 0.42     |
| 1:D:2:LYS:HB2    | 1:D:2:LYS:HZ2    | 1.80        | 0.42     |
| 1:D:606:ASN:HB3  | 1:D:609:SER:OG   | 2.18        | 0.42     |
| 2:E:213:ALA:N    | 8:E:302:F3S:S4   | 2.91        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:188:ASP:O    | 1:A:190:LYS:HG3  | 2.19        | 0.42     |
| 1:J:594:TYR:CE1  | 1:J:600:LYS:HG2  | 2.54        | 0.42     |
| 1:G:515:PRO:O    | 1:G:518:GLU:HB2  | 2.19        | 0.42     |
| 2:B:176:LEU:HD13 | 2:B:228:ILE:HG23 | 2.01        | 0.42     |
| 1:J:484:GLY:HA2  | 1:J:549:ARG:HH12 | 1.83        | 0.42     |
| 1:J:126:ILE:CG2  | 1:J:127:THR:N    | 2.83        | 0.42     |
| 2:K:129:ASP:OD1  | 2:K:131:SER:HB3  | 2.20        | 0.42     |
| 3:F:72:GLU:HB3   | 3:F:73:GLY:H     | 1.47        | 0.42     |
| 3:C:75:LYS:CA    | 3:C:75:LYS:HE2   | 2.48        | 0.42     |
| 2:K:199:ILE:O    | 2:K:205:VAL:HG12 | 2.20        | 0.42     |
| 3:I:209:LEU:HD23 | 3:I:209:LEU:HA   | 1.92        | 0.42     |
| 1:D:287:PHE:O    | 1:D:290:ASP:HB3  | 2.19        | 0.42     |
| 1:J:6:CYS:O      | 1:J:209:ALA:CB   | 2.68        | 0.42     |
| 2:E:188:ASP:OD1  | 2:E:190:ARG:HB2  | 2.20        | 0.42     |
| 3:C:13:VAL:CG2   | 3:C:18:LYS:N     | 2.79        | 0.42     |
| 3:C:21:ARG:N     | 3:C:21:ARG:HD2   | 2.35        | 0.42     |
| 3:C:104:ASN:OD1  | 3:C:107:GLN:HB2  | 2.19        | 0.42     |
| 1:D:420:VAL:HG12 | 1:D:420:VAL:O    | 2.19        | 0.42     |
| 1:D:126:ILE:CG2  | 1:D:127:THR:N    | 2.83        | 0.42     |
| 1:A:126:ILE:CG2  | 1:A:127:THR:N    | 2.83        | 0.42     |
| 1:J:228:ASN:HD22 | 1:J:228:ASN:N    | 2.17        | 0.42     |
| 1:G:287:PHE:O    | 1:G:290:ASP:HB3  | 2.19        | 0.42     |
| 3:F:69:PHE:C     | 3:F:70:ILE:HG13  | 2.40        | 0.42     |
| 1:G:225:ASN:HB3  | 1:G:367:MET:HG2  | 2.01        | 0.42     |
| 1:J:316:LYS:CE   | 1:J:316:LYS:HA   | 2.49        | 0.42     |
| 1:A:316:LYS:CE   | 1:A:316:LYS:HA   | 2.49        | 0.42     |
| 3:F:21:ARG:HD2   | 3:F:21:ARG:N     | 2.35        | 0.42     |
| 3:I:21:ARG:HD2   | 3:I:21:ARG:N     | 2.35        | 0.42     |
| 1:A:531:LEU:O    | 1:A:535:LYS:HB3  | 2.19        | 0.42     |
| 3:C:103:ILE:O    | 3:C:104:ASN:CB   | 2.67        | 0.42     |
| 1:J:420:VAL:HG12 | 1:J:420:VAL:O    | 2.19        | 0.42     |
| 1:G:490:ALA:O    | 1:G:492:LYS:N    | 2.53        | 0.42     |
| 2:K:67:MET:HA    | 2:K:94:LEU:HD23  | 2.02        | 0.42     |
| 2:H:197:GLU:HA   | 3:I:19:LYS:HD3   | 2.02        | 0.42     |
| 1:G:141:PHE:HZ   | 5:G:702:MLA:C2   | 2.31        | 0.42     |
| 1:A:83:GLN:HE21  | 1:A:588:MET:CB   | 2.26        | 0.42     |
| 1:A:225:ASN:HB3  | 1:A:367:MET:HG2  | 2.01        | 0.42     |
| 2:H:123:HIS:HD2  | 2:H:190:ARG:CZ   | 2.32        | 0.42     |
| 1:D:562:ASN:ND2  | 1:D:562:ASN:H    | 2.12        | 0.42     |
| 1:D:29:LEU:O     | 1:D:31:THR:HG23  | 2.19        | 0.42     |
| 1:G:41:ARG:HG2   | 1:G:41:ARG:NH1   | 2.33        | 0.42     |
| 1:J:374:GLY:O    | 1:J:375:ILE:C    | 2.57        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:60:MET:C     | 1:D:62:ASP:N     | 2.73        | 0.42     |
| 1:A:490:ALA:O    | 1:A:492:LYS:N    | 2.53        | 0.42     |
| 2:E:197:GLU:HA   | 3:F:19:LYS:HD3   | 2.02        | 0.42     |
| 1:G:591:ALA:HA   | 1:G:592:PRO:HD3  | 1.83        | 0.42     |
| 2:B:164:LYS:HD3  | 2:B:164:LYS:O    | 2.20        | 0.42     |
| 1:G:328:LEU:O    | 1:G:361:TRP:HA   | 2.19        | 0.42     |
| 1:A:270:GLU:C    | 1:A:272:CYS:N    | 2.73        | 0.42     |
| 1:A:287:PHE:O    | 1:A:290:ASP:HB3  | 2.19        | 0.42     |
| 3:I:103:ILE:O    | 3:I:104:ASN:CB   | 2.67        | 0.42     |
| 3:F:44:HIS:CE1   | 10:F:303:HEM:ND  | 2.88        | 0.42     |
| 1:A:478:VAL:CG1  | 1:A:482:ARG:HE   | 2.33        | 0.42     |
| 3:L:253:THR:HG22 | 3:L:254:HIS:N    | 2.21        | 0.42     |
| 1:J:225:ASN:CB   | 1:J:367:MET:HE2  | 2.43        | 0.42     |
| 1:A:6:CYS:O      | 1:A:209:ALA:CB   | 2.68        | 0.42     |
| 3:I:69:PHE:C     | 3:I:70:ILE:HG13  | 2.40        | 0.42     |
| 3:I:216:MET:O    | 3:I:220:LEU:HG   | 2.20        | 0.42     |
| 4:J:701:FAD:H1'1 | 4:J:701:FAD:H9   | 1.63        | 0.41     |
| 3:F:63:LYS:O     | 3:F:66:GLN:N     | 2.45        | 0.41     |
| 1:J:380:ARG:HA   | 1:J:423:TYR:CD1  | 2.55        | 0.41     |
| 1:A:380:ARG:HA   | 1:A:423:TYR:CD1  | 2.55        | 0.41     |
| 2:K:188:ASP:OD1  | 2:K:190:ARG:HB2  | 2.20        | 0.41     |
| 2:H:188:ASP:OD1  | 2:H:190:ARG:HB2  | 2.20        | 0.41     |
| 1:G:464:PHE:HE2  | 1:G:519:GLU:HG3  | 1.84        | 0.41     |
| 1:G:41:ARG:HH11  | 1:G:41:ARG:CG    | 2.29        | 0.41     |
| 1:G:420:VAL:HG12 | 1:G:420:VAL:O    | 2.20        | 0.41     |
| 1:D:188:ASP:O    | 1:D:190:LYS:HG3  | 2.19        | 0.41     |
| 2:E:150:ARG:O    | 2:E:151:CYS:C    | 2.59        | 0.41     |
| 1:D:490:ALA:O    | 1:D:492:LYS:N    | 2.53        | 0.41     |
| 1:J:164:VAL:O    | 1:J:167:GLU:N    | 2.53        | 0.41     |
| 3:F:216:MET:O    | 3:F:220:LEU:HG   | 2.20        | 0.41     |
| 1:J:551:ASP:N    | 1:J:551:ASP:OD1  | 2.51        | 0.41     |
| 1:A:306:ARG:HG2  | 1:A:481:PHE:CZ   | 2.55        | 0.41     |
| 3:F:136:MET:HE2  | 3:F:179:VAL:N    | 2.35        | 0.41     |
| 1:G:251:MET:O    | 1:G:533:VAL:HG13 | 2.21        | 0.41     |
| 2:H:191:THR:O    | 2:H:195:TYR:CD1  | 2.72        | 0.41     |
| 3:F:29:TRP:HA    | 3:F:32:ALA:CB    | 2.45        | 0.41     |
| 3:L:21:ARG:HD2   | 3:L:21:ARG:N     | 2.35        | 0.41     |
| 1:J:29:LEU:O     | 1:J:31:THR:HG23  | 2.19        | 0.41     |
| 1:G:29:LEU:O     | 1:G:31:THR:HG23  | 2.19        | 0.41     |
| 2:H:213:ALA:N    | 8:H:302:F3S:S4   | 2.91        | 0.41     |
| 1:G:633:ILE:O    | 1:G:636:ALA:HB3  | 2.20        | 0.41     |
| 2:E:129:ASP:OD1  | 2:E:131:SER:HB3  | 2.20        | 0.41     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:G:6:CYS:O      | 1:G:209:ALA:CB    | 2.68        | 0.41     |
| 1:D:228:ASN:HD22 | 1:D:228:ASN:N     | 2.17        | 0.41     |
| 1:J:306:ARG:HG2  | 1:J:481:PHE:CZ    | 2.55        | 0.41     |
| 1:G:281:ASP:HB3  | 1:G:282:VAL:H     | 1.74        | 0.41     |
| 1:G:303:VAL:CG1  | 1:G:304:VAL:N     | 2.80        | 0.41     |
| 3:I:44:HIS:CE1   | 10:I:302:HEM:ND   | 2.88        | 0.41     |
| 2:B:209:MET:O    | 2:B:210:THR:C     | 2.59        | 0.41     |
| 1:D:423:TYR:CZ   | 1:D:643:PRO:HG3   | 2.55        | 0.41     |
| 3:L:69:PHE:C     | 3:L:70:ILE:HG13   | 2.40        | 0.41     |
| 1:D:338:ILE:HD13 | 1:D:358:ALA:HA    | 2.01        | 0.41     |
| 1:A:338:ILE:HD13 | 1:A:358:ALA:HA    | 2.01        | 0.41     |
| 1:D:531:LEU:HD13 | 1:D:574:THR:O     | 2.21        | 0.41     |
| 1:D:419:ILE:C    | 1:D:421:GLY:N     | 2.72        | 0.41     |
| 2:B:150:ARG:O    | 2:B:151:CYS:C     | 2.59        | 0.41     |
| 1:J:490:ALA:O    | 1:J:492:LYS:N     | 2.53        | 0.41     |
| 1:D:222:ILE:HG13 | 1:D:223:TYR:CD1   | 2.56        | 0.41     |
| 1:J:347:GLU:O    | 1:J:351:TYR:HD1   | 2.03        | 0.41     |
| 1:G:164:VAL:O    | 1:G:167:GLU:N     | 2.53        | 0.41     |
| 2:B:129:ASP:OD1  | 2:B:131:SER:HB3   | 2.20        | 0.41     |
| 3:C:216:MET:O    | 3:C:220:LEU:HG    | 2.20        | 0.41     |
| 3:L:72:GLU:HB3   | 3:L:73:GLY:H      | 1.47        | 0.41     |
| 1:G:216:THR:CB   | 1:G:236:GLY:HA3   | 2.51        | 0.41     |
| 3:L:175:LEU:HG   | 10:L:303:HEM:HMD2 | 2.01        | 0.41     |
| 3:C:44:HIS:CE1   | 10:C:302:HEM:ND   | 2.88        | 0.41     |
| 3:F:175:LEU:HG   | 10:F:303:HEM:HMD2 | 2.02        | 0.41     |
| 1:G:478:VAL:CG1  | 1:G:482:ARG:HE    | 2.33        | 0.41     |
| 2:B:191:THR:O    | 2:B:195:TYR:CD1   | 2.72        | 0.41     |
| 2:H:167:ARG:NH1  | 2:H:167:ARG:CG    | 2.82        | 0.41     |
| 1:A:420:VAL:O    | 1:A:420:VAL:HG12  | 2.20        | 0.41     |
| 1:D:164:VAL:O    | 1:D:167:GLU:N     | 2.53        | 0.41     |
| 1:G:126:ILE:CG2  | 1:G:127:THR:N     | 2.83        | 0.41     |
| 1:J:270:GLU:C    | 1:J:272:CYS:N     | 2.73        | 0.41     |
| 4:D:701:FAD:H1'1 | 4:D:701:FAD:H9    | 1.63        | 0.41     |
| 3:C:126:TRP:HE1  | 10:C:301:HEM:HBA1 | 1.83        | 0.41     |
| 3:F:253:THR:HG22 | 3:F:254:HIS:N     | 2.20        | 0.41     |
| 1:A:423:TYR:CZ   | 1:A:643:PRO:HG3   | 2.55        | 0.41     |
| 1:A:5:TYR:CG     | 1:A:6:CYS:N       | 2.89        | 0.41     |
| 2:B:188:ASP:OD1  | 2:B:190:ARG:HB2   | 2.20        | 0.41     |
| 1:D:225:ASN:HB3  | 1:D:367:MET:HG2   | 2.01        | 0.41     |
| 1:D:415:VAL:O    | 1:D:418:MET:N     | 2.52        | 0.41     |
| 1:A:375:ILE:O    | 1:A:395:ALA:HB1   | 2.21        | 0.41     |
| 2:E:67:MET:HA    | 2:E:94:LEU:HD23   | 2.02        | 0.41     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:164:VAL:O    | 1:A:167:GLU:N     | 2.53        | 0.41     |
| 1:G:506:ILE:HG22 | 1:G:516:GLU:HG2   | 2.03        | 0.41     |
| 1:A:506:ILE:HG22 | 1:A:516:GLU:HG2   | 2.03        | 0.41     |
| 3:L:22:MET:HB2   | 3:L:23:PRO:HD3    | 2.02        | 0.41     |
| 1:A:433:VAL:CG1  | 1:A:434:ASP:N     | 2.84        | 0.41     |
| 1:J:506:ILE:HG22 | 1:J:516:GLU:HG2   | 2.03        | 0.41     |
| 1:G:306:ARG:HG2  | 1:G:481:PHE:CZ    | 2.55        | 0.41     |
| 2:K:209:MET:O    | 2:K:210:THR:C     | 2.59        | 0.41     |
| 3:L:136:MET:HE2  | 3:L:179:VAL:N     | 2.35        | 0.41     |
| 3:L:44:HIS:CE1   | 10:L:303:HEM:ND   | 2.88        | 0.41     |
| 1:D:380:ARG:HA   | 1:D:423:TYR:CD1   | 2.55        | 0.41     |
| 1:G:423:TYR:CZ   | 1:G:643:PRO:HG3   | 2.55        | 0.41     |
| 1:A:251:MET:O    | 1:A:533:VAL:HG13  | 2.21        | 0.41     |
| 1:D:41:ARG:NH1   | 1:D:41:ARG:CG     | 2.83        | 0.41     |
| 1:A:419:ILE:O    | 1:A:421:GLY:N     | 2.54        | 0.41     |
| 1:G:419:ILE:O    | 1:G:421:GLY:N     | 2.54        | 0.41     |
| 2:K:150:ARG:O    | 2:K:151:CYS:C     | 2.59        | 0.41     |
| 1:A:408:ASN:HA   | 1:A:408:ASN:HD22  | 1.65        | 0.41     |
| 1:G:222:ILE:HG13 | 1:G:223:TYR:CD1   | 2.56        | 0.41     |
| 1:A:222:ILE:HG13 | 1:A:223:TYR:CD1   | 2.56        | 0.41     |
| 3:F:22:MET:HB2   | 3:F:23:PRO:HD3    | 2.03        | 0.41     |
| 2:H:24:GLN:HG2   | 2:H:26:TYR:CZ     | 2.56        | 0.41     |
| 1:A:228:ASN:N    | 1:A:228:ASN:HD22  | 2.17        | 0.41     |
| 1:D:486:HIS:N    | 1:D:486:HIS:CD2   | 2.88        | 0.41     |
| 3:C:175:LEU:HG   | 10:C:302:HEM:HMD2 | 2.02        | 0.41     |
| 1:J:423:TYR:CZ   | 1:J:643:PRO:HG3   | 2.55        | 0.41     |
| 1:D:3:VAL:HG22   | 1:D:206:ALA:HB3   | 2.02        | 0.41     |
| 2:B:199:ILE:O    | 2:B:205:VAL:HG12  | 2.20        | 0.41     |
| 2:E:123:HIS:HD2  | 2:E:190:ARG:CZ    | 2.32        | 0.41     |
| 1:J:64:ASP:OD1   | 1:J:148:ARG:HB3   | 2.21        | 0.41     |
| 1:J:39:VAL:O     | 1:J:41:ARG:N      | 2.54        | 0.41     |
| 1:J:375:ILE:O    | 1:J:395:ALA:HB1   | 2.21        | 0.41     |
| 1:G:111:HIS:HD2  | 2:H:139:PRO:CG    | 2.34        | 0.41     |
| 1:J:222:ILE:HG13 | 1:J:223:TYR:CD1   | 2.56        | 0.41     |
| 3:L:22:MET:CB    | 3:L:23:PRO:HD3    | 2.51        | 0.41     |
| 3:F:22:MET:CB    | 3:F:23:PRO:HD3    | 2.51        | 0.41     |
| 2:E:24:GLN:HG2   | 2:E:26:TYR:CZ     | 2.56        | 0.41     |
| 2:H:129:ASP:OD1  | 2:H:131:SER:HB3   | 2.20        | 0.41     |
| 1:G:210:LYS:NZ   | 1:J:441:GLU:OE2   | 2.52        | 0.41     |
| 1:D:216:THR:CB   | 1:D:236:GLY:HA3   | 2.51        | 0.41     |
| 1:A:328:LEU:O    | 1:A:361:TRP:HA    | 2.20        | 0.41     |
| 3:I:253:THR:CG2  | 3:I:254:HIS:H     | 2.20        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:3:VAL:HG22   | 1:J:206:ALA:HB3  | 2.03        | 0.41     |
| 1:A:3:VAL:HG22   | 1:A:206:ALA:HB3  | 2.02        | 0.41     |
| 1:A:415:VAL:O    | 1:A:418:MET:N    | 2.52        | 0.41     |
| 1:J:463:VAL:O    | 1:J:467:LYS:HB3  | 2.21        | 0.41     |
| 1:J:39:VAL:C     | 1:J:41:ARG:H     | 2.24        | 0.41     |
| 1:D:375:ILE:O    | 1:D:395:ALA:HB1  | 2.21        | 0.41     |
| 1:A:60:MET:C     | 1:A:62:ASP:H     | 2.24        | 0.41     |
| 1:D:433:VAL:CG1  | 1:D:434:ASP:N    | 2.84        | 0.41     |
| 1:J:141:PHE:CE1  | 1:J:270:GLU:HB3  | 2.56        | 0.41     |
| 1:G:288:MET:C    | 1:G:290:ASP:N    | 2.71        | 0.41     |
| 1:J:216:THR:CB   | 1:J:236:GLY:HA3  | 2.51        | 0.41     |
| 1:D:141:PHE:CE1  | 1:D:270:GLU:HB3  | 2.56        | 0.41     |
| 1:A:216:THR:CB   | 1:A:236:GLY:HA3  | 2.51        | 0.41     |
| 3:F:93:HIS:CD2   | 10:F:302:HEM:NB  | 2.89        | 0.41     |
| 1:A:107:TRP:HA   | 1:A:152:THR:CG2  | 2.38        | 0.41     |
| 2:K:141:VAL:C    | 2:K:143:GLN:N    | 2.75        | 0.41     |
| 2:E:141:VAL:C    | 2:E:143:GLN:H    | 2.25        | 0.41     |
| 1:D:478:VAL:CG1  | 1:D:482:ARG:HE   | 2.33        | 0.41     |
| 3:C:64:LYS:HB3   | 3:C:64:LYS:HE2   | 1.79        | 0.41     |
| 1:G:644:ALA:HA   | 1:G:647:LYS:HG3  | 2.03        | 0.41     |
| 1:G:380:ARG:HA   | 1:G:423:TYR:CD1  | 2.56        | 0.41     |
| 1:G:3:VAL:HG22   | 1:G:206:ALA:HB3  | 2.03        | 0.41     |
| 2:H:206:PHE:HE1  | 3:I:24:ALA:HB2   | 1.86        | 0.41     |
| 3:C:69:PHE:C     | 3:C:70:ILE:HG13  | 2.40        | 0.41     |
| 1:G:265:GLY:HA3  | 1:G:367:MET:HE1  | 2.03        | 0.41     |
| 1:D:64:ASP:OD1   | 1:D:148:ARG:HB3  | 2.21        | 0.41     |
| 1:J:415:VAL:O    | 1:J:418:MET:N    | 2.52        | 0.41     |
| 1:A:531:LEU:HD13 | 1:A:574:THR:O    | 2.21        | 0.41     |
| 1:D:463:VAL:O    | 1:D:467:LYS:HB3  | 2.21        | 0.41     |
| 1:G:463:VAL:O    | 1:G:467:LYS:HB3  | 2.21        | 0.41     |
| 1:G:39:VAL:C     | 1:G:41:ARG:H     | 2.24        | 0.41     |
| 1:G:41:ARG:CG    | 1:G:41:ARG:NH1   | 2.83        | 0.41     |
| 1:A:41:ARG:NH1   | 1:A:41:ARG:CG    | 2.83        | 0.41     |
| 1:J:542:GLU:HG2  | 1:J:560:TRP:CG   | 2.56        | 0.41     |
| 1:A:60:MET:C     | 1:A:62:ASP:N     | 2.73        | 0.41     |
| 1:A:111:HIS:HD2  | 2:B:139:PRO:CG   | 2.34        | 0.41     |
| 1:D:347:GLU:O    | 1:D:351:TYR:HD1  | 2.03        | 0.41     |
| 2:K:197:GLU:HA   | 3:L:19:LYS:HD3   | 2.02        | 0.41     |
| 1:G:433:VAL:CG1  | 1:G:434:ASP:N    | 2.84        | 0.41     |
| 1:J:589:GLU:C    | 1:J:590:ILE:HG13 | 2.41        | 0.41     |
| 1:D:611:LYS:HB3  | 1:D:611:LYS:HE2  | 1.84        | 0.41     |
| 1:D:306:ARG:HG2  | 1:D:481:PHE:CZ   | 2.55        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:328:LEU:O    | 1:D:361:TRP:HA   | 2.20        | 0.41     |
| 2:B:213:ALA:N    | 8:B:302:F3S:S4   | 2.91        | 0.41     |
| 1:A:349:CYS:CB   | 1:A:357:PRO:HG3  | 2.51        | 0.41     |
| 1:J:120:ASN:CG   | 1:J:121:ALA:H    | 2.25        | 0.41     |
| 2:B:148:LEU:HD22 | 2:B:177:ASN:OD1  | 2.21        | 0.41     |
| 1:D:87:ARG:HD2   | 1:D:640:TYR:CD2  | 2.56        | 0.41     |
| 1:J:644:ALA:HA   | 1:J:647:LYS:HG3  | 2.03        | 0.41     |
| 1:J:251:MET:O    | 1:J:533:VAL:HG13 | 2.21        | 0.41     |
| 1:A:64:ASP:OD1   | 1:A:148:ARG:HB3  | 2.21        | 0.41     |
| 1:G:64:ASP:OD1   | 1:G:148:ARG:HB3  | 2.21        | 0.41     |
| 1:J:419:ILE:C    | 1:J:421:GLY:N    | 2.72        | 0.41     |
| 1:G:392:GLY:O    | 1:G:393:GLU:C    | 2.60        | 0.41     |
| 1:D:542:GLU:HG2  | 1:D:560:TRP:CG   | 2.56        | 0.41     |
| 2:E:192:ASP:OD2  | 2:E:234:LYS:HE2  | 2.21        | 0.41     |
| 2:B:192:ASP:OD2  | 2:B:234:LYS:HE2  | 2.21        | 0.41     |
| 3:C:1:MET:HB3    | 3:F:112:LYS:NZ   | 2.35        | 0.41     |
| 3:F:19:LYS:O     | 3:F:20:SER:C     | 2.60        | 0.41     |
| 2:B:24:GLN:HG2   | 2:B:26:TYR:CZ    | 2.56        | 0.41     |
| 1:G:589:GLU:C    | 1:G:590:ILE:HG13 | 2.41        | 0.41     |
| 1:A:589:GLU:C    | 1:A:590:ILE:HG13 | 2.41        | 0.41     |
| 2:E:164:LYS:HD3  | 2:E:164:LYS:O    | 2.20        | 0.41     |
| 1:G:141:PHE:CE1  | 1:G:270:GLU:HB3  | 2.56        | 0.40     |
| 1:G:278:ILE:HG22 | 1:G:297:GLU:HG3  | 2.03        | 0.40     |
| 1:A:262:PHE:H    | 1:A:364:VAL:HA   | 1.86        | 0.40     |
| 3:I:26:LEU:HB3   | 3:I:99:ARG:HH12  | 1.86        | 0.40     |
| 3:F:142:VAL:CG2  | 3:F:143:HIS:N    | 2.66        | 0.40     |
| 2:E:141:VAL:C    | 2:E:143:GLN:N    | 2.74        | 0.40     |
| 3:C:71:PHE:HB3   | 3:C:75:LYS:CG    | 2.51        | 0.40     |
| 1:D:118:ILE:CD1  | 1:D:123:LYS:HE3  | 2.41        | 0.40     |
| 1:D:282:VAL:HG13 | 1:D:318:VAL:HB   | 2.03        | 0.40     |
| 1:J:99:GLU:OE1   | 1:J:418:MET:HE3  | 2.21        | 0.40     |
| 1:J:392:GLY:O    | 1:J:393:GLU:C    | 2.59        | 0.40     |
| 1:G:542:GLU:HG2  | 1:G:560:TRP:CG   | 2.56        | 0.40     |
| 1:J:333:LEU:O    | 1:J:337:HIS:HB2  | 2.21        | 0.40     |
| 1:G:60:MET:C     | 1:G:62:ASP:N     | 2.73        | 0.40     |
| 1:A:347:GLU:O    | 1:A:351:TYR:HD1  | 2.03        | 0.40     |
| 2:B:93:PRO:HB3   | 2:B:103:LEU:HA   | 2.03        | 0.40     |
| 1:A:633:ILE:O    | 1:A:636:ALA:HB3  | 2.20        | 0.40     |
| 3:C:19:LYS:O     | 3:C:20:SER:C     | 2.60        | 0.40     |
| 2:H:93:PRO:HB3   | 2:H:103:LEU:HA   | 2.03        | 0.40     |
| 2:K:164:LYS:HD3  | 2:K:164:LYS:O    | 2.20        | 0.40     |
| 1:G:228:ASN:N    | 1:G:228:ASN:HD22 | 2.17        | 0.40     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:C:3:ASN:HD21   | 2:E:8:ARG:HH12   | 1.69        | 0.40     |
| 1:J:299:ALA:HB1  | 1:J:303:VAL:CG1  | 2.48        | 0.40     |
| 1:A:141:PHE:CE1  | 1:A:270:GLU:HB3  | 2.56        | 0.40     |
| 1:A:268:LEU:HA   | 1:A:345:VAL:HG13 | 2.04        | 0.40     |
| 3:I:145:TYR:CE1  | 3:L:171:LEU:HD12 | 2.56        | 0.40     |
| 1:D:120:ASN:CG   | 1:D:121:ALA:H    | 2.24        | 0.40     |
| 2:K:148:LEU:HD22 | 2:K:177:ASN:OD1  | 2.21        | 0.40     |
| 2:B:141:VAL:C    | 2:B:143:GLN:N    | 2.74        | 0.40     |
| 1:J:5:TYR:CG     | 1:J:6:CYS:N      | 2.89        | 0.40     |
| 1:A:463:VAL:O    | 1:A:467:LYS:HB3  | 2.21        | 0.40     |
| 1:G:333:LEU:O    | 1:G:337:HIS:HB2  | 2.21        | 0.40     |
| 1:J:111:HIS:HD2  | 2:K:139:PRO:CG   | 2.34        | 0.40     |
| 3:I:19:LYS:O     | 3:I:20:SER:C     | 2.60        | 0.40     |
| 2:E:129:ASP:HB3  | 2:E:132:LYS:HB2  | 2.04        | 0.40     |
| 2:K:24:GLN:HG2   | 2:K:26:TYR:CZ    | 2.56        | 0.40     |
| 1:J:385:LEU:O    | 1:J:386:LYS:C    | 2.59        | 0.40     |
| 2:E:93:PRO:HB3   | 2:E:103:LEU:HA   | 2.03        | 0.40     |
| 3:C:22:MET:HB2   | 3:C:23:PRO:HD3   | 2.02        | 0.40     |
| 1:G:603:TYR:CD1  | 1:G:603:TYR:O    | 2.74        | 0.40     |
| 3:L:155:GLY:O    | 3:L:159:SER:HB2  | 2.22        | 0.40     |
| 1:J:262:PHE:H    | 1:J:364:VAL:HA   | 1.86        | 0.40     |
| 1:J:268:LEU:HA   | 1:J:345:VAL:HG13 | 2.04        | 0.40     |
| 3:L:99:ARG:HH21  | 3:L:100:LYS:NZ   | 2.20        | 0.40     |
| 1:D:349:CYS:CB   | 1:D:357:PRO:HG3  | 2.51        | 0.40     |
| 1:J:107:TRP:HA   | 1:J:152:THR:CG2  | 2.38        | 0.40     |
| 1:G:87:ARG:HA    | 1:G:87:ARG:HD3   | 1.95        | 0.40     |
| 1:D:5:TYR:CG     | 1:D:6:CYS:N      | 2.89        | 0.40     |
| 2:B:123:HIS:HD2  | 2:B:190:ARG:CZ   | 2.32        | 0.40     |
| 1:A:540:ARG:NH2  | 1:A:562:ASN:O    | 2.54        | 0.40     |
| 1:J:282:VAL:HG13 | 1:J:318:VAL:HB   | 2.03        | 0.40     |
| 1:G:531:LEU:HD13 | 1:G:574:THR:O    | 2.21        | 0.40     |
| 1:J:531:LEU:HD13 | 1:J:574:THR:O    | 2.21        | 0.40     |
| 3:F:26:LEU:HB3   | 3:F:99:ARG:HH12  | 1.86        | 0.40     |
| 1:D:39:VAL:O     | 1:D:41:ARG:N     | 2.54        | 0.40     |
| 1:G:375:ILE:O    | 1:G:395:ALA:HB1  | 2.21        | 0.40     |
| 2:H:67:MET:HA    | 2:H:94:LEU:HD23  | 2.02        | 0.40     |
| 2:E:176:LEU:CD1  | 2:E:228:ILE:HG23 | 2.52        | 0.40     |
| 2:B:176:LEU:CD1  | 2:B:228:ILE:HG23 | 2.52        | 0.40     |
| 3:L:19:LYS:O     | 3:L:20:SER:C     | 2.60        | 0.40     |
| 1:G:434:ASP:OD1  | 1:J:434:ASP:OD1  | 2.39        | 0.40     |
| 1:D:589:GLU:C    | 1:D:590:ILE:HG13 | 2.41        | 0.40     |
| 3:C:155:GLY:O    | 3:C:159:SER:HB2  | 2.21        | 0.40     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:140:ASP:O    | 1:J:274:GLY:HA3  | 2.22        | 0.40     |
| 1:D:633:ILE:O    | 1:D:636:ALA:HB3  | 2.20        | 0.40     |
| 3:I:125:LEU:HD23 | 3:I:125:LEU:HA   | 1.91        | 0.40     |
| 2:H:164:LYS:HD3  | 2:H:164:LYS:O    | 2.20        | 0.40     |
| 3:L:77:ILE:O     | 3:L:77:ILE:HG12  | 2.22        | 0.40     |
| 1:G:262:PHE:H    | 1:G:364:VAL:HA   | 1.86        | 0.40     |
| 3:I:99:ARG:HH21  | 3:I:100:LYS:NZ   | 2.20        | 0.40     |
| 2:H:141:VAL:C    | 2:H:143:GLN:H    | 2.25        | 0.40     |
| 2:H:148:LEU:HD22 | 2:H:177:ASN:OD1  | 2.21        | 0.40     |
| 2:B:206:PHE:HE1  | 3:C:24:ALA:HB2   | 1.86        | 0.40     |
| 2:K:167:ARG:NH1  | 2:K:167:ARG:CG   | 2.82        | 0.40     |
| 1:J:419:ILE:O    | 1:J:421:GLY:N    | 2.54        | 0.40     |
| 1:A:542:GLU:HG2  | 1:A:560:TRP:CG   | 2.56        | 0.40     |
| 2:K:192:ASP:OD2  | 2:K:234:LYS:HE2  | 2.21        | 0.40     |
| 1:G:129:GLU:HG2  | 1:G:131:PHE:CE2  | 2.57        | 0.40     |
| 2:H:129:ASP:HB3  | 2:H:132:LYS:HB2  | 2.04        | 0.40     |
| 2:K:99:LEU:HD12  | 2:K:100:ILE:H    | 1.87        | 0.40     |
| 2:H:64:SER:O     | 2:H:66:GLY:N     | 2.54        | 0.40     |
| 1:A:385:LEU:O    | 1:A:386:LYS:C    | 2.59        | 0.40     |
| 1:D:506:ILE:HG22 | 1:D:516:GLU:HG2  | 2.03        | 0.40     |
| 3:L:216:MET:O    | 3:L:220:LEU:HG   | 2.20        | 0.40     |
| 1:J:257:HIS:CE1  | 1:J:267:LEU:HD11 | 2.57        | 0.40     |
| 3:I:93:HIS:CD2   | 10:I:301:HEM:NB  | 2.89        | 0.40     |
| 3:L:103:ILE:O    | 3:L:104:ASN:CB   | 2.67        | 0.40     |
| 3:C:44:HIS:O     | 3:C:48:VAL:HB    | 2.22        | 0.40     |
| 1:A:344:ASP:O    | 1:A:346:GLN:N    | 2.53        | 0.40     |
| 2:H:141:VAL:C    | 2:H:143:GLN:N    | 2.75        | 0.40     |
| 1:A:118:ILE:CD1  | 1:A:123:LYS:HE3  | 2.41        | 0.40     |
| 1:D:251:MET:O    | 1:D:533:VAL:HG13 | 2.21        | 0.40     |
| 3:C:29:TRP:HA    | 3:C:32:ALA:CB    | 2.45        | 0.40     |
| 1:D:9:LEU:CD2    | 1:D:10:VAL:H     | 2.28        | 0.40     |
| 3:C:85:PHE:C     | 3:C:87:PHE:N     | 2.75        | 0.40     |
| 3:I:85:PHE:C     | 3:I:87:PHE:N     | 2.75        | 0.40     |
| 1:D:39:VAL:C     | 1:D:41:ARG:H     | 2.24        | 0.40     |
| 1:D:419:ILE:O    | 1:D:421:GLY:N    | 2.54        | 0.40     |
| 1:G:14:GLY:O     | 1:G:18:LEU:HG    | 2.22        | 0.40     |
| 1:D:26:GLN:HE21  | 1:D:27:LYS:HE3   | 1.87        | 0.40     |
| 1:D:129:GLU:HG2  | 1:D:131:PHE:CE2  | 2.57        | 0.40     |
| 2:K:64:SER:O     | 2:K:66:GLY:N     | 2.54        | 0.40     |
| 2:E:64:SER:O     | 2:E:66:GLY:N     | 2.54        | 0.40     |
| 1:G:385:LEU:O    | 1:G:386:LYS:C    | 2.59        | 0.40     |
| 3:C:77:ILE:O     | 3:C:77:ILE:HG12  | 2.22        | 0.40     |

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| Atom-1         | Atom-2           | Distance(Å) | Clash(Å) |
|----------------|------------------|-------------|----------|
| 3:C:221:ILE:HA | 3:C:221:ILE:HD13 | 1.90        | 0.40     |
| 3:F:155:GLY:O  | 3:F:159:SER:HB2  | 2.22        | 0.40     |

All (27) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Distance(Å) | Clash(Å) |
|-----------------|------------------------|-------------|----------|
| 1:D:580:TYR:C   | 1:G:122:GLN:NE2[1_455] | 0.81        | 1.39     |
| 1:A:122:GLN:NE2 | 1:J:581:GLU:N[1_554]   | 0.84        | 1.36     |
| 1:D:581:GLU:N   | 1:G:122:GLN:NE2[1_455] | 1.03        | 1.17     |
| 1:A:122:GLN:NE2 | 1:J:580:TYR:C[1_554]   | 1.10        | 1.10     |
| 1:A:122:GLN:OE1 | 1:J:581:GLU:CA[1_554]  | 1.30        | 0.90     |
| 1:D:580:TYR:C   | 1:G:122:GLN:CD[1_455]  | 1.35        | 0.85     |
| 1:D:580:TYR:O   | 1:G:122:GLN:CD[1_455]  | 1.38        | 0.82     |
| 1:D:581:GLU:CA  | 1:G:122:GLN:OE1[1_455] | 1.44        | 0.76     |
| 1:D:116:MET:CE  | 1:J:332:ILE:CD1[2_546] | 1.45        | 0.75     |
| 1:A:122:GLN:CD  | 1:J:580:TYR:C[1_554]   | 1.62        | 0.58     |
| 1:A:122:GLN:CD  | 1:J:581:GLU:N[1_554]   | 1.62        | 0.58     |
| 1:D:581:GLU:N   | 1:G:122:GLN:CD[1_455]  | 1.63        | 0.57     |
| 1:D:580:TYR:CA  | 1:G:122:GLN:NE2[1_455] | 1.68        | 0.52     |
| 1:A:122:GLN:CD  | 1:J:580:TYR:O[1_554]   | 1.70        | 0.50     |
| 1:D:116:MET:CE  | 1:J:332:ILE:CG1[2_546] | 1.71        | 0.49     |
| 1:A:122:GLN:CD  | 1:J:581:GLU:CA[1_554]  | 1.80        | 0.40     |
| 1:D:122:GLN:NE2 | 1:J:359:GLU:CB[2_546]  | 1.83        | 0.37     |
| 1:D:580:TYR:O   | 1:G:122:GLN:OE1[1_455] | 1.87        | 0.33     |
| 1:D:580:TYR:O   | 1:G:122:GLN:NE2[1_455] | 1.90        | 0.30     |
| 1:D:581:GLU:N   | 1:G:122:GLN:OE1[1_455] | 1.96        | 0.24     |
| 1:D:581:GLU:CA  | 1:G:122:GLN:CD[1_455]  | 2.03        | 0.17     |
| 1:A:122:GLN:NE2 | 1:J:581:GLU:CA[1_554]  | 2.04        | 0.16     |
| 1:A:122:GLN:NE2 | 1:J:580:TYR:CA[1_554]  | 2.05        | 0.15     |
| 1:A:122:GLN:OE1 | 1:J:581:GLU:N[1_554]   | 2.07        | 0.13     |
| 1:D:580:TYR:O   | 1:G:122:GLN:CG[1_455]  | 2.08        | 0.12     |
| 1:A:122:GLN:NE2 | 1:J:580:TYR:O[1_554]   | 2.09        | 0.11     |
| 1:D:580:TYR:C   | 1:G:122:GLN:OE1[1_455] | 2.13        | 0.07     |

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 653/656 (100%)  | 499 (76%)  | 113 (17%) | 41 (6%)  | 2           | 16 |
| 1   | D     | 653/656 (100%)  | 499 (76%)  | 112 (17%) | 42 (6%)  | 2           | 15 |
| 1   | G     | 653/656 (100%)  | 499 (76%)  | 113 (17%) | 41 (6%)  | 2           | 16 |
| 1   | J     | 653/656 (100%)  | 499 (76%)  | 112 (17%) | 42 (6%)  | 2           | 15 |
| 2   | B     | 237/239 (99%)   | 190 (80%)  | 37 (16%)  | 10 (4%)  | 4           | 27 |
| 2   | E     | 237/239 (99%)   | 190 (80%)  | 37 (16%)  | 10 (4%)  | 4           | 27 |
| 2   | H     | 237/239 (99%)   | 190 (80%)  | 37 (16%)  | 10 (4%)  | 4           | 27 |
| 2   | K     | 237/239 (99%)   | 190 (80%)  | 37 (16%)  | 10 (4%)  | 4           | 27 |
| 3   | C     | 252/256 (98%)   | 200 (79%)  | 40 (16%)  | 12 (5%)  | 4           | 23 |
| 3   | F     | 252/256 (98%)   | 200 (79%)  | 40 (16%)  | 12 (5%)  | 4           | 23 |
| 3   | I     | 252/256 (98%)   | 200 (79%)  | 40 (16%)  | 12 (5%)  | 4           | 23 |
| 3   | L     | 252/256 (98%)   | 200 (79%)  | 40 (16%)  | 12 (5%)  | 4           | 23 |
| All | All   | 4568/4604 (99%) | 3556 (78%) | 758 (17%) | 254 (6%) | 3           | 19 |

All (254) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 269 | THR  |
| 1   | A     | 288 | MET  |
| 1   | A     | 294 | GLU  |
| 1   | A     | 319 | GLN  |
| 1   | A     | 333 | LEU  |
| 1   | A     | 345 | VAL  |
| 2   | B     | 65  | CYS  |
| 2   | B     | 85  | GLU  |
| 2   | B     | 109 | ASN  |
| 2   | B     | 132 | LYS  |
| 3   | C     | 54  | GLY  |
| 3   | C     | 103 | ILE  |
| 3   | C     | 104 | ASN  |
| 3   | C     | 147 | MET  |
| 1   | D     | 269 | THR  |
| 1   | D     | 288 | MET  |
| 1   | D     | 294 | GLU  |
| 1   | D     | 319 | GLN  |
| 1   | D     | 333 | LEU  |
| 1   | D     | 345 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 65  | CYS  |
| 2   | E     | 85  | GLU  |
| 2   | E     | 109 | ASN  |
| 2   | E     | 132 | LYS  |
| 3   | F     | 54  | GLY  |
| 3   | F     | 103 | ILE  |
| 3   | F     | 104 | ASN  |
| 3   | F     | 147 | MET  |
| 1   | G     | 269 | THR  |
| 1   | G     | 288 | MET  |
| 1   | G     | 294 | GLU  |
| 1   | G     | 319 | GLN  |
| 1   | G     | 333 | LEU  |
| 1   | G     | 345 | VAL  |
| 2   | H     | 65  | CYS  |
| 2   | H     | 85  | GLU  |
| 2   | H     | 109 | ASN  |
| 2   | H     | 132 | LYS  |
| 3   | I     | 54  | GLY  |
| 3   | I     | 103 | ILE  |
| 3   | I     | 104 | ASN  |
| 3   | I     | 147 | MET  |
| 1   | J     | 269 | THR  |
| 1   | J     | 288 | MET  |
| 1   | J     | 294 | GLU  |
| 1   | J     | 319 | GLN  |
| 1   | J     | 333 | LEU  |
| 1   | J     | 345 | VAL  |
| 2   | K     | 65  | CYS  |
| 2   | K     | 85  | GLU  |
| 2   | K     | 109 | ASN  |
| 2   | K     | 132 | LYS  |
| 3   | L     | 54  | GLY  |
| 3   | L     | 103 | ILE  |
| 3   | L     | 104 | ASN  |
| 3   | L     | 147 | MET  |
| 1   | A     | 14  | GLY  |
| 1   | A     | 49  | GLY  |
| 1   | A     | 119 | ILE  |
| 1   | A     | 129 | GLU  |
| 1   | A     | 218 | GLY  |
| 1   | A     | 304 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 334 | GLY  |
| 1   | A     | 375 | ILE  |
| 1   | A     | 393 | GLU  |
| 1   | A     | 513 | ALA  |
| 1   | A     | 573 | GLN  |
| 2   | B     | 47  | TYR  |
| 2   | B     | 108 | GLY  |
| 2   | B     | 147 | GLU  |
| 3   | C     | 253 | THR  |
| 1   | D     | 14  | GLY  |
| 1   | D     | 49  | GLY  |
| 1   | D     | 119 | ILE  |
| 1   | D     | 129 | GLU  |
| 1   | D     | 218 | GLY  |
| 1   | D     | 304 | VAL  |
| 1   | D     | 334 | GLY  |
| 1   | D     | 375 | ILE  |
| 1   | D     | 393 | GLU  |
| 1   | D     | 513 | ALA  |
| 1   | D     | 573 | GLN  |
| 2   | E     | 47  | TYR  |
| 2   | E     | 108 | GLY  |
| 2   | E     | 147 | GLU  |
| 3   | F     | 253 | THR  |
| 1   | G     | 14  | GLY  |
| 1   | G     | 49  | GLY  |
| 1   | G     | 119 | ILE  |
| 1   | G     | 129 | GLU  |
| 1   | G     | 218 | GLY  |
| 1   | G     | 304 | VAL  |
| 1   | G     | 334 | GLY  |
| 1   | G     | 375 | ILE  |
| 1   | G     | 393 | GLU  |
| 1   | G     | 513 | ALA  |
| 1   | G     | 573 | GLN  |
| 2   | H     | 47  | TYR  |
| 2   | H     | 108 | GLY  |
| 2   | H     | 147 | GLU  |
| 3   | I     | 253 | THR  |
| 1   | J     | 14  | GLY  |
| 1   | J     | 49  | GLY  |
| 1   | J     | 119 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 129 | GLU  |
| 1   | J     | 218 | GLY  |
| 1   | J     | 304 | VAL  |
| 1   | J     | 334 | GLY  |
| 1   | J     | 375 | ILE  |
| 1   | J     | 393 | GLU  |
| 1   | J     | 513 | ALA  |
| 1   | J     | 573 | GLN  |
| 2   | K     | 47  | TYR  |
| 2   | K     | 108 | GLY  |
| 2   | K     | 147 | GLU  |
| 3   | L     | 253 | THR  |
| 1   | A     | 10  | VAL  |
| 1   | A     | 40  | LYS  |
| 1   | A     | 42  | SER  |
| 1   | A     | 54  | SER  |
| 1   | A     | 125 | THR  |
| 1   | A     | 146 | LYS  |
| 1   | A     | 540 | ARG  |
| 1   | A     | 553 | PRO  |
| 1   | A     | 555 | ARG  |
| 1   | A     | 620 | GLN  |
| 1   | A     | 648 | ALA  |
| 2   | B     | 64  | SER  |
| 2   | B     | 102 | ASP  |
| 3   | C     | 198 | ASP  |
| 1   | D     | 10  | VAL  |
| 1   | D     | 40  | LYS  |
| 1   | D     | 42  | SER  |
| 1   | D     | 54  | SER  |
| 1   | D     | 125 | THR  |
| 1   | D     | 146 | LYS  |
| 1   | D     | 540 | ARG  |
| 1   | D     | 553 | PRO  |
| 1   | D     | 555 | ARG  |
| 1   | D     | 620 | GLN  |
| 1   | D     | 648 | ALA  |
| 2   | E     | 64  | SER  |
| 2   | E     | 102 | ASP  |
| 3   | F     | 198 | ASP  |
| 1   | G     | 10  | VAL  |
| 1   | G     | 40  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 42  | SER  |
| 1   | G     | 54  | SER  |
| 1   | G     | 125 | THR  |
| 1   | G     | 146 | LYS  |
| 1   | G     | 540 | ARG  |
| 1   | G     | 553 | PRO  |
| 1   | G     | 555 | ARG  |
| 1   | G     | 620 | GLN  |
| 1   | G     | 648 | ALA  |
| 2   | H     | 64  | SER  |
| 2   | H     | 102 | ASP  |
| 3   | I     | 198 | ASP  |
| 1   | J     | 10  | VAL  |
| 1   | J     | 40  | LYS  |
| 1   | J     | 42  | SER  |
| 1   | J     | 54  | SER  |
| 1   | J     | 125 | THR  |
| 1   | J     | 146 | LYS  |
| 1   | J     | 540 | ARG  |
| 1   | J     | 553 | PRO  |
| 1   | J     | 555 | ARG  |
| 1   | J     | 620 | GLN  |
| 1   | J     | 648 | ALA  |
| 2   | K     | 64  | SER  |
| 2   | K     | 102 | ASP  |
| 3   | L     | 198 | ASP  |
| 1   | A     | 89  | PHE  |
| 1   | A     | 261 | LEU  |
| 1   | A     | 286 | ARG  |
| 1   | A     | 564 | THR  |
| 3   | C     | 214 | THR  |
| 1   | D     | 89  | PHE  |
| 1   | D     | 261 | LEU  |
| 1   | D     | 286 | ARG  |
| 1   | D     | 564 | THR  |
| 3   | F     | 214 | THR  |
| 1   | G     | 89  | PHE  |
| 1   | G     | 261 | LEU  |
| 1   | G     | 286 | ARG  |
| 1   | G     | 564 | THR  |
| 3   | I     | 214 | THR  |
| 1   | J     | 89  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 261 | LEU  |
| 1   | J     | 286 | ARG  |
| 1   | J     | 564 | THR  |
| 3   | L     | 214 | THR  |
| 1   | A     | 198 | ASP  |
| 1   | A     | 281 | ASP  |
| 1   | A     | 295 | LYS  |
| 1   | A     | 365 | LEU  |
| 3   | C     | 70  | ILE  |
| 3   | C     | 112 | LYS  |
| 1   | D     | 198 | ASP  |
| 1   | D     | 281 | ASP  |
| 1   | D     | 295 | LYS  |
| 1   | D     | 365 | LEU  |
| 3   | F     | 70  | ILE  |
| 1   | G     | 198 | ASP  |
| 1   | G     | 281 | ASP  |
| 1   | G     | 295 | LYS  |
| 1   | G     | 365 | LEU  |
| 3   | I     | 70  | ILE  |
| 3   | I     | 112 | LYS  |
| 1   | J     | 198 | ASP  |
| 1   | J     | 281 | ASP  |
| 1   | J     | 295 | LYS  |
| 1   | J     | 365 | LEU  |
| 3   | L     | 70  | ILE  |
| 3   | L     | 112 | LYS  |
| 1   | A     | 153 | ALA  |
| 3   | C     | 121 | GLY  |
| 3   | C     | 127 | TRP  |
| 1   | D     | 153 | ALA  |
| 3   | F     | 112 | LYS  |
| 3   | F     | 121 | GLY  |
| 3   | F     | 127 | TRP  |
| 1   | G     | 153 | ALA  |
| 3   | I     | 121 | GLY  |
| 3   | I     | 127 | TRP  |
| 1   | J     | 153 | ALA  |
| 3   | L     | 121 | GLY  |
| 3   | L     | 127 | TRP  |
| 1   | A     | 419 | ILE  |
| 1   | D     | 419 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 419 | ILE  |
| 1   | J     | 419 | ILE  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 406 | GLY  |
| 1   | D     | 303 | VAL  |
| 1   | D     | 406 | GLY  |
| 1   | G     | 303 | VAL  |
| 1   | G     | 406 | GLY  |
| 1   | J     | 303 | VAL  |
| 1   | J     | 406 | GLY  |
| 2   | B     | 21  | PRO  |
| 3   | C     | 142 | VAL  |
| 2   | E     | 21  | PRO  |
| 3   | F     | 142 | VAL  |
| 2   | H     | 21  | PRO  |
| 3   | I     | 142 | VAL  |
| 2   | K     | 21  | PRO  |
| 3   | L     | 142 | VAL  |
| 1   | A     | 592 | PRO  |
| 1   | D     | 592 | PRO  |
| 1   | G     | 592 | PRO  |
| 1   | J     | 592 | PRO  |
| 1   | D     | 105 | VAL  |
| 1   | J     | 105 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 532/533 (100%) | 497 (93%) | 35 (7%)  | 24          | 64 |
| 1   | D     | 532/533 (100%) | 497 (93%) | 35 (7%)  | 24          | 64 |
| 1   | G     | 532/533 (100%) | 497 (93%) | 35 (7%)  | 24          | 64 |
| 1   | J     | 532/533 (100%) | 497 (93%) | 35 (7%)  | 24          | 64 |
| 2   | B     | 211/211 (100%) | 199 (94%) | 12 (6%)  | 29          | 70 |
| 2   | E     | 211/211 (100%) | 199 (94%) | 12 (6%)  | 29          | 70 |
| 2   | H     | 211/211 (100%) | 199 (94%) | 12 (6%)  | 29          | 70 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 2   | K     | 211/211 (100%)   | 199 (94%)  | 12 (6%)  | 29          | 70 |
| 3   | C     | 221/223 (99%)    | 198 (90%)  | 23 (10%) | 10          | 36 |
| 3   | F     | 221/223 (99%)    | 198 (90%)  | 23 (10%) | 10          | 36 |
| 3   | I     | 221/223 (99%)    | 198 (90%)  | 23 (10%) | 10          | 36 |
| 3   | L     | 221/223 (99%)    | 198 (90%)  | 23 (10%) | 10          | 36 |
| All | All   | 3856/3868 (100%) | 3576 (93%) | 280 (7%) | 20          | 59 |

All (280) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | LYS  |
| 1   | A     | 9   | LEU  |
| 1   | A     | 40  | LYS  |
| 1   | A     | 72  | ASP  |
| 1   | A     | 84  | LYS  |
| 1   | A     | 97  | ILE  |
| 1   | A     | 109 | ARG  |
| 1   | A     | 116 | MET  |
| 1   | A     | 141 | PHE  |
| 1   | A     | 145 | LYS  |
| 1   | A     | 268 | LEU  |
| 1   | A     | 278 | ILE  |
| 1   | A     | 285 | HIS  |
| 1   | A     | 286 | ARG  |
| 1   | A     | 287 | PHE  |
| 1   | A     | 294 | GLU  |
| 1   | A     | 302 | ASP  |
| 1   | A     | 307 | ARG  |
| 1   | A     | 314 | LYS  |
| 1   | A     | 322 | TYR  |
| 1   | A     | 337 | HIS  |
| 1   | A     | 361 | TRP  |
| 1   | A     | 368 | GLN  |
| 1   | A     | 371 | SER  |
| 1   | A     | 385 | LEU  |
| 1   | A     | 390 | SER  |
| 1   | A     | 398 | ASP  |
| 1   | A     | 403 | ASN  |
| 1   | A     | 408 | ASN  |
| 1   | A     | 426 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 467 | LYS  |
| 1   | A     | 509 | LYS  |
| 1   | A     | 511 | LEU  |
| 1   | A     | 562 | ASN  |
| 1   | A     | 628 | LYS  |
| 2   | B     | 1   | MET  |
| 2   | B     | 40  | LEU  |
| 2   | B     | 41  | ASN  |
| 2   | B     | 50  | ASP  |
| 2   | B     | 79  | THR  |
| 2   | B     | 101 | LYS  |
| 2   | B     | 114 | MET  |
| 2   | B     | 140 | GLU  |
| 2   | B     | 147 | GLU  |
| 2   | B     | 167 | ARG  |
| 2   | B     | 181 | ARG  |
| 2   | B     | 189 | GLU  |
| 3   | C     | 1   | MET  |
| 3   | C     | 14  | THR  |
| 3   | C     | 40  | PHE  |
| 3   | C     | 47  | PHE  |
| 3   | C     | 56  | ASN  |
| 3   | C     | 58  | MET  |
| 3   | C     | 65  | PHE  |
| 3   | C     | 69  | PHE  |
| 3   | C     | 75  | LYS  |
| 3   | C     | 78  | VAL  |
| 3   | C     | 100 | LYS  |
| 3   | C     | 101 | PHE  |
| 3   | C     | 106 | ARG  |
| 3   | C     | 123 | THR  |
| 3   | C     | 137 | PHE  |
| 3   | C     | 154 | ILE  |
| 3   | C     | 164 | VAL  |
| 3   | C     | 197 | PHE  |
| 3   | C     | 203 | ASP  |
| 3   | C     | 212 | LEU  |
| 3   | C     | 223 | LEU  |
| 3   | C     | 234 | LYS  |
| 3   | C     | 239 | THR  |
| 1   | D     | 2   | LYS  |
| 1   | D     | 9   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 40  | LYS  |
| 1   | D     | 72  | ASP  |
| 1   | D     | 84  | LYS  |
| 1   | D     | 97  | ILE  |
| 1   | D     | 109 | ARG  |
| 1   | D     | 116 | MET  |
| 1   | D     | 141 | PHE  |
| 1   | D     | 145 | LYS  |
| 1   | D     | 268 | LEU  |
| 1   | D     | 278 | ILE  |
| 1   | D     | 285 | HIS  |
| 1   | D     | 286 | ARG  |
| 1   | D     | 287 | PHE  |
| 1   | D     | 294 | GLU  |
| 1   | D     | 302 | ASP  |
| 1   | D     | 307 | ARG  |
| 1   | D     | 314 | LYS  |
| 1   | D     | 322 | TYR  |
| 1   | D     | 337 | HIS  |
| 1   | D     | 361 | TRP  |
| 1   | D     | 368 | GLN  |
| 1   | D     | 371 | SER  |
| 1   | D     | 385 | LEU  |
| 1   | D     | 390 | SER  |
| 1   | D     | 398 | ASP  |
| 1   | D     | 403 | ASN  |
| 1   | D     | 408 | ASN  |
| 1   | D     | 426 | GLU  |
| 1   | D     | 467 | LYS  |
| 1   | D     | 509 | LYS  |
| 1   | D     | 511 | LEU  |
| 1   | D     | 562 | ASN  |
| 1   | D     | 628 | LYS  |
| 2   | E     | 1   | MET  |
| 2   | E     | 40  | LEU  |
| 2   | E     | 41  | ASN  |
| 2   | E     | 50  | ASP  |
| 2   | E     | 79  | THR  |
| 2   | E     | 101 | LYS  |
| 2   | E     | 114 | MET  |
| 2   | E     | 140 | GLU  |
| 2   | E     | 147 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 167 | ARG  |
| 2   | E     | 181 | ARG  |
| 2   | E     | 189 | GLU  |
| 3   | F     | 1   | MET  |
| 3   | F     | 14  | THR  |
| 3   | F     | 40  | PHE  |
| 3   | F     | 47  | PHE  |
| 3   | F     | 56  | ASN  |
| 3   | F     | 58  | MET  |
| 3   | F     | 65  | PHE  |
| 3   | F     | 69  | PHE  |
| 3   | F     | 75  | LYS  |
| 3   | F     | 78  | VAL  |
| 3   | F     | 100 | LYS  |
| 3   | F     | 101 | PHE  |
| 3   | F     | 106 | ARG  |
| 3   | F     | 123 | THR  |
| 3   | F     | 137 | PHE  |
| 3   | F     | 154 | ILE  |
| 3   | F     | 164 | VAL  |
| 3   | F     | 197 | PHE  |
| 3   | F     | 203 | ASP  |
| 3   | F     | 212 | LEU  |
| 3   | F     | 223 | LEU  |
| 3   | F     | 234 | LYS  |
| 3   | F     | 239 | THR  |
| 1   | G     | 2   | LYS  |
| 1   | G     | 9   | LEU  |
| 1   | G     | 40  | LYS  |
| 1   | G     | 72  | ASP  |
| 1   | G     | 84  | LYS  |
| 1   | G     | 97  | ILE  |
| 1   | G     | 109 | ARG  |
| 1   | G     | 116 | MET  |
| 1   | G     | 141 | PHE  |
| 1   | G     | 145 | LYS  |
| 1   | G     | 268 | LEU  |
| 1   | G     | 278 | ILE  |
| 1   | G     | 285 | HIS  |
| 1   | G     | 286 | ARG  |
| 1   | G     | 287 | PHE  |
| 1   | G     | 294 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 302 | ASP  |
| 1   | G     | 307 | ARG  |
| 1   | G     | 314 | LYS  |
| 1   | G     | 322 | TYR  |
| 1   | G     | 337 | HIS  |
| 1   | G     | 361 | TRP  |
| 1   | G     | 368 | GLN  |
| 1   | G     | 371 | SER  |
| 1   | G     | 385 | LEU  |
| 1   | G     | 390 | SER  |
| 1   | G     | 398 | ASP  |
| 1   | G     | 403 | ASN  |
| 1   | G     | 408 | ASN  |
| 1   | G     | 426 | GLU  |
| 1   | G     | 467 | LYS  |
| 1   | G     | 509 | LYS  |
| 1   | G     | 511 | LEU  |
| 1   | G     | 562 | ASN  |
| 1   | G     | 628 | LYS  |
| 2   | H     | 1   | MET  |
| 2   | H     | 40  | LEU  |
| 2   | H     | 41  | ASN  |
| 2   | H     | 50  | ASP  |
| 2   | H     | 79  | THR  |
| 2   | H     | 101 | LYS  |
| 2   | H     | 114 | MET  |
| 2   | H     | 140 | GLU  |
| 2   | H     | 147 | GLU  |
| 2   | H     | 167 | ARG  |
| 2   | H     | 181 | ARG  |
| 2   | H     | 189 | GLU  |
| 3   | I     | 1   | MET  |
| 3   | I     | 14  | THR  |
| 3   | I     | 40  | PHE  |
| 3   | I     | 47  | PHE  |
| 3   | I     | 56  | ASN  |
| 3   | I     | 58  | MET  |
| 3   | I     | 65  | PHE  |
| 3   | I     | 69  | PHE  |
| 3   | I     | 75  | LYS  |
| 3   | I     | 78  | VAL  |
| 3   | I     | 100 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 101 | PHE  |
| 3   | I     | 106 | ARG  |
| 3   | I     | 123 | THR  |
| 3   | I     | 137 | PHE  |
| 3   | I     | 154 | ILE  |
| 3   | I     | 164 | VAL  |
| 3   | I     | 197 | PHE  |
| 3   | I     | 203 | ASP  |
| 3   | I     | 212 | LEU  |
| 3   | I     | 223 | LEU  |
| 3   | I     | 234 | LYS  |
| 3   | I     | 239 | THR  |
| 1   | J     | 2   | LYS  |
| 1   | J     | 9   | LEU  |
| 1   | J     | 40  | LYS  |
| 1   | J     | 72  | ASP  |
| 1   | J     | 84  | LYS  |
| 1   | J     | 97  | ILE  |
| 1   | J     | 109 | ARG  |
| 1   | J     | 116 | MET  |
| 1   | J     | 141 | PHE  |
| 1   | J     | 145 | LYS  |
| 1   | J     | 268 | LEU  |
| 1   | J     | 278 | ILE  |
| 1   | J     | 285 | HIS  |
| 1   | J     | 286 | ARG  |
| 1   | J     | 287 | PHE  |
| 1   | J     | 294 | GLU  |
| 1   | J     | 302 | ASP  |
| 1   | J     | 307 | ARG  |
| 1   | J     | 314 | LYS  |
| 1   | J     | 322 | TYR  |
| 1   | J     | 337 | HIS  |
| 1   | J     | 361 | TRP  |
| 1   | J     | 368 | GLN  |
| 1   | J     | 371 | SER  |
| 1   | J     | 385 | LEU  |
| 1   | J     | 390 | SER  |
| 1   | J     | 398 | ASP  |
| 1   | J     | 403 | ASN  |
| 1   | J     | 408 | ASN  |
| 1   | J     | 426 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 467 | LYS  |
| 1   | J     | 509 | LYS  |
| 1   | J     | 511 | LEU  |
| 1   | J     | 562 | ASN  |
| 1   | J     | 628 | LYS  |
| 2   | K     | 1   | MET  |
| 2   | K     | 40  | LEU  |
| 2   | K     | 41  | ASN  |
| 2   | K     | 50  | ASP  |
| 2   | K     | 79  | THR  |
| 2   | K     | 101 | LYS  |
| 2   | K     | 114 | MET  |
| 2   | K     | 140 | GLU  |
| 2   | K     | 147 | GLU  |
| 2   | K     | 167 | ARG  |
| 2   | K     | 181 | ARG  |
| 2   | K     | 189 | GLU  |
| 3   | L     | 1   | MET  |
| 3   | L     | 14  | THR  |
| 3   | L     | 40  | PHE  |
| 3   | L     | 47  | PHE  |
| 3   | L     | 56  | ASN  |
| 3   | L     | 58  | MET  |
| 3   | L     | 65  | PHE  |
| 3   | L     | 69  | PHE  |
| 3   | L     | 75  | LYS  |
| 3   | L     | 78  | VAL  |
| 3   | L     | 100 | LYS  |
| 3   | L     | 101 | PHE  |
| 3   | L     | 106 | ARG  |
| 3   | L     | 123 | THR  |
| 3   | L     | 137 | PHE  |
| 3   | L     | 154 | ILE  |
| 3   | L     | 164 | VAL  |
| 3   | L     | 197 | PHE  |
| 3   | L     | 203 | ASP  |
| 3   | L     | 212 | LEU  |
| 3   | L     | 223 | LEU  |
| 3   | L     | 234 | LYS  |
| 3   | L     | 239 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | GLN  |
| 1   | A     | 48  | GLN  |
| 1   | A     | 83  | GLN  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 111 | HIS  |
| 1   | A     | 158 | HIS  |
| 1   | A     | 228 | ASN  |
| 1   | A     | 257 | HIS  |
| 1   | A     | 325 | HIS  |
| 1   | A     | 368 | GLN  |
| 1   | A     | 403 | ASN  |
| 1   | A     | 408 | ASN  |
| 1   | A     | 468 | ASN  |
| 1   | A     | 486 | HIS  |
| 1   | A     | 547 | HIS  |
| 1   | A     | 548 | ASN  |
| 1   | A     | 562 | ASN  |
| 1   | A     | 631 | HIS  |
| 2   | B     | 116 | GLN  |
| 2   | B     | 225 | GLN  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 30  | GLN  |
| 3   | C     | 107 | GLN  |
| 3   | C     | 152 | GLN  |
| 1   | D     | 26  | GLN  |
| 1   | D     | 48  | GLN  |
| 1   | D     | 83  | GLN  |
| 1   | D     | 91  | ASN  |
| 1   | D     | 111 | HIS  |
| 1   | D     | 158 | HIS  |
| 1   | D     | 228 | ASN  |
| 1   | D     | 257 | HIS  |
| 1   | D     | 325 | HIS  |
| 1   | D     | 368 | GLN  |
| 1   | D     | 403 | ASN  |
| 1   | D     | 408 | ASN  |
| 1   | D     | 468 | ASN  |
| 1   | D     | 486 | HIS  |
| 1   | D     | 547 | HIS  |
| 1   | D     | 548 | ASN  |
| 1   | D     | 562 | ASN  |
| 1   | D     | 631 | HIS  |
| 2   | E     | 116 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 225 | GLN  |
| 3   | F     | 3   | ASN  |
| 3   | F     | 30  | GLN  |
| 3   | F     | 107 | GLN  |
| 3   | F     | 152 | GLN  |
| 1   | G     | 26  | GLN  |
| 1   | G     | 48  | GLN  |
| 1   | G     | 83  | GLN  |
| 1   | G     | 91  | ASN  |
| 1   | G     | 111 | HIS  |
| 1   | G     | 158 | HIS  |
| 1   | G     | 228 | ASN  |
| 1   | G     | 257 | HIS  |
| 1   | G     | 325 | HIS  |
| 1   | G     | 368 | GLN  |
| 1   | G     | 403 | ASN  |
| 1   | G     | 408 | ASN  |
| 1   | G     | 468 | ASN  |
| 1   | G     | 486 | HIS  |
| 1   | G     | 547 | HIS  |
| 1   | G     | 548 | ASN  |
| 1   | G     | 562 | ASN  |
| 1   | G     | 631 | HIS  |
| 2   | H     | 116 | GLN  |
| 2   | H     | 225 | GLN  |
| 3   | I     | 3   | ASN  |
| 3   | I     | 30  | GLN  |
| 3   | I     | 107 | GLN  |
| 3   | I     | 152 | GLN  |
| 1   | J     | 26  | GLN  |
| 1   | J     | 48  | GLN  |
| 1   | J     | 83  | GLN  |
| 1   | J     | 91  | ASN  |
| 1   | J     | 111 | HIS  |
| 1   | J     | 158 | HIS  |
| 1   | J     | 228 | ASN  |
| 1   | J     | 257 | HIS  |
| 1   | J     | 325 | HIS  |
| 1   | J     | 368 | GLN  |
| 1   | J     | 403 | ASN  |
| 1   | J     | 408 | ASN  |
| 1   | J     | 468 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 486 | HIS  |
| 1   | J     | 547 | HIS  |
| 1   | J     | 548 | ASN  |
| 1   | J     | 562 | ASN  |
| 1   | J     | 631 | HIS  |
| 2   | K     | 116 | GLN  |
| 2   | K     | 225 | GLN  |
| 3   | L     | 3   | ASN  |
| 3   | L     | 30  | GLN  |
| 3   | L     | 107 | GLN  |
| 3   | L     | 152 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | FAD  | A     | 701 | 1    | 58,58,58     | 2.17 | 14 (24%)    | 85,89,89    | 1.75 | 16 (18%)    |
| 5   | MLA  | A     | 702 | -    | 6,6,6        | 1.92 | 2 (33%)     | 7,7,7       | 0.65 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |       |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|-------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ  | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | FES  | B     | 301 | 2    | 0,4,4        | 0.00  | -        | 0,4,4       | 0.00 | -        |
| 8   | F3S  | B     | 302 | 2    | 3,9,9        | 14.47 | 3 (100%) | 0,15,15     | 0.00 | -        |
| 9   | SF4  | B     | 303 | 2    | 12,12,12     | 13.32 | 11 (91%) | 0,24,24     | 0.00 | -        |
| 10  | HEM  | C     | 301 | 3    | 49,50,50     | 1.97  | 14 (28%) | 46,82,82    | 1.79 | 6 (13%)  |
| 10  | HEM  | C     | 302 | 3    | 49,50,50     | 2.14  | 15 (30%) | 46,82,82    | 1.53 | 5 (10%)  |
| 11  | LMT  | C     | 303 | -    | 36,36,36     | 1.11  | 2 (5%)   | 47,47,47    | 1.23 | 4 (8%)   |
| 4   | FAD  | D     | 701 | 1    | 58,58,58     | 2.17  | 14 (24%) | 85,89,89    | 1.75 | 16 (18%) |
| 5   | MLA  | D     | 702 | -    | 6,6,6        | 1.92  | 2 (33%)  | 7,7,7       | 0.66 | 0        |
| 7   | FES  | E     | 301 | 2    | 0,4,4        | 0.00  | -        | 0,4,4       | 0.00 | -        |
| 8   | F3S  | E     | 302 | 2    | 3,9,9        | 14.47 | 3 (100%) | 0,15,15     | 0.00 | -        |
| 9   | SF4  | E     | 303 | 2    | 12,12,12     | 13.32 | 11 (91%) | 0,24,24     | 0.00 | -        |
| 11  | LMT  | F     | 301 | -    | 36,36,36     | 1.11  | 2 (5%)   | 47,47,47    | 1.23 | 4 (8%)   |
| 10  | HEM  | F     | 302 | 3    | 49,50,50     | 1.97  | 14 (28%) | 46,82,82    | 1.79 | 6 (13%)  |
| 10  | HEM  | F     | 303 | 3    | 49,50,50     | 2.12  | 15 (30%) | 46,82,82    | 1.52 | 5 (10%)  |
| 4   | FAD  | G     | 701 | 1    | 58,58,58     | 2.16  | 14 (24%) | 85,89,89    | 1.75 | 16 (18%) |
| 5   | MLA  | G     | 702 | -    | 6,6,6        | 1.92  | 2 (33%)  | 7,7,7       | 0.65 | 0        |
| 7   | FES  | H     | 301 | 2    | 0,4,4        | 0.00  | -        | 0,4,4       | 0.00 | -        |
| 8   | F3S  | H     | 302 | 2    | 3,9,9        | 14.50 | 3 (100%) | 0,15,15     | 0.00 | -        |
| 9   | SF4  | H     | 303 | 2    | 12,12,12     | 13.32 | 11 (91%) | 0,24,24     | 0.00 | -        |
| 10  | HEM  | I     | 301 | 3    | 49,50,50     | 1.98  | 14 (28%) | 46,82,82    | 1.78 | 6 (13%)  |
| 10  | HEM  | I     | 302 | 3    | 49,50,50     | 2.15  | 15 (30%) | 46,82,82    | 1.53 | 5 (10%)  |
| 11  | LMT  | I     | 303 | -    | 36,36,36     | 1.11  | 2 (5%)   | 47,47,47    | 1.23 | 4 (8%)   |
| 4   | FAD  | J     | 701 | 1    | 58,58,58     | 2.17  | 14 (24%) | 85,89,89    | 1.75 | 16 (18%) |
| 5   | MLA  | J     | 702 | -    | 6,6,6        | 1.94  | 2 (33%)  | 7,7,7       | 0.65 | 0        |
| 7   | FES  | K     | 301 | 2    | 0,4,4        | 0.00  | -        | 0,4,4       | 0.00 | -        |
| 8   | F3S  | K     | 302 | 2    | 3,9,9        | 14.50 | 3 (100%) | 0,15,15     | 0.00 | -        |
| 9   | SF4  | K     | 303 | 2    | 12,12,12     | 13.34 | 11 (91%) | 0,24,24     | 0.00 | -        |
| 11  | LMT  | L     | 301 | -    | 36,36,36     | 1.11  | 2 (5%)   | 47,47,47    | 1.23 | 4 (8%)   |
| 10  | HEM  | L     | 302 | 3    | 49,50,50     | 1.97  | 14 (28%) | 46,82,82    | 1.78 | 5 (10%)  |
| 10  | HEM  | L     | 303 | 3    | 49,50,50     | 2.13  | 15 (30%) | 46,82,82    | 1.53 | 5 (10%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 4   | FAD  | A     | 701 | 1    | -       | 0/34/50/50   | 0/1/6/6 |
| 5   | MLA  | A     | 702 | -    | -       | 0/4/4/4      | 0/0/0/0 |
| 7   | FES  | B     | 301 | 2    | -       | 0/0/4/4      | 0/0/1/1 |
| 8   | F3S  | B     | 302 | 2    | -       | 0/0/24/24    | 0/0/3/3 |
| 9   | SF4  | B     | 303 | 2    | -       | 0/0/48/48    | 0/0/5/5 |
| 10  | HEM  | C     | 301 | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 10  | HEM  | C     | 302 | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 11  | LMT  | C     | 303 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 4   | FAD  | D     | 701 | 1    | -       | 0/34/50/50   | 0/1/6/6 |
| 5   | MLA  | D     | 702 | -    | -       | 0/4/4/4      | 0/0/0/0 |
| 7   | FES  | E     | 301 | 2    | -       | 0/0/4/4      | 0/0/1/1 |
| 8   | F3S  | E     | 302 | 2    | -       | 0/0/24/24    | 0/0/3/3 |
| 9   | SF4  | E     | 303 | 2    | -       | 0/0/48/48    | 0/0/5/5 |
| 11  | LMT  | F     | 301 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 10  | HEM  | F     | 302 | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 10  | HEM  | F     | 303 | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 4   | FAD  | G     | 701 | 1    | -       | 0/34/50/50   | 0/1/6/6 |
| 5   | MLA  | G     | 702 | -    | -       | 0/4/4/4      | 0/0/0/0 |
| 7   | FES  | H     | 301 | 2    | -       | 0/0/4/4      | 0/0/1/1 |
| 8   | F3S  | H     | 302 | 2    | -       | 0/0/24/24    | 0/0/3/3 |
| 9   | SF4  | H     | 303 | 2    | -       | 0/0/48/48    | 0/0/5/5 |
| 10  | HEM  | I     | 301 | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 10  | HEM  | I     | 302 | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 11  | LMT  | I     | 303 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 4   | FAD  | J     | 701 | 1    | -       | 0/34/50/50   | 0/1/6/6 |
| 5   | MLA  | J     | 702 | -    | -       | 0/4/4/4      | 0/0/0/0 |
| 7   | FES  | K     | 301 | 2    | -       | 0/0/4/4      | 0/0/1/1 |
| 8   | F3S  | K     | 302 | 2    | -       | 0/0/24/24    | 0/0/3/3 |
| 9   | SF4  | K     | 303 | 2    | -       | 0/0/48/48    | 0/0/5/5 |
| 11  | LMT  | L     | 301 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 10  | HEM  | L     | 302 | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 10  | HEM  | L     | 303 | 3    | -       | 0/14/114/114 | 0/0/8/8 |

All (244) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 9   | E     | 303 | SF4  | S4-FE3 | -24.81 | 2.16        | 2.33     |
| 9   | B     | 303 | SF4  | S4-FE3 | -24.76 | 2.16        | 2.33     |
| 9   | K     | 303 | SF4  | S4-FE3 | -24.73 | 2.16        | 2.33     |
| 9   | H     | 303 | SF4  | S4-FE3 | -24.69 | 2.16        | 2.33     |
| 8   | K     | 302 | F3S  | S3-FE3 | -24.24 | 2.16        | 2.33     |
| 8   | H     | 302 | F3S  | S3-FE3 | -24.24 | 2.17        | 2.33     |
| 8   | E     | 302 | F3S  | S3-FE3 | -24.23 | 2.17        | 2.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 8   | B     | 302 | F3S  | S3-FE3  | -24.19 | 2.17        | 2.33     |
| 9   | K     | 303 | SF4  | S1-FE3  | -23.19 | 2.17        | 2.33     |
| 9   | E     | 303 | SF4  | S1-FE3  | -23.14 | 2.17        | 2.33     |
| 9   | H     | 303 | SF4  | S1-FE3  | -23.13 | 2.17        | 2.33     |
| 9   | B     | 303 | SF4  | S1-FE3  | -23.12 | 2.17        | 2.33     |
| 9   | H     | 303 | SF4  | S2-FE3  | -16.38 | 2.22        | 2.33     |
| 9   | K     | 303 | SF4  | S2-FE3  | -16.35 | 2.22        | 2.33     |
| 9   | B     | 303 | SF4  | S2-FE3  | -16.29 | 2.22        | 2.33     |
| 9   | E     | 303 | SF4  | S2-FE3  | -16.23 | 2.22        | 2.33     |
| 9   | E     | 303 | SF4  | S3-FE2  | -16.14 | 2.22        | 2.33     |
| 9   | K     | 303 | SF4  | S3-FE2  | -16.14 | 2.22        | 2.33     |
| 9   | B     | 303 | SF4  | S3-FE2  | -16.11 | 2.22        | 2.33     |
| 9   | H     | 303 | SF4  | S3-FE2  | -16.11 | 2.22        | 2.33     |
| 9   | H     | 303 | SF4  | S3-FE4  | -11.31 | 2.25        | 2.33     |
| 9   | B     | 303 | SF4  | S3-FE4  | -11.14 | 2.25        | 2.33     |
| 9   | K     | 303 | SF4  | S3-FE4  | -11.07 | 2.25        | 2.33     |
| 9   | E     | 303 | SF4  | S3-FE4  | -11.07 | 2.25        | 2.33     |
| 9   | B     | 303 | SF4  | S2-FE1  | -9.88  | 2.26        | 2.33     |
| 9   | H     | 303 | SF4  | S2-FE1  | -9.87  | 2.26        | 2.33     |
| 9   | E     | 303 | SF4  | S2-FE1  | -9.86  | 2.26        | 2.33     |
| 9   | K     | 303 | SF4  | S2-FE1  | -9.84  | 2.26        | 2.33     |
| 9   | H     | 303 | SF4  | S3-FE1  | -9.30  | 2.27        | 2.33     |
| 9   | K     | 303 | SF4  | S3-FE1  | -9.27  | 2.27        | 2.33     |
| 9   | B     | 303 | SF4  | S3-FE1  | -9.26  | 2.27        | 2.33     |
| 9   | E     | 303 | SF4  | S3-FE1  | -9.23  | 2.27        | 2.33     |
| 9   | K     | 303 | SF4  | S4-FE2  | -8.11  | 2.27        | 2.33     |
| 9   | B     | 303 | SF4  | S4-FE2  | -7.97  | 2.27        | 2.33     |
| 9   | E     | 303 | SF4  | S4-FE2  | -7.90  | 2.27        | 2.33     |
| 9   | H     | 303 | SF4  | S4-FE2  | -7.84  | 2.28        | 2.33     |
| 9   | E     | 303 | SF4  | S1-FE2  | -7.34  | 2.28        | 2.33     |
| 9   | K     | 303 | SF4  | S1-FE2  | -7.29  | 2.28        | 2.33     |
| 9   | B     | 303 | SF4  | S1-FE2  | -7.28  | 2.28        | 2.33     |
| 9   | H     | 303 | SF4  | S1-FE2  | -7.27  | 2.28        | 2.33     |
| 4   | J     | 701 | FAD  | C1'-C2' | 6.25   | 1.57        | 1.51     |
| 4   | A     | 701 | FAD  | C1'-C2' | 6.19   | 1.57        | 1.51     |
| 4   | G     | 701 | FAD  | C1'-C2' | 6.19   | 1.57        | 1.51     |
| 4   | D     | 701 | FAD  | C1'-C2' | 6.11   | 1.57        | 1.51     |
| 4   | D     | 701 | FAD  | P-O3P   | -5.58  | 1.49        | 1.59     |
| 4   | J     | 701 | FAD  | P-O3P   | -5.57  | 1.49        | 1.59     |
| 4   | A     | 701 | FAD  | P-O3P   | -5.56  | 1.49        | 1.59     |
| 4   | G     | 701 | FAD  | P-O3P   | -5.54  | 1.49        | 1.59     |
| 10  | F     | 302 | HEM  | C3B-C2B | -5.52  | 1.34        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | I     | 301 | HEM  | C3B-C2B | -5.51 | 1.34        | 1.43     |
| 10  | C     | 301 | HEM  | C3B-C2B | -5.48 | 1.34        | 1.43     |
| 8   | H     | 302 | F3S  | S3-FE1  | -5.48 | 2.29        | 2.33     |
| 8   | K     | 302 | F3S  | S3-FE1  | -5.47 | 2.29        | 2.33     |
| 10  | L     | 302 | HEM  | C3B-C2B | -5.46 | 1.34        | 1.43     |
| 8   | B     | 302 | F3S  | S3-FE1  | -5.40 | 2.29        | 2.33     |
| 8   | E     | 302 | F3S  | S3-FE1  | -5.32 | 2.29        | 2.33     |
| 10  | L     | 303 | HEM  | C3D-C2D | -5.17 | 1.34        | 1.43     |
| 10  | C     | 302 | HEM  | C3D-C2D | -5.15 | 1.34        | 1.43     |
| 10  | I     | 302 | HEM  | C3D-C2D | -5.14 | 1.34        | 1.43     |
| 10  | F     | 303 | HEM  | C3D-C2D | -5.12 | 1.34        | 1.43     |
| 10  | C     | 302 | HEM  | C3B-C2B | -4.77 | 1.35        | 1.43     |
| 10  | F     | 303 | HEM  | C3B-C2B | -4.76 | 1.35        | 1.43     |
| 10  | I     | 302 | HEM  | C3B-C2B | -4.75 | 1.35        | 1.43     |
| 10  | L     | 303 | HEM  | C3B-C2B | -4.73 | 1.35        | 1.43     |
| 10  | C     | 301 | HEM  | C3D-C2D | -4.64 | 1.35        | 1.43     |
| 10  | I     | 301 | HEM  | C3D-C2D | -4.64 | 1.35        | 1.43     |
| 10  | I     | 302 | HEM  | C3D-C4D | -4.63 | 1.43        | 1.44     |
| 10  | F     | 302 | HEM  | C3D-C2D | -4.62 | 1.35        | 1.43     |
| 10  | L     | 302 | HEM  | C3D-C2D | -4.60 | 1.35        | 1.43     |
| 10  | F     | 302 | HEM  | C3C-C2C | -4.60 | 1.35        | 1.43     |
| 10  | C     | 301 | HEM  | C3C-C2C | -4.58 | 1.35        | 1.43     |
| 10  | L     | 302 | HEM  | C3C-C2C | -4.56 | 1.35        | 1.43     |
| 10  | I     | 301 | HEM  | C3C-C2C | -4.54 | 1.35        | 1.43     |
| 9   | K     | 303 | SF4  | S1-FE4  | -4.52 | 2.30        | 2.33     |
| 10  | F     | 303 | HEM  | C3C-C2C | -4.49 | 1.35        | 1.43     |
| 10  | C     | 302 | HEM  | C3C-C2C | -4.47 | 1.35        | 1.43     |
| 10  | I     | 302 | HEM  | C3C-C2C | -4.45 | 1.36        | 1.43     |
| 4   | D     | 701 | FAD  | O4B-C1B | 4.45  | 1.48        | 1.41     |
| 10  | L     | 303 | HEM  | C3C-C2C | -4.44 | 1.36        | 1.43     |
| 4   | G     | 701 | FAD  | C9A-N10 | 4.44  | 1.45        | 1.38     |
| 9   | B     | 303 | SF4  | S1-FE4  | -4.44 | 2.30        | 2.33     |
| 4   | J     | 701 | FAD  | C9A-N10 | 4.42  | 1.45        | 1.38     |
| 4   | G     | 701 | FAD  | O4B-C1B | 4.41  | 1.48        | 1.41     |
| 9   | E     | 303 | SF4  | S1-FE4  | -4.41 | 2.30        | 2.33     |
| 4   | A     | 701 | FAD  | O4B-C1B | 4.41  | 1.48        | 1.41     |
| 4   | A     | 701 | FAD  | C9A-N10 | 4.39  | 1.45        | 1.38     |
| 4   | D     | 701 | FAD  | C9A-N10 | 4.38  | 1.45        | 1.38     |
| 4   | J     | 701 | FAD  | O4B-C1B | 4.37  | 1.48        | 1.41     |
| 9   | H     | 303 | SF4  | S1-FE4  | -4.34 | 2.30        | 2.33     |
| 4   | A     | 701 | FAD  | PA-O2A  | -4.29 | 1.35        | 1.55     |
| 4   | J     | 701 | FAD  | PA-O2A  | -4.28 | 1.35        | 1.55     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | G     | 701 | FAD  | PA-O2A  | -4.28 | 1.35        | 1.55     |
| 4   | D     | 701 | FAD  | PA-O2A  | -4.28 | 1.35        | 1.55     |
| 10  | I     | 302 | HEM  | C4A-C3A | 4.22  | 1.45        | 1.40     |
| 10  | C     | 302 | HEM  | C4A-C3A | 4.21  | 1.45        | 1.40     |
| 10  | F     | 303 | HEM  | C4A-C3A | 4.20  | 1.45        | 1.40     |
| 10  | C     | 302 | HEM  | C3D-C4D | -4.20 | 1.43        | 1.44     |
| 4   | J     | 701 | FAD  | C4X-C10 | 4.17  | 1.48        | 1.40     |
| 10  | F     | 303 | HEM  | C3D-C4D | -4.15 | 1.43        | 1.44     |
| 4   | A     | 701 | FAD  | C4X-C10 | 4.15  | 1.48        | 1.40     |
| 10  | L     | 303 | HEM  | C4A-C3A | 4.15  | 1.45        | 1.40     |
| 4   | G     | 701 | FAD  | C4X-C10 | 4.14  | 1.48        | 1.40     |
| 4   | D     | 701 | FAD  | C4X-C10 | 4.11  | 1.48        | 1.40     |
| 10  | I     | 301 | HEM  | C4A-C3A | 3.98  | 1.45        | 1.40     |
| 10  | C     | 301 | HEM  | C4A-C3A | 3.97  | 1.45        | 1.40     |
| 10  | L     | 302 | HEM  | C4A-C3A | 3.95  | 1.45        | 1.40     |
| 10  | F     | 302 | HEM  | C4A-C3A | 3.95  | 1.45        | 1.40     |
| 10  | L     | 303 | HEM  | C2B-C1B | 3.87  | 1.45        | 1.44     |
| 10  | L     | 303 | HEM  | C3D-C4D | -3.85 | 1.43        | 1.44     |
| 4   | J     | 701 | FAD  | O5'-C5' | 3.80  | 1.60        | 1.44     |
| 4   | G     | 701 | FAD  | O5'-C5' | 3.79  | 1.60        | 1.44     |
| 4   | A     | 701 | FAD  | O5'-C5' | 3.79  | 1.60        | 1.44     |
| 4   | D     | 701 | FAD  | O5'-C5' | 3.78  | 1.60        | 1.44     |
| 10  | C     | 302 | HEM  | C2B-C1B | 3.72  | 1.45        | 1.44     |
| 8   | K     | 302 | F3S  | S3-FE4  | -3.67 | 2.30        | 2.33     |
| 8   | H     | 302 | F3S  | S3-FE4  | -3.67 | 2.30        | 2.33     |
| 8   | B     | 302 | F3S  | S3-FE4  | -3.63 | 2.30        | 2.33     |
| 10  | F     | 303 | HEM  | C2B-C1B | 3.61  | 1.45        | 1.44     |
| 10  | I     | 302 | HEM  | C2B-C1B | 3.59  | 1.45        | 1.44     |
| 8   | E     | 302 | F3S  | S3-FE4  | -3.60 | 2.30        | 2.33     |
| 4   | G     | 701 | FAD  | P-O2P   | -3.59 | 1.39        | 1.55     |
| 4   | J     | 701 | FAD  | P-O2P   | -3.58 | 1.39        | 1.55     |
| 4   | A     | 701 | FAD  | P-O2P   | -3.58 | 1.39        | 1.55     |
| 4   | D     | 701 | FAD  | P-O2P   | -3.58 | 1.39        | 1.55     |
| 10  | L     | 303 | HEM  | C2D-C1D | 3.49  | 1.45        | 1.44     |
| 9   | H     | 303 | SF4  | S2-FE4  | -3.47 | 2.30        | 2.33     |
| 4   | D     | 701 | FAD  | C2B-C1B | -3.47 | 1.48        | 1.53     |
| 9   | K     | 303 | SF4  | S2-FE4  | -3.47 | 2.30        | 2.33     |
| 9   | B     | 303 | SF4  | S2-FE4  | -3.44 | 2.30        | 2.33     |
| 9   | E     | 303 | SF4  | S2-FE4  | -3.44 | 2.30        | 2.33     |
| 4   | J     | 701 | FAD  | C2B-C1B | -3.42 | 1.48        | 1.53     |
| 4   | A     | 701 | FAD  | C2B-C1B | -3.41 | 1.48        | 1.53     |
| 4   | G     | 701 | FAD  | C2B-C1B | -3.40 | 1.48        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 10  | C     | 302 | HEM  | CBB-CAB | 3.39 | 1.48        | 1.28     |
| 10  | L     | 303 | HEM  | CBB-CAB | 3.39 | 1.48        | 1.28     |
| 10  | I     | 302 | HEM  | CBB-CAB | 3.39 | 1.48        | 1.28     |
| 10  | F     | 303 | HEM  | CBB-CAB | 3.38 | 1.48        | 1.28     |
| 10  | I     | 302 | HEM  | C2D-C1D | 3.35 | 1.45        | 1.44     |
| 10  | C     | 302 | HEM  | C2D-C1D | 3.32 | 1.45        | 1.44     |
| 4   | D     | 701 | FAD  | C4-C4X  | 3.31 | 1.46        | 1.41     |
| 11  | C     | 303 | LMT  | O5B-C1B | 3.31 | 1.50        | 1.41     |
| 11  | I     | 303 | LMT  | O5B-C1B | 3.31 | 1.50        | 1.41     |
| 11  | L     | 301 | LMT  | O5B-C1B | 3.30 | 1.50        | 1.41     |
| 11  | F     | 301 | LMT  | O5B-C1B | 3.30 | 1.50        | 1.41     |
| 4   | A     | 701 | FAD  | C4-C4X  | 3.29 | 1.46        | 1.41     |
| 4   | G     | 701 | FAD  | C4-C4X  | 3.27 | 1.46        | 1.41     |
| 4   | J     | 701 | FAD  | C4-C4X  | 3.26 | 1.46        | 1.41     |
| 10  | F     | 302 | HEM  | CBC-CAC | 3.17 | 1.47        | 1.28     |
| 10  | C     | 301 | HEM  | CBC-CAC | 3.17 | 1.47        | 1.28     |
| 10  | I     | 301 | HEM  | CBC-CAC | 3.16 | 1.47        | 1.28     |
| 10  | L     | 302 | HEM  | CBC-CAC | 3.15 | 1.47        | 1.28     |
| 5   | J     | 702 | MLA  | C2-C1   | 3.13 | 1.55        | 1.51     |
| 5   | G     | 702 | MLA  | C2-C1   | 3.11 | 1.55        | 1.51     |
| 10  | F     | 303 | HEM  | FE-NB   | 3.11 | 2.09        | 1.97     |
| 10  | C     | 302 | HEM  | FE-NB   | 3.11 | 2.09        | 1.97     |
| 10  | I     | 302 | HEM  | FE-NB   | 3.10 | 2.09        | 1.97     |
| 10  | L     | 303 | HEM  | FE-NB   | 3.10 | 2.09        | 1.97     |
| 5   | A     | 702 | MLA  | C2-C1   | 3.08 | 1.55        | 1.51     |
| 10  | C     | 302 | HEM  | CMB-C2B | 3.07 | 1.57        | 1.47     |
| 10  | F     | 303 | HEM  | CMB-C2B | 3.06 | 1.56        | 1.47     |
| 10  | L     | 303 | HEM  | CMB-C2B | 3.06 | 1.56        | 1.47     |
| 10  | I     | 302 | HEM  | CMB-C2B | 3.05 | 1.56        | 1.47     |
| 5   | D     | 702 | MLA  | C2-C1   | 3.05 | 1.55        | 1.51     |
| 10  | F     | 303 | HEM  | C2D-C1D | 3.05 | 1.45        | 1.44     |
| 10  | F     | 302 | HEM  | CBB-CAB | 2.99 | 1.46        | 1.28     |
| 10  | L     | 302 | HEM  | CBB-CAB | 2.99 | 1.46        | 1.28     |
| 10  | I     | 301 | HEM  | CBB-CAB | 2.98 | 1.46        | 1.28     |
| 10  | C     | 301 | HEM  | CBB-CAB | 2.98 | 1.46        | 1.28     |
| 10  | I     | 302 | HEM  | CHB-C1B | 2.97 | 1.40        | 1.35     |
| 10  | C     | 302 | HEM  | CHB-C1B | 2.97 | 1.40        | 1.35     |
| 10  | F     | 303 | HEM  | CHB-C1B | 2.96 | 1.40        | 1.35     |
| 10  | I     | 302 | HEM  | CHD-C4C | 2.93 | 1.41        | 1.36     |
| 10  | L     | 303 | HEM  | CHB-C1B | 2.93 | 1.40        | 1.35     |
| 10  | C     | 302 | HEM  | CHD-C4C | 2.91 | 1.41        | 1.36     |
| 10  | F     | 303 | HEM  | CHD-C4C | 2.90 | 1.41        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | L     | 302 | HEM  | CAA-C2A | 2.87  | 1.57        | 1.52     |
| 10  | L     | 303 | HEM  | CHD-C4C | 2.87  | 1.41        | 1.36     |
| 10  | I     | 301 | HEM  | CAA-C2A | 2.86  | 1.57        | 1.52     |
| 10  | F     | 302 | HEM  | CAA-C2A | 2.85  | 1.57        | 1.52     |
| 10  | C     | 301 | HEM  | CAA-C2A | 2.84  | 1.57        | 1.52     |
| 10  | I     | 301 | HEM  | C3D-C4D | -2.81 | 1.43        | 1.44     |
| 10  | F     | 302 | HEM  | C2B-C1B | -2.80 | 1.43        | 1.44     |
| 10  | L     | 302 | HEM  | C2B-C1B | -2.77 | 1.43        | 1.44     |
| 11  | C     | 303 | LMT  | C3'-C4' | 2.74  | 1.60        | 1.52     |
| 5   | J     | 702 | MLA  | C2-C3   | 2.74  | 1.55        | 1.51     |
| 10  | I     | 301 | HEM  | C2B-C1B | -2.74 | 1.43        | 1.44     |
| 5   | A     | 702 | MLA  | C2-C3   | 2.74  | 1.55        | 1.51     |
| 11  | L     | 301 | LMT  | C3'-C4' | 2.74  | 1.60        | 1.52     |
| 11  | F     | 301 | LMT  | C3'-C4' | 2.73  | 1.60        | 1.52     |
| 10  | L     | 302 | HEM  | FE-NA   | 2.73  | 2.04        | 1.92     |
| 10  | I     | 301 | HEM  | FE-NA   | 2.73  | 2.04        | 1.92     |
| 10  | F     | 302 | HEM  | FE-NA   | 2.73  | 2.04        | 1.92     |
| 5   | D     | 702 | MLA  | C2-C3   | 2.73  | 1.55        | 1.51     |
| 11  | I     | 303 | LMT  | C3'-C4' | 2.72  | 1.60        | 1.52     |
| 10  | C     | 301 | HEM  | FE-NA   | 2.72  | 2.04        | 1.92     |
| 4   | D     | 701 | FAD  | C5'-C4' | 2.71  | 1.56        | 1.51     |
| 4   | G     | 701 | FAD  | C5'-C4' | 2.70  | 1.56        | 1.51     |
| 5   | G     | 702 | MLA  | C2-C3   | 2.69  | 1.55        | 1.51     |
| 4   | A     | 701 | FAD  | C5'-C4' | 2.69  | 1.55        | 1.51     |
| 10  | F     | 302 | HEM  | C3D-C4D | -2.69 | 1.43        | 1.44     |
| 10  | L     | 302 | HEM  | C3D-C4D | -2.67 | 1.43        | 1.44     |
| 10  | I     | 302 | HEM  | FE-NA   | 2.66  | 2.03        | 1.92     |
| 4   | J     | 701 | FAD  | C5'-C4' | 2.66  | 1.55        | 1.51     |
| 10  | C     | 302 | HEM  | FE-NA   | 2.65  | 2.03        | 1.92     |
| 10  | L     | 303 | HEM  | FE-NA   | 2.65  | 2.03        | 1.92     |
| 10  | F     | 303 | HEM  | FE-NA   | 2.64  | 2.03        | 1.92     |
| 10  | C     | 301 | HEM  | C2B-C1B | -2.63 | 1.43        | 1.44     |
| 10  | F     | 303 | HEM  | CBC-CAC | 2.61  | 1.44        | 1.28     |
| 10  | I     | 302 | HEM  | CBC-CAC | 2.60  | 1.43        | 1.28     |
| 10  | C     | 302 | HEM  | CBC-CAC | 2.60  | 1.43        | 1.28     |
| 10  | L     | 303 | HEM  | CBC-CAC | 2.59  | 1.43        | 1.28     |
| 10  | C     | 301 | HEM  | C3D-C4D | -2.59 | 1.43        | 1.44     |
| 4   | D     | 701 | FAD  | C4A-N9A | 2.55  | 1.41        | 1.37     |
| 4   | J     | 701 | FAD  | C4A-N9A | 2.54  | 1.41        | 1.37     |
| 4   | A     | 701 | FAD  | C4A-N9A | 2.53  | 1.41        | 1.37     |
| 4   | G     | 701 | FAD  | C4A-N9A | 2.49  | 1.41        | 1.37     |
| 10  | L     | 302 | HEM  | CHB-C1B | 2.45  | 1.39        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | I     | 301 | HEM  | CHB-C1B | 2.43  | 1.39        | 1.35     |
| 10  | F     | 302 | HEM  | CHB-C1B | 2.43  | 1.39        | 1.35     |
| 10  | C     | 301 | HEM  | CHB-C1B | 2.43  | 1.39        | 1.35     |
| 4   | A     | 701 | FAD  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 4   | D     | 701 | FAD  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 4   | J     | 701 | FAD  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 4   | G     | 701 | FAD  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 4   | D     | 701 | FAD  | C2-N3   | 2.28  | 1.41        | 1.37     |
| 10  | I     | 301 | HEM  | CHA-C4D | 2.26  | 1.39        | 1.35     |
| 10  | L     | 302 | HEM  | CHA-C4D | 2.26  | 1.39        | 1.35     |
| 4   | A     | 701 | FAD  | C2-N3   | 2.23  | 1.41        | 1.37     |
| 10  | C     | 301 | HEM  | CHA-C4D | 2.23  | 1.39        | 1.35     |
| 4   | G     | 701 | FAD  | C2-N3   | 2.23  | 1.41        | 1.37     |
| 4   | J     | 701 | FAD  | C2-N3   | 2.22  | 1.41        | 1.37     |
| 10  | F     | 302 | HEM  | CHA-C4D | 2.21  | 1.39        | 1.35     |
| 10  | F     | 302 | HEM  | CMD-C2D | 2.16  | 1.54        | 1.47     |
| 10  | L     | 302 | HEM  | CMD-C2D | 2.16  | 1.54        | 1.47     |
| 10  | I     | 301 | HEM  | CMD-C2D | 2.16  | 1.54        | 1.47     |
| 10  | C     | 301 | HEM  | CMD-C2D | 2.16  | 1.54        | 1.47     |
| 10  | C     | 301 | HEM  | CMC-C2C | 2.13  | 1.54        | 1.47     |
| 10  | F     | 302 | HEM  | CMC-C2C | 2.13  | 1.54        | 1.47     |
| 10  | I     | 301 | HEM  | CMC-C2C | 2.12  | 1.54        | 1.47     |
| 10  | L     | 302 | HEM  | CMC-C2C | 2.11  | 1.54        | 1.47     |
| 10  | L     | 303 | HEM  | CHC-C1C | 2.03  | 1.39        | 1.36     |
| 10  | F     | 303 | HEM  | CHC-C1C | 2.03  | 1.39        | 1.36     |
| 10  | C     | 302 | HEM  | CHC-C1C | 2.02  | 1.39        | 1.36     |
| 10  | I     | 302 | HEM  | CHC-C1C | 2.02  | 1.39        | 1.36     |

All (123) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | L     | 302 | HEM  | C3B-C4B-NB  | -6.89 | 109.07      | 114.00   |
| 10  | C     | 301 | HEM  | C3B-C4B-NB  | -6.87 | 109.08      | 114.00   |
| 10  | I     | 301 | HEM  | C3B-C4B-NB  | -6.87 | 109.08      | 114.00   |
| 10  | F     | 302 | HEM  | C3B-C4B-NB  | -6.86 | 109.09      | 114.00   |
| 10  | I     | 301 | HEM  | CBA-CAA-C2A | 6.11  | 123.46      | 112.69   |
| 10  | L     | 302 | HEM  | CBA-CAA-C2A | 6.11  | 123.45      | 112.69   |
| 10  | C     | 301 | HEM  | CBA-CAA-C2A | 6.10  | 123.44      | 112.69   |
| 4   | G     | 701 | FAD  | C1'-N10-C9A | -6.10 | 112.94      | 118.87   |
| 4   | D     | 701 | FAD  | C1'-N10-C9A | -6.09 | 112.95      | 118.87   |
| 10  | F     | 302 | HEM  | CBA-CAA-C2A | 6.09  | 123.42      | 112.69   |
| 4   | A     | 701 | FAD  | C1'-N10-C9A | -6.08 | 112.96      | 118.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | J     | 701 | FAD  | C1'-N10-C9A | -6.07 | 112.97      | 118.87   |
| 10  | I     | 302 | HEM  | C3B-C4B-NB  | -6.05 | 109.67      | 114.00   |
| 10  | C     | 302 | HEM  | C3B-C4B-NB  | -6.00 | 109.70      | 114.00   |
| 10  | F     | 303 | HEM  | C3B-C4B-NB  | -5.97 | 109.73      | 114.00   |
| 10  | L     | 303 | HEM  | C3B-C4B-NB  | -5.92 | 109.76      | 114.00   |
| 4   | D     | 701 | FAD  | O4B-C1B-N9A | -5.65 | 103.18      | 108.44   |
| 4   | A     | 701 | FAD  | O4B-C1B-N9A | -5.61 | 103.22      | 108.44   |
| 4   | G     | 701 | FAD  | O4B-C1B-N9A | -5.61 | 103.22      | 108.44   |
| 4   | J     | 701 | FAD  | O4B-C1B-N9A | -5.58 | 103.25      | 108.44   |
| 4   | J     | 701 | FAD  | C2-N1-C10   | 5.30  | 120.32      | 114.98   |
| 4   | A     | 701 | FAD  | C2-N1-C10   | 5.30  | 120.32      | 114.98   |
| 4   | G     | 701 | FAD  | C2-N1-C10   | 5.30  | 120.31      | 114.98   |
| 4   | D     | 701 | FAD  | C2-N1-C10   | 5.29  | 120.31      | 114.98   |
| 4   | D     | 701 | FAD  | C1'-N10-C10 | 5.24  | 126.60      | 119.17   |
| 4   | G     | 701 | FAD  | C1'-N10-C10 | 5.23  | 126.59      | 119.17   |
| 4   | J     | 701 | FAD  | C1'-N10-C10 | 5.22  | 126.58      | 119.17   |
| 4   | A     | 701 | FAD  | C1'-N10-C10 | 5.21  | 126.56      | 119.17   |
| 10  | I     | 302 | HEM  | CBA-CAA-C2A | 4.63  | 120.84      | 112.69   |
| 10  | C     | 302 | HEM  | CBA-CAA-C2A | 4.63  | 120.84      | 112.69   |
| 10  | L     | 303 | HEM  | CBA-CAA-C2A | 4.62  | 120.82      | 112.69   |
| 10  | F     | 303 | HEM  | CBA-CAA-C2A | 4.60  | 120.80      | 112.69   |
| 11  | L     | 301 | LMT  | C1-O1'-C1'  | 4.44  | 121.95      | 113.96   |
| 11  | I     | 303 | LMT  | C1-O1'-C1'  | 4.43  | 121.93      | 113.96   |
| 11  | F     | 301 | LMT  | C1-O1'-C1'  | 4.43  | 121.93      | 113.96   |
| 11  | C     | 303 | LMT  | C1-O1'-C1'  | 4.43  | 121.93      | 113.96   |
| 4   | A     | 701 | FAD  | C4X-C10-N10 | -4.39 | 118.32      | 120.51   |
| 4   | G     | 701 | FAD  | C4X-C10-N10 | -4.34 | 118.34      | 120.51   |
| 4   | J     | 701 | FAD  | C4X-C10-N10 | -4.33 | 118.35      | 120.51   |
| 4   | D     | 701 | FAD  | C4X-C10-N10 | -4.33 | 118.35      | 120.51   |
| 10  | F     | 302 | HEM  | C2D-C1D-ND  | -3.79 | 108.45      | 112.93   |
| 10  | C     | 301 | HEM  | C2D-C1D-ND  | -3.79 | 108.46      | 112.93   |
| 10  | L     | 303 | HEM  | C2D-C1D-ND  | -3.78 | 108.47      | 112.93   |
| 10  | I     | 301 | HEM  | C2D-C1D-ND  | -3.77 | 108.48      | 112.93   |
| 10  | L     | 302 | HEM  | C2D-C1D-ND  | -3.77 | 108.48      | 112.93   |
| 10  | F     | 303 | HEM  | C2D-C1D-ND  | -3.75 | 108.50      | 112.93   |
| 10  | C     | 302 | HEM  | C2D-C1D-ND  | -3.75 | 108.50      | 112.93   |
| 10  | I     | 302 | HEM  | C2D-C1D-ND  | -3.73 | 108.53      | 112.93   |
| 4   | J     | 701 | FAD  | C4X-C10-N1  | -3.33 | 119.40      | 122.73   |
| 4   | A     | 701 | FAD  | C4X-C10-N1  | -3.31 | 119.43      | 122.73   |
| 4   | G     | 701 | FAD  | C4X-C10-N1  | -3.30 | 119.43      | 122.73   |
| 4   | D     | 701 | FAD  | C4X-C10-N1  | -3.29 | 119.45      | 122.73   |
| 4   | J     | 701 | FAD  | C5'-C4'-C3' | -3.23 | 105.97      | 112.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | A     | 701 | FAD  | C5'-C4'-C3' | -3.23 | 105.97      | 112.06   |
| 4   | G     | 701 | FAD  | C5'-C4'-C3' | -3.22 | 105.98      | 112.06   |
| 4   | D     | 701 | FAD  | C5'-C4'-C3' | -3.21 | 106.00      | 112.06   |
| 11  | I     | 303 | LMT  | C3'-C4'-C5' | -3.13 | 103.82      | 110.85   |
| 11  | L     | 301 | LMT  | C3'-C4'-C5' | -3.13 | 103.83      | 110.85   |
| 11  | F     | 301 | LMT  | C3'-C4'-C5' | -3.12 | 103.84      | 110.85   |
| 11  | C     | 303 | LMT  | C3'-C4'-C5' | -3.11 | 103.86      | 110.85   |
| 4   | D     | 701 | FAD  | N3A-C2A-N1A | -2.85 | 126.33      | 128.71   |
| 4   | A     | 701 | FAD  | N3A-C2A-N1A | -2.84 | 126.33      | 128.71   |
| 4   | J     | 701 | FAD  | N3A-C2A-N1A | -2.82 | 126.35      | 128.71   |
| 4   | G     | 701 | FAD  | N3A-C2A-N1A | -2.78 | 126.38      | 128.71   |
| 11  | F     | 301 | LMT  | O1'-C1'-C2' | -2.72 | 104.72      | 108.18   |
| 11  | I     | 303 | LMT  | O1'-C1'-C2' | -2.71 | 104.73      | 108.18   |
| 11  | L     | 301 | LMT  | O1'-C1'-C2' | -2.71 | 104.73      | 108.18   |
| 11  | C     | 303 | LMT  | O1'-C1'-C2' | -2.71 | 104.73      | 108.18   |
| 4   | G     | 701 | FAD  | N3A-C4A-N9A | 2.62  | 130.16      | 125.43   |
| 10  | L     | 303 | HEM  | C1A-CHA-C4D | -2.62 | 124.03      | 127.47   |
| 4   | A     | 701 | FAD  | N3A-C4A-N9A | 2.61  | 130.15      | 125.43   |
| 4   | D     | 701 | FAD  | N3A-C4A-N9A | 2.60  | 130.12      | 125.43   |
| 4   | J     | 701 | FAD  | N3A-C4A-N9A | 2.59  | 130.10      | 125.43   |
| 10  | C     | 302 | HEM  | C1A-CHA-C4D | -2.55 | 124.12      | 127.47   |
| 10  | F     | 303 | HEM  | C1A-CHA-C4D | -2.54 | 124.13      | 127.47   |
| 10  | I     | 302 | HEM  | C1A-CHA-C4D | -2.50 | 124.18      | 127.47   |
| 4   | A     | 701 | FAD  | N1-C10-N10  | 2.39  | 122.25      | 115.97   |
| 4   | J     | 701 | FAD  | N1-C10-N10  | 2.39  | 122.24      | 115.97   |
| 4   | G     | 701 | FAD  | N1-C10-N10  | 2.38  | 122.22      | 115.97   |
| 4   | D     | 701 | FAD  | N1-C10-N10  | 2.37  | 122.19      | 115.97   |
| 4   | D     | 701 | FAD  | O3P-P-O5'   | 2.32  | 113.80      | 103.41   |
| 4   | G     | 701 | FAD  | O3P-P-O5'   | 2.32  | 113.78      | 103.41   |
| 4   | A     | 701 | FAD  | O3P-P-O5'   | 2.32  | 113.77      | 103.41   |
| 4   | J     | 701 | FAD  | O3P-P-O5'   | 2.31  | 113.73      | 103.41   |
| 10  | I     | 302 | HEM  | CMA-C3A-C4A | -2.26 | 125.14      | 128.62   |
| 10  | C     | 302 | HEM  | CMA-C3A-C4A | -2.26 | 125.15      | 128.62   |
| 10  | L     | 303 | HEM  | CMA-C3A-C4A | -2.26 | 125.15      | 128.62   |
| 10  | F     | 303 | HEM  | CMA-C3A-C4A | -2.24 | 125.18      | 128.62   |
| 10  | L     | 302 | HEM  | CMA-C3A-C4A | -2.21 | 125.22      | 128.62   |
| 4   | G     | 701 | FAD  | O4B-C1B-C2B | -2.19 | 103.42      | 106.77   |
| 4   | A     | 701 | FAD  | O4B-C1B-C2B | -2.19 | 103.42      | 106.77   |
| 4   | D     | 701 | FAD  | C4-N3-C2    | -2.18 | 120.91      | 125.39   |
| 10  | C     | 301 | HEM  | CMA-C3A-C4A | -2.18 | 125.27      | 128.62   |
| 4   | D     | 701 | FAD  | O4B-C1B-C2B | -2.18 | 103.43      | 106.77   |
| 4   | J     | 701 | FAD  | O4B-C1B-C2B | -2.18 | 103.44      | 106.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | I     | 301 | HEM  | CMA-C3A-C4A | -2.17 | 125.28      | 128.62   |
| 10  | F     | 302 | HEM  | CHA-C4D-ND  | 2.17  | 127.28      | 124.31   |
| 4   | J     | 701 | FAD  | C4-N3-C2    | -2.16 | 120.95      | 125.39   |
| 10  | F     | 302 | HEM  | CMA-C3A-C4A | -2.16 | 125.30      | 128.62   |
| 4   | A     | 701 | FAD  | C4-N3-C2    | -2.15 | 120.98      | 125.39   |
| 4   | G     | 701 | FAD  | C4-N3-C2    | -2.15 | 120.98      | 125.39   |
| 10  | C     | 301 | HEM  | CHA-C4D-ND  | 2.15  | 127.26      | 124.31   |
| 11  | F     | 301 | LMT  | O1B-C4'-C3' | 2.15  | 112.67      | 107.16   |
| 11  | L     | 301 | LMT  | O1B-C4'-C3' | 2.14  | 112.66      | 107.16   |
| 4   | D     | 701 | FAD  | C4B-O4B-C1B | -2.14 | 107.42      | 109.75   |
| 11  | I     | 303 | LMT  | O1B-C4'-C3' | 2.14  | 112.66      | 107.16   |
| 11  | C     | 303 | LMT  | O1B-C4'-C3' | 2.14  | 112.64      | 107.16   |
| 10  | L     | 302 | HEM  | CHA-C4D-ND  | 2.13  | 127.24      | 124.31   |
| 4   | A     | 701 | FAD  | C4B-O4B-C1B | -2.12 | 107.45      | 109.75   |
| 4   | J     | 701 | FAD  | C4B-O4B-C1B | -2.11 | 107.46      | 109.75   |
| 4   | G     | 701 | FAD  | C4B-O4B-C1B | -2.10 | 107.47      | 109.75   |
| 10  | I     | 301 | HEM  | CHA-C4D-ND  | 2.10  | 127.19      | 124.31   |
| 4   | D     | 701 | FAD  | C2A-N1A-C6A | 2.07  | 122.50      | 118.77   |
| 4   | A     | 701 | FAD  | C2A-N1A-C6A | 2.06  | 122.49      | 118.77   |
| 4   | J     | 701 | FAD  | C2A-N1A-C6A | 2.05  | 122.47      | 118.77   |
| 4   | G     | 701 | FAD  | C2A-N1A-C6A | 2.05  | 122.46      | 118.77   |
| 10  | I     | 301 | HEM  | CHD-C1D-ND  | 2.04  | 126.28      | 124.58   |
| 10  | C     | 301 | HEM  | CHD-C1D-ND  | 2.03  | 126.27      | 124.58   |
| 10  | F     | 302 | HEM  | CHD-C1D-ND  | 2.03  | 126.27      | 124.58   |
| 4   | G     | 701 | FAD  | C5A-C4A-N9A | -2.03 | 104.23      | 107.16   |
| 4   | D     | 701 | FAD  | C5A-C4A-N9A | -2.03 | 104.23      | 107.16   |
| 4   | A     | 701 | FAD  | C5A-C4A-N9A | -2.03 | 104.24      | 107.16   |
| 4   | J     | 701 | FAD  | C5A-C4A-N9A | -2.01 | 104.26      | 107.16   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.