



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:50 PM GMT

PDB ID : 3S27  
Title : The crystal structure of sucrose synthase-1 from Arabidopsis thaliana and its functional implications.  
Authors : Zheng, Y.; Garavito, R.M.  
Deposited on : 2011-05-16  
Resolution : 2.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

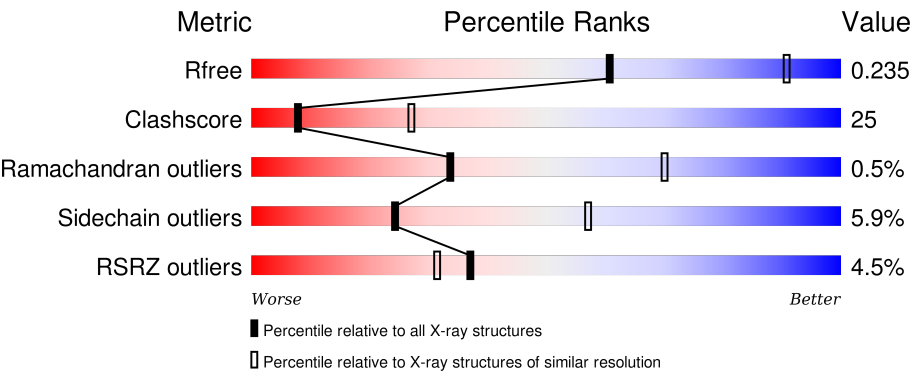
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1643 (2.94-2.90)                                      |
| Clashscore            | 102246                      | 1871 (2.94-2.90)                                      |
| Ramachandran outliers | 100387                      | 1824 (2.94-2.90)                                      |
| Sidechain outliers    | 100360                      | 1826 (2.94-2.90)                                      |
| RSRZ outliers         | 91569                       | 1650 (2.94-2.90)                                      |

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 816    | <div><div>4%</div><div><div></div><div>58%</div><div>34%</div><div></div><div></div></div><div></div></div> |
| 1   | B     | 816    | <div><div>7%</div><div><div></div><div>58%</div><div>36%</div><div></div><div></div></div><div></div></div> |
| 1   | C     | 816    | <div><div>3%</div><div><div></div><div>54%</div><div>38%</div><div></div><div></div></div><div></div></div> |
| 1   | D     | 816    | <div><div>3%</div><div><div></div><div>60%</div><div>34%</div><div></div><div></div></div><div></div></div> |
| 1   | E     | 816    | <div><div>4%</div><div><div></div><div>60%</div><div>31%</div><div></div><div></div></div><div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 816    |                  |
| 1   | G     | 816    |                  |
| 1   | H     | 816    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | SO4  | A     | 911 | -         | -        | -       | X                |
| 4   | SO4  | B     | 913 | -         | -        | X       | X                |
| 4   | SO4  | D     | 911 | -         | -        | -       | X                |
| 4   | SO4  | E     | 913 | -         | -        | -       | X                |
| 4   | SO4  | F     | 911 | -         | -        | -       | X                |
| 4   | SO4  | F     | 913 | -         | -        | X       | -                |
| 4   | SO4  | G     | 911 | -         | -        | -       | X                |
| 4   | SO4  | H     | 913 | -         | -        | -       | X                |
| 5   | MLA  | B     | 921 | -         | -        | -       | X                |
| 5   | MLA  | C     | 921 | -         | -        | -       | X                |
| 5   | MLA  | D     | 921 | -         | -        | -       | X                |
| 5   | MLA  | E     | 921 | -         | -        | X       | X                |
| 5   | MLA  | F     | 921 | -         | -        | -       | X                |
| 5   | MLA  | G     | 921 | -         | -        | -       | X                |
| 5   | MLA  | H     | 921 | -         | -        | -       | X                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 51483 atoms, of which 200 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sucrose synthase 1.

| Mol | Chain | Residues | Atoms |      |      |      |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|----|---------|---------|-------|
| 1   | A     | 781      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6277  | 4031 | 1065 | 1159 | 10 | 12 |         |         |       |
| 1   | B     | 793      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6313  | 4046 | 1074 | 1171 | 10 | 12 |         |         |       |
| 1   | C     | 781      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6268  | 4028 | 1064 | 1154 | 10 | 12 |         |         |       |
| 1   | D     | 781      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6243  | 4014 | 1059 | 1148 | 10 | 12 |         |         |       |
| 1   | E     | 781      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6249  | 4014 | 1061 | 1152 | 10 | 12 |         |         |       |
| 1   | F     | 781      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6275  | 4031 | 1064 | 1158 | 10 | 12 |         |         |       |
| 1   | G     | 781      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6279  | 4032 | 1068 | 1157 | 10 | 12 |         |         |       |
| 1   | H     | 797      | Total | C    | N    | O    | S  | Se | 0       | 0       | 0     |
|     |       |          | 6336  | 4060 | 1087 | 1167 | 10 | 12 |         |         |       |

There are 64 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| A     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| A     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| A     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| A     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| A     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| A     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| A     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| B     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| B     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| B     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| B     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| B     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |

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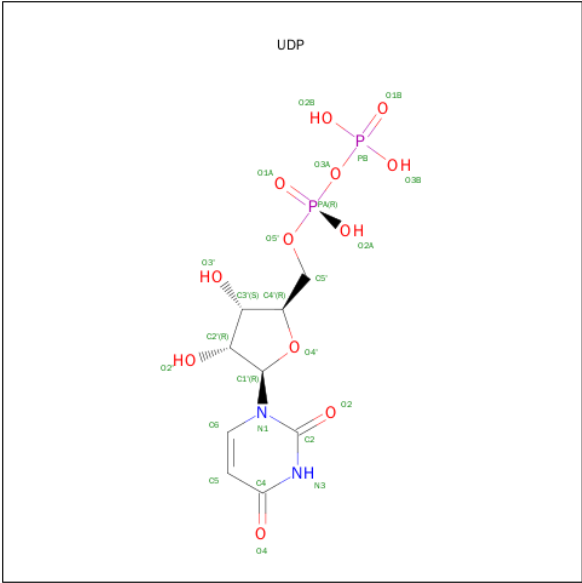
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| B     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| B     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| C     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| D     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| E     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| F     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| G     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| G     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| G     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| G     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| G     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| G     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| G     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 809     | VAL      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 810     | GLU      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 811     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 812     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 813     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 814     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 815     | HIS      | -      | EXPRESSION TAG | UNP P49040 |
| H     | 816     | HIS      | -      | EXPRESSION TAG | UNP P49040 |

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



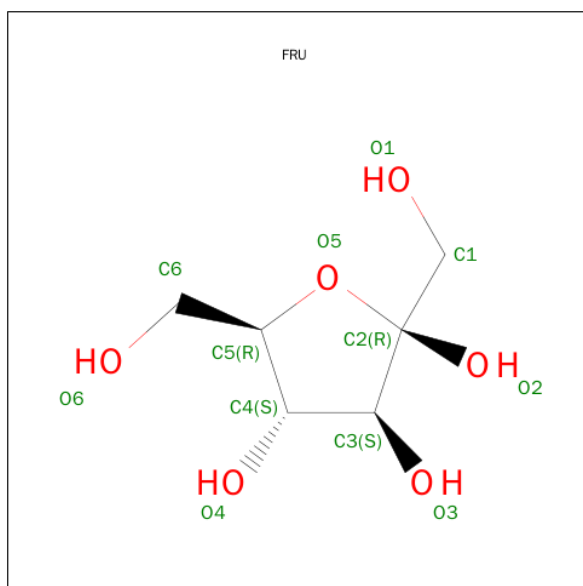
| Mol | Chain | Residues | Atoms |   |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2 |         |         |
| 2   | B     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2 |         |         |
| 2   | C     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2 |         |         |
| 2   | D     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2 |         |         |
| 2   | E     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2 |         |         |
| 2   | F     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2 |         |         |
| 2   | G     | 1        | Total | C | H  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|----|---------|---------|
| 2   | H     | 1        | Total | C | H  | N | O  | P       |         |
|     |       |          | 36    | 9 | 11 | 2 | 12 | 2       |         |
|     |       |          |       |   |    |   |    | 0       | 0       |

- Molecule 3 is SUGAR (FRUCTOSE) (three-letter code: FRU) (formula:  $C_6H_{12}O_6$ ).



| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |
| 3   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |
| 3   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |
| 3   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |
| 3   | E     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |
| 3   | F     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |
| 3   | G     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |
| 3   | H     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 24    | 6 | 12 | 6 |         |         |

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

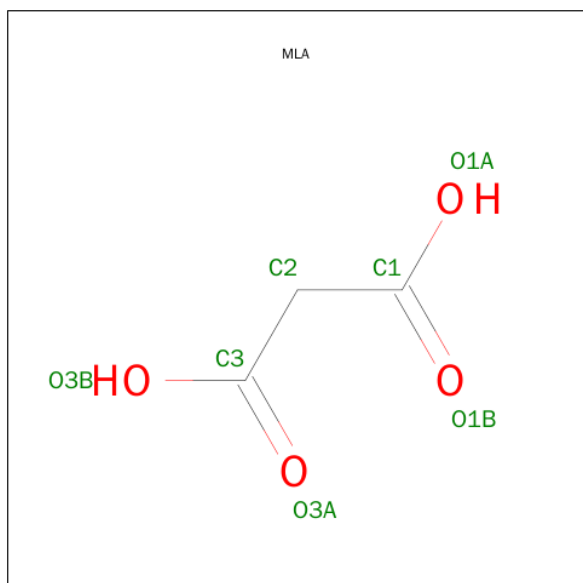
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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- 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 | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | B     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 5   | C     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 5   | D     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 5   | E     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 5   | F     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 5   | G     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 5   | H     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6   | G     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | D     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | E     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | H     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | B     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | C     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | A     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | F     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 7 is water.

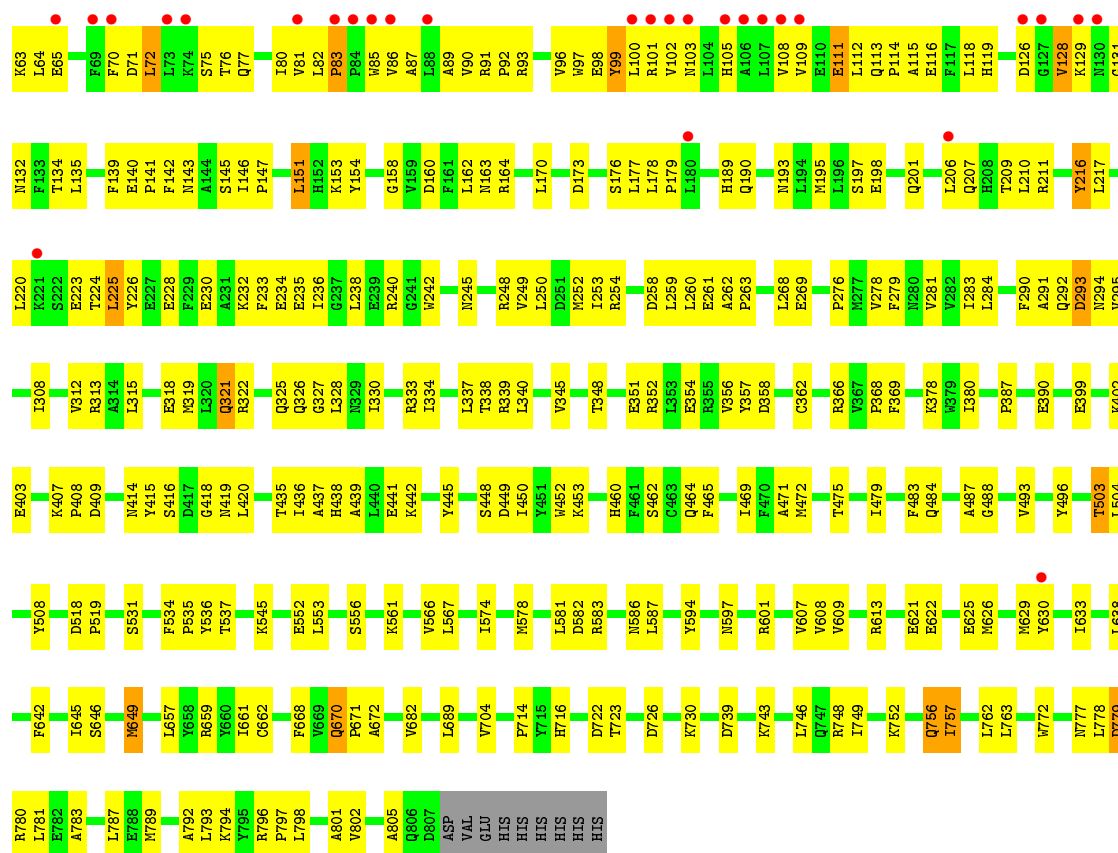
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | A     | 82       | Total | O  | 0       | 0       |
|     |       |          | 82    | 82 |         |         |
| 7   | B     | 72       | Total | O  | 0       | 0       |
|     |       |          | 72    | 72 |         |         |

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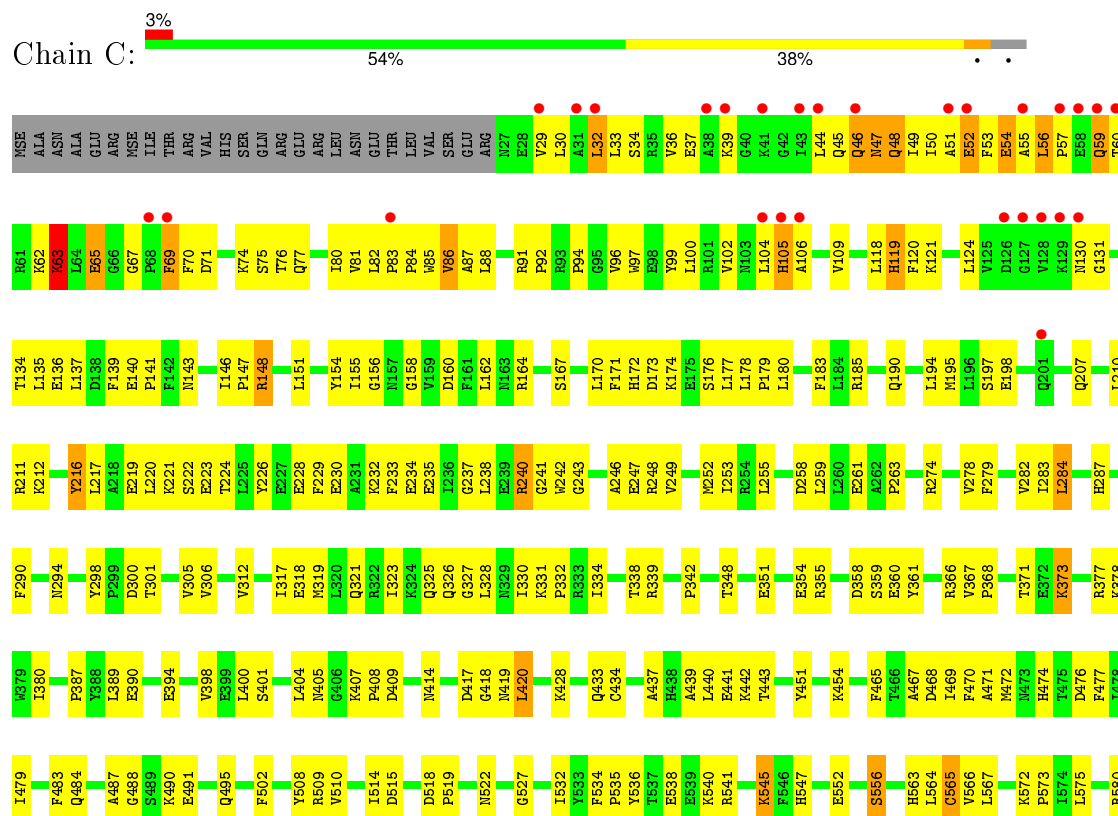
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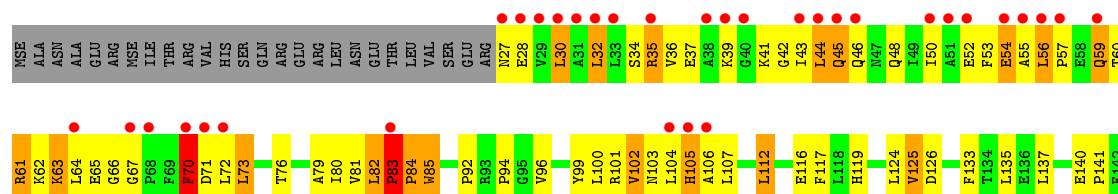
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 7   | C     | 45       | Total<br>45 | O<br>45 | 0       | 0       |
| 7   | D     | 67       | Total<br>67 | O<br>67 | 0       | 0       |
| 7   | E     | 66       | Total<br>66 | O<br>66 | 0       | 0       |
| 7   | F     | 90       | Total<br>90 | O<br>90 | 0       | 0       |
| 7   | G     | 81       | Total<br>81 | O<br>81 | 0       | 0       |
| 7   | H     | 60       | Total<br>60 | O<br>60 | 0       | 0       |

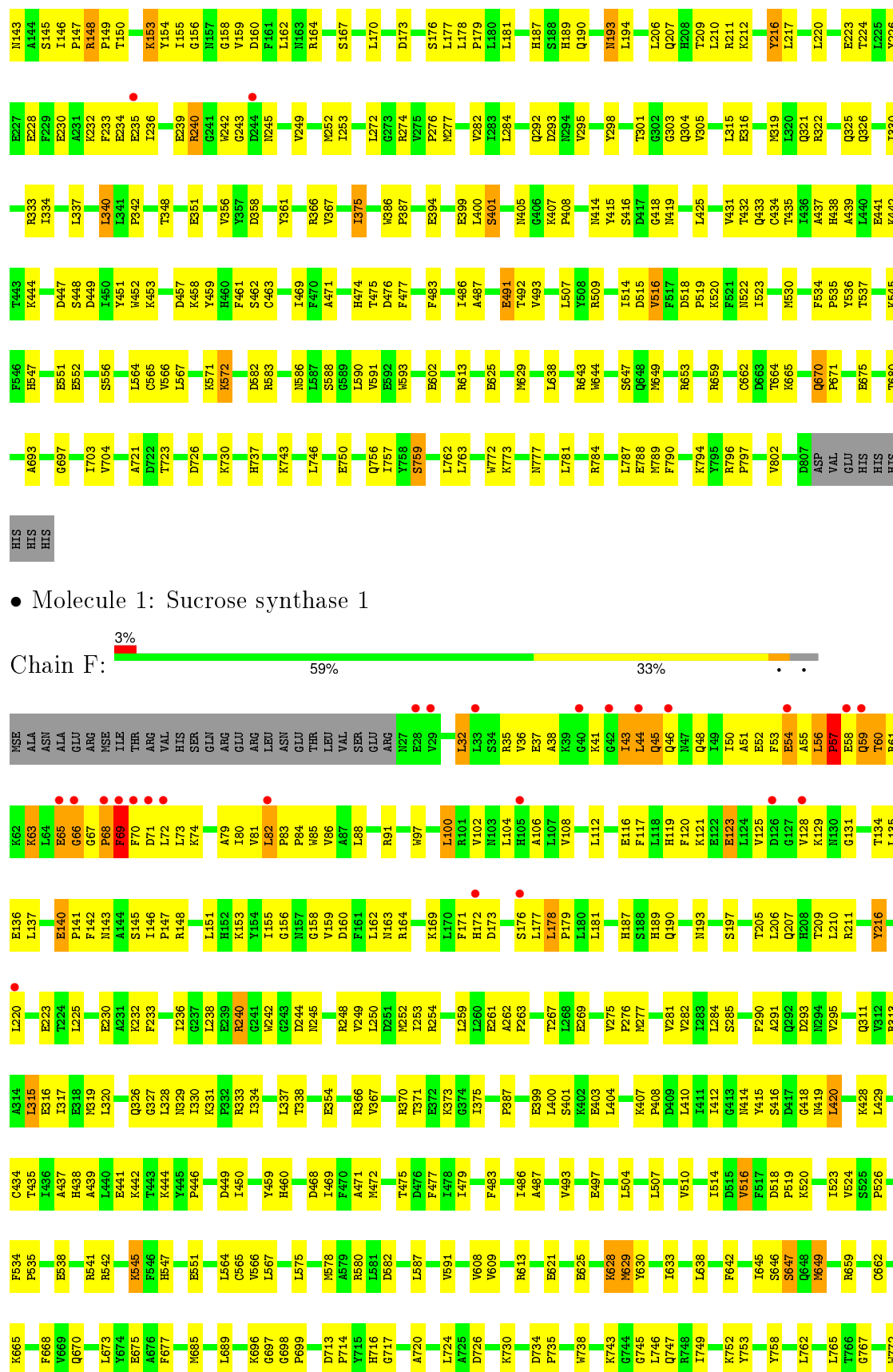




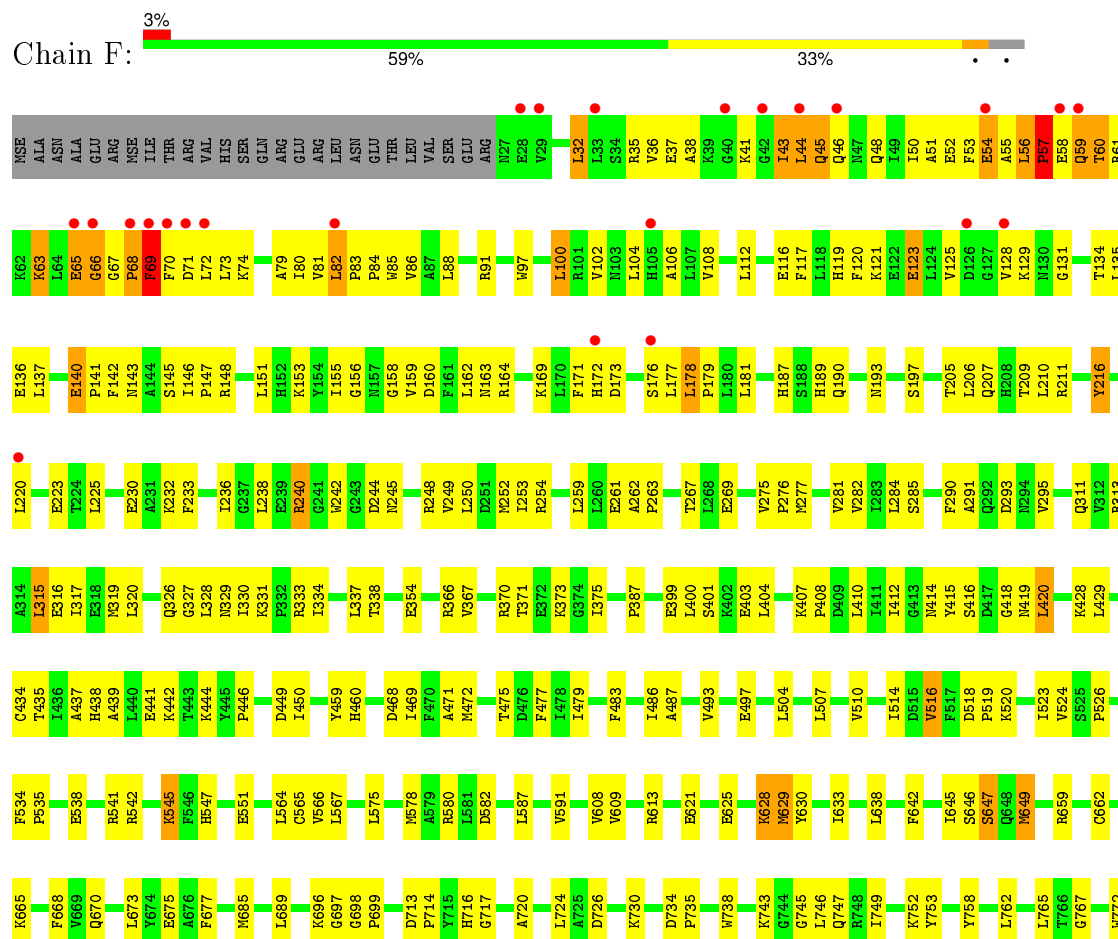
• Molecule 1: Sucrose synthase 1

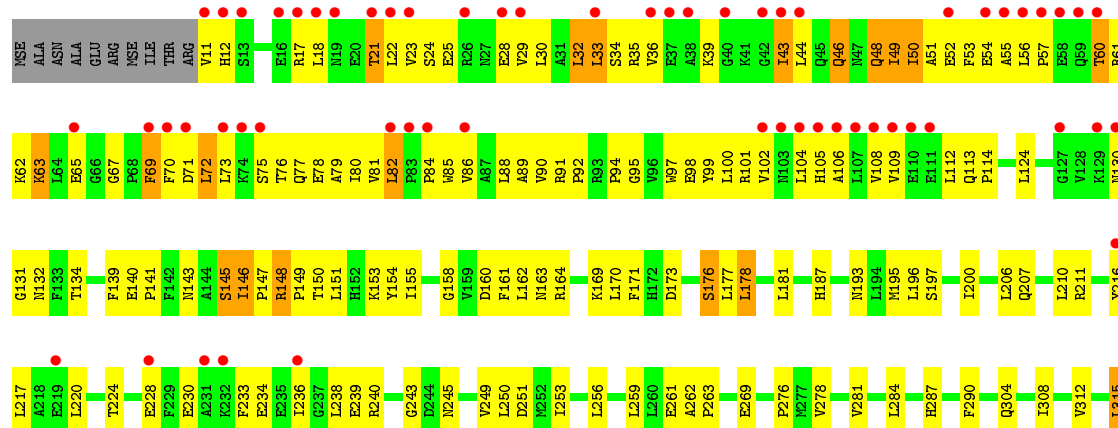






• Molecule 1: Sucrose synthase 1







|      |      |      |      |      |
|------|------|------|------|------|
| Y791 | A672 | L553 | A437 | K319 |
| A792 | E675 | S556 | H438 | R322 |
| L793 | A676 | K561 | A439 | I323 |
| K794 | F677 | E562 | K444 | Q326 |
| Y795 | G678 | H563 | D449 | I336 |
| R796 | L679 | L564 | I450 | L337 |
| P797 | T680 | C565 | W452 | T338 |
| V802 | V681 | V566 | K453 | R339 |
| D807 | V682 | K572 | T466 | Y345 |
| ASP  | A684 | V584 | M472 | T348 |
| VAL  | H685 | S588 | T475 | E351 |
| GLU  | I689 | G589 | D476 | R352 |
| HIS  | F692 | L590 | S481 | L353 |
| HIS  | A693 | K596 | T482 | E354 |
| HIS  | T694 | R599 | F483 | R355 |
| HIS  | G697 | V609 | I486 | S359 |
| HIS  | G698 | R613 | A487 | L365 |
| HIS  | P699 | K614 | T492 | R366 |
|      | H705 | K615 | V493 | V367 |
|      | Q719 | E616 | T503 | P368 |
|      | D726 | S617 | L504 | I375 |
|      | E743 | K623 | Y508 | K378 |
|      | R748 | A624 | H512 | P387 |
|      | I749 | E525 | G513 | E390 |
|      | E750 | M626 | I514 | L400 |
|      | E761 | M629 | D515 | K407 |
|      | K762 | Y630 | F517 | P408 |
|      | L763 | Y636 | D518 | I411 |
|      | T757 | G640 | K520 | M414 |
|      | Y758 | Q641 | A528 | Y414 |
|      | S759 | F642 | I532 | S416 |
|      | Q760 | I645 | Y533 | D417 |
|      | R761 | R651 | F534 | O418 |
|      | L762 | L657 | P535 | M419 |
|      | L763 | Y658 | E538 | L425 |
|      | T766 | R659 | E539 | V431 |
|      | W772 | I661 | K540 | T432 |
|      | D779 | C662 | R541 | Q433 |
|      | E782 | F668 | R542 | C434 |
|      | A783 | V669 | K545 | T435 |
|      | R784 | Q670 | E552 | I436 |
|      | L787 | P671 |      |      |
|      | E788 |      |      |      |
|      | M789 |      |      |      |
|      | F790 |      |      |      |

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 276.21 Å   263.70 Å   159.66 Å<br>90.00°   108.80°   90.00° | Depositor        |
| Resolution (Å)  | 25.00 – 2.91<br>49.68 – 2.91                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.0 (25.00-2.91)<br>90.8 (49.68-2.91)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.18  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.75 (at 2.91 Å)  | Xtriage          |
| Refinement program  | PHENIX (PHENIX.REFINE: 1.7_650)                             | Depositor        |
| R, $R_{free}$   | 0.186   ,   0.237<br>0.186   ,   0.235                      | Depositor<br>DCC |
| $R_{free}$ test set   | 11567 reflections (5.68%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 35.1  | Xtriage          |
| Anisotropy  | 0.252   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33   ,   45.1   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 5 of 231037 reflections (0.002%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 51483   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 36.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.21 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7500e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, MLA, K, FRU, SO4

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     | 0.40         | 0/6412  | 0.56        | 0/8664  |
| 1   | B     | 0.37         | 0/6447  | 0.55        | 0/8717  |
| 1   | C     | 0.36         | 0/6403  | 0.55        | 0/8654  |
| 1   | D     | 0.39         | 0/6378  | 0.57        | 0/8624  |
| 1   | E     | 0.39         | 0/6383  | 0.56        | 0/8629  |
| 1   | F     | 0.41         | 0/6410  | 0.59        | 0/8663  |
| 1   | G     | 0.38         | 0/6414  | 0.56        | 0/8667  |
| 1   | H     | 0.37         | 0/6471  | 0.55        | 0/8749  |
| All | All   | 0.38         | 0/51318 | 0.56        | 0/69367 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 2                   |
| 1   | F     | 0                   | 3                   |
| 1   | G     | 0                   | 1                   |
| All | All   | 0                   | 9                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 83  | PRO  | Peptide |
| 1   | C     | 47  | ASN  | Peptide |
| 1   | D     | 56  | LEU  | Peptide |
| 1   | E     | 70  | PHE  | Peptide |
| 1   | E     | 83  | PRO  | Peptide |
| 1   | F     | 106 | ALA  | Peptide |
| 1   | F     | 57  | PRO  | Peptide |
| 1   | F     | 66  | GLY  | Peptide |
| 1   | G     | 68  | PRO  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6277  | 0        | 6191     | 319     | 0            |
| 1   | B     | 6313  | 0        | 6170     | 321     | 0            |
| 1   | C     | 6268  | 0        | 6189     | 314     | 0            |
| 1   | D     | 6243  | 0        | 6143     | 311     | 0            |
| 1   | E     | 6249  | 0        | 6158     | 348     | 0            |
| 1   | F     | 6275  | 0        | 6195     | 360     | 0            |
| 1   | G     | 6279  | 0        | 6201     | 329     | 0            |
| 1   | H     | 6336  | 0        | 6196     | 308     | 0            |
| 2   | A     | 25    | 11       | 11       | 0       | 0            |
| 2   | B     | 25    | 11       | 11       | 0       | 0            |
| 2   | C     | 25    | 11       | 11       | 1       | 0            |
| 2   | D     | 25    | 11       | 11       | 2       | 0            |
| 2   | E     | 25    | 11       | 11       | 4       | 0            |
| 2   | F     | 25    | 11       | 11       | 1       | 0            |
| 2   | G     | 25    | 11       | 11       | 1       | 0            |
| 2   | H     | 25    | 11       | 11       | 0       | 0            |
| 3   | A     | 12    | 12       | 12       | 1       | 0            |
| 3   | B     | 12    | 12       | 12       | 0       | 0            |
| 3   | C     | 12    | 12       | 12       | 1       | 0            |
| 3   | D     | 12    | 12       | 12       | 0       | 0            |
| 3   | E     | 12    | 12       | 12       | 1       | 0            |
| 3   | F     | 12    | 12       | 12       | 1       | 0            |
| 3   | G     | 12    | 12       | 12       | 4       | 0            |
| 3   | H     | 12    | 12       | 12       | 1       | 0            |
| 4   | A     | 15    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 15    | 0        | 0        | 3       | 0            |
| 4   | C     | 15    | 0        | 0        | 0       | 0            |
| 4   | D     | 15    | 0        | 0        | 0       | 0            |
| 4   | E     | 15    | 0        | 0        | 1       | 0            |
| 4   | F     | 15    | 0        | 0        | 2       | 0            |
| 4   | G     | 15    | 0        | 0        | 1       | 0            |
| 4   | H     | 15    | 0        | 0        | 1       | 0            |
| 5   | A     | 7     | 2        | 2        | 0       | 0            |
| 5   | B     | 7     | 2        | 2        | 1       | 0            |
| 5   | C     | 7     | 2        | 2        | 0       | 0            |
| 5   | D     | 7     | 2        | 2        | 0       | 0            |
| 5   | E     | 7     | 2        | 2        | 5       | 0            |
| 5   | F     | 7     | 2        | 2        | 0       | 0            |
| 5   | G     | 7     | 2        | 2        | 0       | 0            |
| 5   | H     | 7     | 2        | 2        | 0       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 1     | 0        | 0        | 0       | 0            |
| 6   | G     | 1     | 0        | 0        | 0       | 0            |
| 6   | H     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 82    | 0        | 0        | 5       | 0            |
| 7   | B     | 72    | 0        | 0        | 7       | 0            |
| 7   | C     | 45    | 0        | 0        | 3       | 0            |
| 7   | D     | 67    | 0        | 0        | 3       | 0            |
| 7   | E     | 66    | 0        | 0        | 2       | 0            |
| 7   | F     | 90    | 0        | 0        | 10      | 0            |
| 7   | G     | 81    | 0        | 0        | 5       | 0            |
| 7   | H     | 60    | 0        | 0        | 6       | 0            |
| All | All   | 51283 | 200      | 49643    | 2497    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:C:83:PRO:HG2  | 1:C:84:PRO:HD3 | 1.22                     | 1.19              |
| 1:G:82:LEU:HD12 | 1:G:83:PRO:CG  | 1.72                     | 1.18              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:83:PRO:HG2   | 1:B:85:TRP:HB2   | 1.19                     | 1.16              |
| 1:G:65:GLU:HB3   | 1:G:70:PHE:CD1   | 1.79                     | 1.16              |
| 1:A:789:MSE:CE   | 1:D:789:MSE:HB3  | 1.76                     | 1.14              |
| 1:F:319:MSE:CE   | 1:F:334:ILE:HD11 | 1.78                     | 1.14              |
| 1:G:65:GLU:HB3   | 1:G:70:PHE:HD1   | 0.96                     | 1.13              |
| 1:C:681:VAL:HG12 | 1:C:685:MSE:CE   | 1.79                     | 1.13              |
| 1:G:83:PRO:HG2   | 1:G:85:TRP:HB2   | 1.20                     | 1.12              |
| 1:E:315:LEU:HG   | 1:E:319:MSE:HE2  | 1.29                     | 1.12              |
| 1:E:45:GLN:HB3   | 1:E:80:ILE:HA    | 1.27                     | 1.12              |
| 1:H:17:ARG:NH2   | 1:H:72:LEU:HB3   | 1.63                     | 1.12              |
| 1:D:56:LEU:HD12  | 1:D:57:PRO:HD3   | 1.31                     | 1.11              |
| 1:E:148:ARG:HH11 | 1:E:148:ARG:HG3  | 1.14                     | 1.11              |
| 1:E:46:GLN:HB3   | 1:E:50:ILE:HB    | 1.16                     | 1.10              |
| 1:C:148:ARG:HH11 | 1:C:148:ARG:HG2  | 0.93                     | 1.09              |
| 1:B:72:LEU:HD13  | 1:B:90:VAL:HG11  | 1.26                     | 1.09              |
| 1:F:316:GLU:HA   | 1:F:319:MSE:HE3  | 1.29                     | 1.09              |
| 1:F:53:PHE:CA    | 1:F:57:PRO:HG2   | 1.81                     | 1.09              |
| 1:C:48:GLN:HG3   | 1:C:76:THR:O     | 1.50                     | 1.09              |
| 1:B:583:ARG:HA   | 1:B:625:GLU:OE1  | 1.51                     | 1.09              |
| 1:H:146:ILE:HG12 | 1:H:147:PRO:HD2  | 1.33                     | 1.08              |
| 1:F:469:ILE:HD13 | 1:F:472:MSE:HE1  | 1.28                     | 1.08              |
| 1:F:469:ILE:HD13 | 1:F:472:MSE:CE   | 1.85                     | 1.07              |
| 1:A:45:GLN:HA    | 1:A:45:GLN:HE21  | 0.91                     | 1.07              |
| 1:A:103:ASN:CB   | 1:A:106:ALA:HB3  | 1.83                     | 1.07              |
| 1:E:789:MSE:HE2  | 1:H:789:MSE:CE   | 1.85                     | 1.07              |
| 1:C:681:VAL:HG12 | 1:C:685:MSE:HE3  | 1.30                     | 1.06              |
| 1:F:53:PHE:HA    | 1:F:57:PRO:HG2   | 1.10                     | 1.05              |
| 1:E:789:MSE:HE2  | 1:H:789:MSE:HE2  | 1.37                     | 1.05              |
| 1:G:82:LEU:HD12  | 1:G:83:PRO:HG3   | 1.13                     | 1.05              |
| 1:B:82:LEU:CB    | 1:B:83:PRO:HD2   | 1.86                     | 1.05              |
| 1:H:46:GLN:HB3   | 1:H:51:ALA:HB2   | 1.39                     | 1.05              |
| 1:C:54:GLU:HG3   | 1:C:55:ALA:N     | 1.70                     | 1.05              |
| 1:G:276:PRO:HG3  | 1:G:326:GLN:HG3  | 1.37                     | 1.04              |
| 1:G:82:LEU:CD1   | 1:G:83:PRO:HG3   | 1.85                     | 1.04              |
| 1:A:45:GLN:HA    | 1:A:45:GLN:NE2   | 1.73                     | 1.04              |
| 1:B:131:GLY:HA3  | 1:B:134:THR:CG2  | 1.87                     | 1.04              |
| 1:F:789:MSE:CE   | 1:G:789:MSE:HB3  | 1.87                     | 1.04              |
| 1:A:319:MSE:HE1  | 1:A:334:ILE:HD11 | 1.04                     | 1.03              |
| 1:H:39:LYS:HB2   | 1:H:104:LEU:CD2  | 1.67                     | 1.03              |
| 1:E:217:LEU:HD11 | 1:E:233:PHE:HZ   | 1.15                     | 1.03              |
| 1:F:319:MSE:HE1  | 1:F:334:ILE:CD1  | 1.89                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:61:ARG:HG3   | 1:E:61:ARG:HH11  | 1.17                     | 1.03              |
| 1:G:148:ARG:HG2  | 1:G:148:ARG:HH11 | 0.89                     | 1.02              |
| 1:A:789:MSE:HE2  | 1:D:789:MSE:HB3  | 1.38                     | 1.02              |
| 1:B:170:LEU:HD22 | 1:B:177:LEU:HD23 | 1.41                     | 1.01              |
| 1:E:85:TRP:HB3   | 1:E:103:ASN:HA   | 1.42                     | 1.01              |
| 1:F:82:LEU:N     | 1:F:83:PRO:HD3   | 1.73                     | 1.01              |
| 1:C:148:ARG:CG   | 1:C:148:ARG:HH11 | 1.73                     | 1.01              |
| 1:D:298:TYR:CE1  | 1:D:649:MSE:HE1  | 1.96                     | 1.01              |
| 1:H:39:LYS:CB    | 1:H:104:LEU:HD22 | 1.91                     | 1.01              |
| 1:C:50:ILE:HD12  | 1:C:54:GLU:HB3   | 1.42                     | 1.00              |
| 1:C:50:ILE:CD1   | 1:C:54:GLU:HB3   | 1.90                     | 1.00              |
| 1:D:146:ILE:HG23 | 1:D:147:PRO:HD2  | 1.43                     | 1.00              |
| 1:B:92:PRO:HG2   | 1:B:96:VAL:HG23  | 1.43                     | 1.00              |
| 1:B:80:ILE:CG1   | 1:B:87:ALA:HB3   | 1.91                     | 0.99              |
| 1:D:552:GLU:O    | 1:D:556:SER:HB3  | 1.61                     | 0.99              |
| 1:F:469:ILE:HA   | 1:F:472:MSE:HE2  | 1.41                     | 0.99              |
| 1:H:216:TYR:CE1  | 1:H:220:LEU:HD11 | 1.97                     | 0.99              |
| 1:C:32:LEU:O     | 1:C:36:VAL:HG23  | 1.63                     | 0.99              |
| 1:D:217:LEU:HA   | 1:D:220:LEU:HD12 | 1.44                     | 0.98              |
| 1:A:65:GLU:HB3   | 1:A:70:PHE:HB3   | 1.42                     | 0.98              |
| 1:C:681:VAL:O    | 1:C:685:MSE:HG3  | 1.63                     | 0.98              |
| 1:A:373:LYS:N    | 1:A:373:LYS:HD2  | 1.79                     | 0.98              |
| 1:B:99:TYR:CE2   | 1:B:114:PRO:HG3  | 1.98                     | 0.98              |
| 1:H:39:LYS:HB2   | 1:H:104:LEU:HD22 | 0.98                     | 0.97              |
| 1:H:216:TYR:HE1  | 1:H:220:LEU:HD11 | 1.27                     | 0.97              |
| 1:A:195:MSE:HE3  | 1:A:242:TRP:CD2  | 1.99                     | 0.97              |
| 1:B:76:THR:HA    | 1:B:89:ALA:O     | 1.63                     | 0.97              |
| 1:A:319:MSE:CE   | 1:A:334:ILE:HD11 | 1.95                     | 0.97              |
| 1:E:304:GLN:HB3  | 3:E:902:FRU:H12  | 1.46                     | 0.97              |
| 1:B:327:GLY:O    | 1:B:328:LEU:HD23 | 1.64                     | 0.97              |
| 1:C:148:ARG:HG2  | 1:C:148:ARG:NH1  | 1.69                     | 0.96              |
| 1:B:55:ALA:O     | 1:B:59:GLN:HB2   | 1.65                     | 0.96              |
| 1:G:48:GLN:HE21  | 1:G:48:GLN:HA    | 1.30                     | 0.96              |
| 1:C:366:ARG:HD3  | 7:C:821:HOH:O    | 1.65                     | 0.96              |
| 1:G:148:ARG:HG2  | 1:G:148:ARG:NH1  | 1.67                     | 0.96              |
| 1:A:124:LEU:O    | 1:A:124:LEU:HD23 | 1.64                     | 0.95              |
| 1:F:789:MSE:HE2  | 1:G:789:MSE:HB3  | 1.44                     | 0.95              |
| 1:A:45:GLN:HE21  | 1:A:45:GLN:CA    | 1.80                     | 0.94              |
| 1:E:315:LEU:HD11 | 1:E:762:LEU:HD23 | 1.50                     | 0.94              |
| 1:G:366:ARG:HD3  | 7:G:826:HOH:O    | 1.66                     | 0.94              |
| 1:F:319:MSE:HE1  | 1:F:334:ILE:HD11 | 0.96                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:53:PHE:HA    | 1:F:57:PRO:CG    | 1.96                     | 0.94              |
| 1:E:351:GLU:O    | 1:E:366:ARG:HD2  | 1.68                     | 0.94              |
| 1:E:217:LEU:HD11 | 1:E:233:PHE:CZ   | 2.02                     | 0.94              |
| 1:B:99:TYR:HE2   | 1:B:114:PRO:HG3  | 1.28                     | 0.94              |
| 1:F:276:PRO:HG3  | 1:F:326:GLN:HG3  | 1.50                     | 0.94              |
| 1:E:82:LEU:HB3   | 1:E:83:PRO:HD2   | 1.50                     | 0.93              |
| 1:F:48:GLN:HG2   | 7:F:871:HOH:O    | 1.67                     | 0.93              |
| 1:A:319:MSE:HE1  | 1:A:334:ILE:CD1  | 1.98                     | 0.93              |
| 1:F:52:GLU:O     | 1:F:57:PRO:HD2   | 1.68                     | 0.93              |
| 1:H:17:ARG:HH21  | 1:H:72:LEU:HB3   | 1.31                     | 0.93              |
| 1:H:173:ASP:HB3  | 1:H:176:SER:HB2  | 1.49                     | 0.93              |
| 1:A:45:GLN:HE22  | 1:A:80:ILE:HD13  | 1.31                     | 0.93              |
| 1:E:41:LYS:HE2   | 1:E:54:GLU:OE1   | 1.68                     | 0.92              |
| 1:G:518:ASP:OD1  | 1:G:520:LYS:HG2  | 1.70                     | 0.92              |
| 1:D:591:VAL:HG21 | 1:D:629:MSE:HE1  | 1.48                     | 0.92              |
| 1:C:47:ASN:O     | 1:C:49:ILE:N     | 2.02                     | 0.92              |
| 1:G:56:LEU:HB3   | 1:G:57:PRO:HD3   | 1.50                     | 0.92              |
| 1:E:44:LEU:HA    | 1:E:124:LEU:HD11 | 1.51                     | 0.92              |
| 1:G:304:GLN:HB3  | 3:G:902:FRU:H11  | 1.51                     | 0.92              |
| 1:F:37:GLU:HG2   | 1:F:54:GLU:OE2   | 1.68                     | 0.92              |
| 1:B:72:LEU:CD1   | 1:B:90:VAL:HG11  | 1.99                     | 0.91              |
| 1:H:46:GLN:HB2   | 1:H:79:ALA:HB3   | 1.53                     | 0.91              |
| 1:G:148:ARG:CG   | 1:G:148:ARG:HH11 | 1.82                     | 0.91              |
| 1:D:163:ASN:ND2  | 1:D:269:GLU:HG3  | 1.86                     | 0.91              |
| 1:C:39:LYS:HB2   | 1:C:104:LEU:HD13 | 1.51                     | 0.91              |
| 1:H:24:SER:O     | 1:H:28:GLU:HB2   | 1.71                     | 0.91              |
| 1:E:789:MSE:CE   | 1:H:789:MSE:HE2  | 2.01                     | 0.90              |
| 1:G:545:LYS:HD2  | 1:G:545:LYS:H    | 1.34                     | 0.90              |
| 1:B:92:PRO:HG2   | 1:B:96:VAL:CG2   | 2.01                     | 0.90              |
| 1:H:72:LEU:HA    | 1:H:75:SER:HB3   | 1.54                     | 0.90              |
| 1:A:47:ASN:O     | 1:A:51:ALA:HB2   | 1.72                     | 0.90              |
| 1:G:82:LEU:N     | 1:G:83:PRO:HD3   | 1.88                     | 0.89              |
| 1:B:20:GLU:OE1   | 1:B:72:LEU:HD23  | 1.71                     | 0.89              |
| 1:A:789:MSE:CE   | 1:D:789:MSE:CB   | 2.51                     | 0.88              |
| 1:C:83:PRO:CG    | 1:C:84:PRO:HD3   | 2.03                     | 0.88              |
| 1:A:56:LEU:HB3   | 1:A:57:PRO:HD3   | 1.56                     | 0.88              |
| 1:F:45:GLN:HB3   | 1:F:80:ILE:HA    | 1.56                     | 0.88              |
| 1:C:34:SER:HA    | 1:C:59:GLN:HE22  | 1.38                     | 0.88              |
| 1:E:61:ARG:CG    | 1:E:61:ARG:HH11  | 1.87                     | 0.88              |
| 1:G:31:ALA:CB    | 1:G:35:ARG:HH21  | 1.86                     | 0.88              |
| 1:D:146:ILE:HD11 | 1:D:772:TRP:CZ2  | 2.09                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:48:GLN:HE21  | 1:G:48:GLN:CA    | 1.87                     | 0.88              |
| 1:D:173:ASP:HB3  | 1:D:176:SER:HB3  | 1.56                     | 0.88              |
| 1:E:45:GLN:HG2   | 1:E:80:ILE:CD1   | 2.03                     | 0.87              |
| 1:A:195:MSE:HE1  | 1:A:242:TRP:HA   | 1.53                     | 0.87              |
| 1:D:61:ARG:HA    | 1:D:63:LYS:HD3   | 1.56                     | 0.87              |
| 1:A:316:GLU:HA   | 1:A:319:MSE:HE3  | 1.55                     | 0.87              |
| 1:E:65:GLU:HG3   | 1:E:70:PHE:HB3   | 1.56                     | 0.87              |
| 1:G:596:LYS:HG2  | 1:G:636:TYR:CE1  | 2.10                     | 0.87              |
| 1:D:173:ASP:HB3  | 1:D:176:SER:CB   | 2.04                     | 0.87              |
| 1:D:83:PRO:HG2   | 1:D:84:PRO:HD3   | 1.55                     | 0.87              |
| 1:F:143:ASN:HB3  | 1:F:148:ARG:NH2  | 1.89                     | 0.87              |
| 1:G:216:TYR:HE1  | 1:G:220:LEU:HD11 | 1.38                     | 0.87              |
| 1:E:789:MSE:HB3  | 1:H:789:MSE:CE   | 2.04                     | 0.86              |
| 1:G:82:LEU:HD12  | 1:G:83:PRO:CD    | 2.05                     | 0.86              |
| 1:B:131:GLY:HA3  | 1:B:134:THR:HG21 | 1.56                     | 0.86              |
| 1:D:629:MSE:HE3  | 1:D:629:MSE:HA   | 1.56                     | 0.86              |
| 1:D:163:ASN:HD21 | 1:D:269:GLU:HG3  | 1.40                     | 0.86              |
| 1:G:83:PRO:CG    | 1:G:85:TRP:HB2   | 2.06                     | 0.86              |
| 1:A:52:GLU:HG2   | 1:A:56:LEU:HB2   | 1.54                     | 0.86              |
| 1:G:48:GLN:NE2   | 1:G:48:GLN:HA    | 1.90                     | 0.85              |
| 1:F:50:ILE:O     | 1:F:54:GLU:HB3   | 1.75                     | 0.85              |
| 1:E:35:ARG:CZ    | 1:E:35:ARG:HB2   | 2.06                     | 0.85              |
| 1:G:83:PRO:HB2   | 1:G:85:TRP:H     | 1.41                     | 0.85              |
| 1:E:45:GLN:HG2   | 1:E:80:ILE:HD13  | 1.56                     | 0.85              |
| 1:F:789:MSE:CG   | 1:G:789:MSE:HE3  | 2.07                     | 0.85              |
| 1:F:789:MSE:HE2  | 1:G:789:MSE:CB   | 2.05                     | 0.85              |
| 1:C:748:ARG:HH11 | 1:C:752:LYS:HG3  | 1.42                     | 0.85              |
| 1:C:796:ARG:HB2  | 1:C:797:PRO:HD3  | 1.57                     | 0.85              |
| 1:G:83:PRO:HG2   | 1:G:85:TRP:CB    | 2.05                     | 0.85              |
| 1:F:82:LEU:HD12  | 1:F:83:PRO:HD3   | 1.57                     | 0.85              |
| 1:H:210:LEU:HD22 | 1:H:253:ILE:HG23 | 1.58                     | 0.84              |
| 1:D:44:LEU:HD13  | 1:D:45:GLN:H     | 1.41                     | 0.84              |
| 1:F:81:VAL:HG13  | 1:F:86:VAL:HG23  | 1.56                     | 0.84              |
| 1:G:304:GLN:H    | 3:G:902:FRU:H12  | 1.42                     | 0.84              |
| 1:F:173:ASP:HB3  | 1:F:176:SER:HB3  | 1.60                     | 0.84              |
| 1:G:65:GLU:CB    | 1:G:70:PHE:HD1   | 1.87                     | 0.84              |
| 1:F:789:MSE:HB3  | 1:G:789:MSE:CE   | 2.07                     | 0.84              |
| 1:A:60:THR:HG23  | 1:A:62:LYS:H     | 1.40                     | 0.84              |
| 1:G:83:PRO:HD2   | 1:G:85:TRP:O     | 1.77                     | 0.84              |
| 1:D:56:LEU:CD1   | 1:D:57:PRO:HD3   | 2.07                     | 0.84              |
| 1:A:32:LEU:O     | 1:A:36:VAL:HG23  | 1.77                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:315:LEU:CG   | 1:E:319:MSE:HE2  | 2.06                     | 0.84              |
| 1:A:28:GLU:O     | 1:A:32:LEU:HG    | 1.75                     | 0.84              |
| 1:B:53:PHE:HA    | 1:B:57:PRO:HG2   | 1.59                     | 0.84              |
| 1:B:56:LEU:HB3   | 1:B:57:PRO:HD3   | 1.60                     | 0.84              |
| 1:E:148:ARG:HH11 | 1:E:148:ARG:CG   | 1.91                     | 0.84              |
| 1:F:43:ILE:HG23  | 1:F:44:LEU:N     | 1.92                     | 0.83              |
| 1:E:216:TYR:HD2  | 1:E:232:LYS:HE2  | 1.41                     | 0.83              |
| 1:F:146:ILE:HG22 | 1:F:147:PRO:O    | 1.77                     | 0.83              |
| 1:G:298:TYR:HE1  | 1:G:649:MSE:HE1  | 1.40                     | 0.83              |
| 1:C:143:ASN:HB3  | 1:C:148:ARG:NH2  | 1.92                     | 0.83              |
| 1:F:59:GLN:O     | 1:F:60:THR:HG22  | 1.77                     | 0.83              |
| 1:B:668:PHE:HB2  | 1:B:689:LEU:HD23 | 1.60                     | 0.83              |
| 1:E:789:MSE:HE2  | 1:H:789:MSE:CG   | 2.09                     | 0.83              |
| 1:H:72:LEU:HD12  | 1:H:72:LEU:O     | 1.77                     | 0.83              |
| 1:D:106:ALA:HB1  | 1:D:108:VAL:HG23 | 1.59                     | 0.83              |
| 1:B:131:GLY:HA3  | 1:B:134:THR:HG23 | 1.61                     | 0.83              |
| 1:D:103:ASN:CB   | 1:D:106:ALA:HB3  | 2.09                     | 0.82              |
| 1:E:789:MSE:CE   | 1:H:789:MSE:HG2  | 2.09                     | 0.82              |
| 1:F:35:ARG:HD2   | 1:F:104:LEU:HA   | 1.60                     | 0.82              |
| 1:A:681:VAL:HG13 | 1:A:691:THR:HG21 | 1.60                     | 0.82              |
| 1:E:789:MSE:HG2  | 1:H:789:MSE:HE3  | 1.61                     | 0.82              |
| 1:A:54:GLU:HG3   | 1:A:55:ALA:N     | 1.93                     | 0.82              |
| 1:G:390:GLU:OE1  | 1:G:796:ARG:HD2  | 1.80                     | 0.81              |
| 1:F:82:LEU:H     | 1:F:83:PRO:HD3   | 1.43                     | 0.81              |
| 1:E:27:ASN:OD1   | 1:E:30:LEU:HB2   | 1.80                     | 0.81              |
| 1:D:41:LYS:HG2   | 7:D:868:HOH:O    | 1.79                     | 0.81              |
| 1:E:46:GLN:HB3   | 1:E:50:ILE:CB    | 2.06                     | 0.81              |
| 1:B:37:GLU:HB3   | 1:B:55:ALA:HB2   | 1.63                     | 0.81              |
| 1:E:65:GLU:HG3   | 1:E:70:PHE:CB    | 2.10                     | 0.81              |
| 1:D:83:PRO:HG2   | 1:D:84:PRO:CD    | 2.11                     | 0.81              |
| 1:C:625:GLU:O    | 1:C:629:MSE:HG2  | 1.79                     | 0.81              |
| 1:G:82:LEU:H     | 1:G:83:PRO:HD3   | 1.45                     | 0.81              |
| 1:D:41:LYS:HE3   | 1:D:54:GLU:HG2   | 1.62                     | 0.81              |
| 1:E:135:LEU:HD11 | 1:H:789:MSE:HG3  | 1.62                     | 0.81              |
| 1:C:48:GLN:CG    | 1:C:76:THR:O     | 2.26                     | 0.80              |
| 1:B:146:ILE:CG2  | 1:B:147:PRO:HD2  | 2.11                     | 0.80              |
| 1:E:315:LEU:HG   | 1:E:319:MSE:CE   | 2.09                     | 0.80              |
| 1:F:472:MSE:HG2  | 1:F:514:ILE:HD13 | 1.63                     | 0.80              |
| 1:D:146:ILE:CG2  | 1:D:147:PRO:HD2  | 2.11                     | 0.80              |
| 1:F:81:VAL:CG1   | 1:F:86:VAL:HG23  | 2.11                     | 0.80              |
| 1:C:590:LEU:HB2  | 1:C:671:PRO:HG3  | 1.63                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:53:PHE:O     | 1:E:57:PRO:HG2   | 1.81                     | 0.80              |
| 1:D:360:GLU:HG3  | 1:D:361:TYR:CE2  | 2.16                     | 0.80              |
| 1:H:82:LEU:HG    | 1:H:85:TRP:O     | 1.82                     | 0.80              |
| 1:B:54:GLU:HA    | 1:B:54:GLU:OE1   | 1.79                     | 0.80              |
| 1:C:319:MSE:O    | 1:C:323:ILE:HG13 | 1.81                     | 0.80              |
| 1:G:170:LEU:HD22 | 1:G:176:SER:HB3  | 1.63                     | 0.80              |
| 1:F:143:ASN:HA   | 1:F:780:ARG:HH12 | 1.47                     | 0.80              |
| 1:A:789:MSE:HE2  | 1:D:789:MSE:CB   | 2.12                     | 0.80              |
| 1:H:39:LYS:CB    | 1:H:104:LEU:CD2  | 2.57                     | 0.80              |
| 1:D:216:TYR:CE2  | 1:D:232:LYS:HG2  | 2.15                     | 0.79              |
| 1:E:143:ASN:HB3  | 1:E:148:ARG:NH2  | 1.98                     | 0.79              |
| 1:B:756:GLN:HG2  | 1:B:757:ILE:HD13 | 1.62                     | 0.79              |
| 1:A:80:ILE:O     | 1:A:86:VAL:HG22  | 1.83                     | 0.79              |
| 1:E:217:LEU:HA   | 1:E:220:LEU:HD12 | 1.63                     | 0.79              |
| 1:F:316:GLU:CA   | 1:F:319:MSE:HE3  | 2.12                     | 0.79              |
| 1:F:789:MSE:HE2  | 1:G:789:MSE:CE   | 2.12                     | 0.79              |
| 1:A:83:PRO:HB2   | 1:A:84:PRO:HD2   | 1.64                     | 0.79              |
| 1:A:85:TRP:CE3   | 1:A:101:ARG:HG2  | 2.18                     | 0.79              |
| 1:F:173:ASP:O    | 1:F:177:LEU:HD12 | 1.82                     | 0.79              |
| 1:C:131:GLY:HA3  | 1:C:134:THR:HG23 | 1.63                     | 0.79              |
| 1:F:81:VAL:HG12  | 1:F:86:VAL:HA    | 1.65                     | 0.79              |
| 1:G:756:GLN:HG2  | 1:G:757:ILE:N    | 1.97                     | 0.79              |
| 1:E:789:MSE:HE1  | 1:H:789:MSE:HB3  | 1.63                     | 0.79              |
| 1:F:121:LYS:HD3  | 1:F:450:ILE:HD12 | 1.65                     | 0.79              |
| 1:E:789:MSE:CE   | 1:H:789:MSE:CG   | 2.61                     | 0.79              |
| 1:F:789:MSE:CE   | 1:G:789:MSE:CB   | 2.60                     | 0.79              |
| 1:F:789:MSE:HE1  | 1:G:789:MSE:HB3  | 1.64                     | 0.79              |
| 1:E:319:MSE:CE   | 1:E:334:ILE:HD11 | 2.12                     | 0.78              |
| 1:B:216:TYR:HE1  | 1:B:220:LEU:HD11 | 1.49                     | 0.78              |
| 1:H:76:THR:O     | 1:H:89:ALA:O     | 2.00                     | 0.78              |
| 1:B:80:ILE:CD1   | 1:B:87:ALA:HB3   | 2.14                     | 0.78              |
| 1:A:373:LYS:H    | 1:A:373:LYS:HD2  | 1.45                     | 0.78              |
| 1:A:65:GLU:HB3   | 1:A:70:PHE:CB    | 2.12                     | 0.78              |
| 1:C:56:LEU:HD12  | 7:C:842:HOH:O    | 1.84                     | 0.78              |
| 1:B:80:ILE:HG13  | 1:B:80:ILE:O     | 1.83                     | 0.78              |
| 1:B:54:GLU:O     | 1:B:57:PRO:HD2   | 1.82                     | 0.78              |
| 1:F:35:ARG:HB2   | 1:F:35:ARG:CZ    | 2.12                     | 0.78              |
| 1:H:39:LYS:C     | 1:H:39:LYS:HD3   | 2.04                     | 0.78              |
| 1:E:162:LEU:HD11 | 1:E:772:TRP:CE3  | 2.18                     | 0.78              |
| 1:E:789:MSE:HB3  | 1:H:789:MSE:HE1  | 1.65                     | 0.78              |
| 1:F:789:MSE:HE2  | 1:G:789:MSE:CG   | 2.13                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:360:GLU:HG3  | 1:D:361:TYR:CD2  | 2.19                     | 0.78              |
| 1:F:207:GLN:HE21 | 1:F:211:ARG:HH22 | 1.28                     | 0.78              |
| 1:D:32:LEU:HD21  | 1:D:106:ALA:H    | 1.48                     | 0.77              |
| 1:G:547:HIS:O    | 1:G:551:GLU:HG3  | 1.84                     | 0.77              |
| 1:F:52:GLU:HG2   | 1:F:53:PHE:N     | 1.98                     | 0.77              |
| 1:H:89:ALA:HB1   | 1:H:99:TYR:HD1   | 1.49                     | 0.77              |
| 1:D:195:MSE:HE1  | 1:D:241:GLY:C    | 2.05                     | 0.77              |
| 1:E:789:MSE:SE   | 1:H:789:MSE:HE2  | 2.35                     | 0.77              |
| 1:F:82:LEU:CD1   | 1:F:83:PRO:HG3   | 2.15                     | 0.77              |
| 1:D:125:VAL:HG11 | 1:D:505:PRO:HG2  | 1.66                     | 0.77              |
| 1:G:145:SER:HB2  | 1:G:779:ASP:OD2  | 1.85                     | 0.77              |
| 1:B:216:TYR:CE1  | 1:B:220:LEU:HD11 | 2.20                     | 0.77              |
| 1:F:591:VAL:HG21 | 1:F:629:MSE:HE1  | 1.67                     | 0.77              |
| 1:F:333:ARG:HH12 | 1:F:403:GLU:HB3  | 1.48                     | 0.77              |
| 1:G:276:PRO:HG3  | 1:G:326:GLN:CG   | 2.15                     | 0.77              |
| 1:A:185:ARG:HD2  | 1:A:198:GLU:OE1  | 1.85                     | 0.77              |
| 1:C:146:ILE:HG22 | 1:C:147:PRO:O    | 1.85                     | 0.77              |
| 1:B:30:LEU:HG    | 1:B:62:LYS:O     | 1.85                     | 0.77              |
| 1:H:82:LEU:HD12  | 1:H:84:PRO:HG2   | 1.67                     | 0.76              |
| 1:A:43:ILE:O     | 1:A:44:LEU:HG    | 1.85                     | 0.76              |
| 1:B:553:LEU:HG   | 1:B:645:ILE:HD13 | 1.67                     | 0.76              |
| 1:B:582:ASP:HB2  | 1:B:621:GLU:OE1  | 1.84                     | 0.76              |
| 1:E:789:MSE:CE   | 1:H:789:MSE:HB3  | 2.14                     | 0.76              |
| 1:B:170:LEU:HD22 | 1:B:177:LEU:CD2  | 2.15                     | 0.76              |
| 1:G:545:LYS:CD   | 1:G:545:LYS:H    | 1.89                     | 0.76              |
| 1:D:171:PHE:HD1  | 1:D:263:PRO:HD2  | 1.51                     | 0.76              |
| 1:G:479:ILE:CD1  | 1:G:762:LEU:HD13 | 2.16                     | 0.76              |
| 1:G:131:GLY:H    | 1:G:134:THR:HG21 | 1.50                     | 0.76              |
| 1:D:441:GLU:HA   | 1:D:441:GLU:OE1  | 1.86                     | 0.76              |
| 1:E:36:VAL:HA    | 1:E:39:LYS:CB    | 2.15                     | 0.76              |
| 1:F:538:GLU:OE1  | 1:F:541:ARG:HD3  | 1.85                     | 0.76              |
| 1:B:24:SER:O     | 1:B:28:GLU:CB    | 2.33                     | 0.76              |
| 1:C:60:THR:C     | 1:C:62:LYS:H     | 1.88                     | 0.76              |
| 1:F:210:LEU:HD22 | 1:F:253:ILE:HG23 | 1.68                     | 0.76              |
| 1:A:146:ILE:HG23 | 1:A:147:PRO:HD2  | 1.67                     | 0.75              |
| 1:B:83:PRO:HG2   | 1:B:85:TRP:CB    | 2.10                     | 0.75              |
| 1:A:29:VAL:O     | 1:A:33:LEU:HG    | 1.86                     | 0.75              |
| 1:B:460:HIS:CD2  | 1:B:802:VAL:HG13 | 2.21                     | 0.75              |
| 1:E:210:LEU:CD2  | 1:E:253:ILE:HG23 | 2.16                     | 0.75              |
| 1:G:298:TYR:CE1  | 1:G:649:MSE:HE1  | 2.21                     | 0.75              |
| 1:E:796:ARG:HB2  | 1:E:797:PRO:HD3  | 1.68                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:70:PHE:CD2   | 1:G:70:PHE:C     | 2.56                     | 0.75              |
| 1:F:207:GLN:HE21 | 1:F:211:ARG:NH2  | 1.84                     | 0.75              |
| 1:G:54:GLU:HG3   | 1:G:55:ALA:H     | 1.52                     | 0.75              |
| 1:G:545:LYS:N    | 1:G:545:LYS:HD2  | 2.01                     | 0.75              |
| 1:F:70:PHE:CD2   | 1:F:71:ASP:N     | 2.55                     | 0.75              |
| 1:D:146:ILE:HD11 | 1:D:772:TRP:CH2  | 2.21                     | 0.75              |
| 1:G:54:GLU:HG3   | 1:G:55:ALA:N     | 2.01                     | 0.75              |
| 1:E:230:GLU:O    | 1:E:234:GLU:HG3  | 1.86                     | 0.75              |
| 1:G:216:TYR:CE1  | 1:G:220:LEU:HD11 | 2.20                     | 0.75              |
| 1:D:264:ASP:OD1  | 1:D:267:THR:HB   | 1.87                     | 0.75              |
| 1:C:119:HIS:HE1  | 1:C:509:ARG:NH1  | 1.85                     | 0.75              |
| 1:D:784:ARG:O    | 1:D:788:GLU:HG3  | 1.87                     | 0.75              |
| 1:B:82:LEU:CB    | 1:B:83:PRO:CD    | 2.63                     | 0.74              |
| 1:F:32:LEU:O     | 1:F:36:VAL:HG23  | 1.87                     | 0.74              |
| 1:H:48:GLN:O     | 1:H:52:GLU:HB3   | 1.86                     | 0.74              |
| 1:H:76:THR:HA    | 1:H:90:VAL:HG12  | 1.68                     | 0.74              |
| 1:F:82:LEU:HD21  | 1:F:123:GLU:HB3  | 1.68                     | 0.74              |
| 1:G:31:ALA:HB1   | 1:G:35:ARG:HH21  | 1.52                     | 0.74              |
| 1:B:210:LEU:HD22 | 1:B:253:ILE:HG23 | 1.69                     | 0.74              |
| 1:G:692:PHE:CE2  | 1:G:724:LEU:HD23 | 2.22                     | 0.74              |
| 1:E:789:MSE:HE2  | 1:H:789:MSE:SE   | 2.37                     | 0.74              |
| 1:E:82:LEU:HB3   | 1:E:83:PRO:CD    | 2.14                     | 0.74              |
| 1:B:80:ILE:HD11  | 1:B:87:ALA:HB3   | 1.67                     | 0.74              |
| 1:A:46:GLN:HB2   | 1:A:79:ALA:O     | 1.87                     | 0.74              |
| 1:B:333:ARG:HG2  | 1:B:333:ARG:HH11 | 1.52                     | 0.74              |
| 1:E:44:LEU:HD21  | 1:E:451:TYR:OH   | 1.87                     | 0.74              |
| 1:A:81:VAL:HA    | 1:A:86:VAL:CG2   | 2.18                     | 0.74              |
| 1:F:789:MSE:HE1  | 1:G:790:PHE:N    | 2.01                     | 0.74              |
| 1:F:74:LYS:HA    | 7:F:891:HOH:O    | 1.87                     | 0.74              |
| 1:D:105:HIS:O    | 1:D:106:ALA:HB2  | 1.86                     | 0.74              |
| 1:C:261:GLU:HG2  | 1:D:151:LEU:HD12 | 1.68                     | 0.74              |
| 1:F:82:LEU:N     | 1:F:83:PRO:CD    | 2.50                     | 0.74              |
| 1:F:83:PRO:HB2   | 1:F:85:TRP:H     | 1.53                     | 0.74              |
| 1:B:756:GLN:HG2  | 1:B:757:ILE:N    | 1.99                     | 0.74              |
| 1:B:93:ARG:O     | 1:B:96:VAL:HG22  | 1.88                     | 0.73              |
| 1:D:39:LYS:NZ    | 1:D:39:LYS:HB2   | 2.02                     | 0.73              |
| 1:E:789:MSE:CB   | 1:H:789:MSE:CE   | 2.66                     | 0.73              |
| 1:A:400:LEU:C    | 1:A:400:LEU:HD12 | 2.07                     | 0.73              |
| 1:E:83:PRO:HB2   | 1:E:84:PRO:HD2   | 1.68                     | 0.73              |
| 1:D:217:LEU:HD11 | 1:D:233:PHE:HZ   | 1.51                     | 0.73              |
| 1:D:44:LEU:CD1   | 1:D:45:GLN:H     | 2.00                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:685:MSE:HE3  | 1:A:745:GLY:HA2  | 1.71                     | 0.73              |
| 1:A:786:TYR:CZ   | 1:D:789:MSE:HE3  | 2.23                     | 0.73              |
| 1:F:59:GLN:O     | 1:F:60:THR:CG2   | 2.36                     | 0.73              |
| 1:F:131:GLY:O    | 1:F:134:THR:HG23 | 1.89                     | 0.73              |
| 1:A:789:MSE:HE1  | 1:D:789:MSE:HB3  | 1.71                     | 0.73              |
| 1:B:72:LEU:HD13  | 1:B:90:VAL:CG1   | 2.15                     | 0.73              |
| 1:B:99:TYR:O     | 1:B:112:LEU:HB2  | 1.89                     | 0.73              |
| 1:H:131:GLY:O    | 1:H:134:THR:HG23 | 1.89                     | 0.73              |
| 1:F:53:PHE:C     | 1:F:57:PRO:HG2   | 2.09                     | 0.73              |
| 1:A:298:TYR:CE1  | 1:A:649:MSE:HE1  | 2.23                     | 0.73              |
| 1:G:667:ALA:HA   | 1:G:689:LEU:HD11 | 1.71                     | 0.73              |
| 1:B:114:PRO:HA   | 7:B:876:HOH:O    | 1.88                     | 0.72              |
| 1:G:131:GLY:CA   | 1:G:134:THR:HG23 | 2.18                     | 0.72              |
| 1:H:33:LEU:HA    | 1:H:36:VAL:HB    | 1.70                     | 0.72              |
| 1:E:35:ARG:CG    | 1:E:104:LEU:HA   | 2.18                     | 0.72              |
| 1:D:36:VAL:HG22  | 1:D:105:HIS:CE1  | 2.24                     | 0.72              |
| 1:B:103:ASN:CB   | 1:B:108:VAL:CB   | 2.67                     | 0.72              |
| 1:E:164:ARG:HD2  | 1:F:262:ALA:HB1  | 1.71                     | 0.72              |
| 1:D:195:MSE:CE   | 1:D:241:GLY:HA3  | 2.19                     | 0.72              |
| 1:G:315:LEU:HD21 | 1:G:762:LEU:HD23 | 1.72                     | 0.72              |
| 1:B:613:ARG:HH11 | 1:B:613:ARG:HG3  | 1.53                     | 0.72              |
| 1:E:70:PHE:CD2   | 1:E:70:PHE:C     | 2.62                     | 0.72              |
| 1:F:69:PHE:HD1   | 1:F:70:PHE:N     | 1.87                     | 0.72              |
| 1:E:789:MSE:CG   | 1:H:789:MSE:CE   | 2.67                     | 0.72              |
| 1:C:216:TYR:HE1  | 1:C:220:LEU:HD11 | 1.55                     | 0.72              |
| 1:E:625:GLU:HG2  | 7:E:839:HOH:O    | 1.90                     | 0.72              |
| 1:E:319:MSE:HE3  | 1:E:334:ILE:HD11 | 1.72                     | 0.72              |
| 1:E:216:TYR:CE1  | 1:E:220:LEU:HD21 | 2.25                     | 0.72              |
| 1:A:184:LEU:HD22 | 1:A:195:MSE:HG2  | 1.72                     | 0.72              |
| 1:E:52:GLU:OE1   | 1:E:57:PRO:HD3   | 1.89                     | 0.72              |
| 1:H:130:ASN:HB3  | 1:H:134:THR:HG21 | 1.72                     | 0.72              |
| 1:F:216:TYR:CE1  | 1:F:220:LEU:HD11 | 2.25                     | 0.71              |
| 1:A:298:TYR:HE1  | 1:A:649:MSE:HE1  | 1.54                     | 0.71              |
| 1:A:36:VAL:HA    | 1:A:39:LYS:HD2   | 1.73                     | 0.71              |
| 1:F:789:MSE:HB3  | 1:G:789:MSE:HE1  | 1.71                     | 0.71              |
| 1:H:89:ALA:CB    | 1:H:99:TYR:HD1   | 2.03                     | 0.71              |
| 1:F:575:LEU:HD21 | 1:F:724:LEU:HD13 | 1.72                     | 0.71              |
| 1:D:56:LEU:HB3   | 1:D:57:PRO:HD2   | 1.72                     | 0.71              |
| 1:F:82:LEU:HD12  | 1:F:83:PRO:CD    | 2.21                     | 0.71              |
| 1:F:629:MSE:HA   | 1:F:629:MSE:CE   | 2.20                     | 0.71              |
| 1:A:210:LEU:HD22 | 1:A:253:ILE:HG23 | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:115:ALA:N    | 7:B:876:HOH:O    | 2.23                     | 0.71              |
| 1:E:486:ILE:HG22 | 1:E:516:VAL:HG22 | 1.73                     | 0.71              |
| 1:E:170:LEU:HD22 | 1:E:177:LEU:HD23 | 1.71                     | 0.71              |
| 1:B:153:LYS:HD3  | 1:B:154:TYR:CE2  | 2.26                     | 0.71              |
| 1:H:48:GLN:OE1   | 1:H:492:THR:HG22 | 1.89                     | 0.70              |
| 1:G:27:ASN:CA    | 1:G:30:LEU:HD12  | 2.21                     | 0.70              |
| 1:F:469:ILE:HA   | 1:F:472:MSE:CE   | 2.17                     | 0.70              |
| 1:A:60:THR:O     | 1:A:63:LYS:HG3   | 1.91                     | 0.70              |
| 1:D:112:LEU:HD22 | 1:D:116:GLU:HB3  | 1.73                     | 0.70              |
| 1:D:91:ARG:HD2   | 1:D:97:TRP:CZ2   | 2.26                     | 0.70              |
| 1:G:441:GLU:HA   | 1:G:441:GLU:OE1  | 1.90                     | 0.70              |
| 1:B:83:PRO:O     | 1:B:85:TRP:N     | 2.23                     | 0.70              |
| 1:C:216:TYR:CE1  | 1:C:220:LEU:HD11 | 2.26                     | 0.70              |
| 1:F:400:LEU:HD12 | 1:F:400:LEU:C    | 2.12                     | 0.70              |
| 1:E:789:MSE:CE   | 1:H:789:MSE:CB   | 2.69                     | 0.70              |
| 1:F:83:PRO:HD2   | 1:F:85:TRP:O     | 1.91                     | 0.70              |
| 1:C:105:HIS:O    | 1:C:106:ALA:HB3  | 1.91                     | 0.70              |
| 1:A:82:LEU:HB3   | 1:A:83:PRO:HD2   | 1.72                     | 0.70              |
| 1:E:35:ARG:HB2   | 1:E:35:ARG:NH1   | 2.07                     | 0.70              |
| 1:G:284:LEU:HD13 | 1:G:337:LEU:HB2  | 1.74                     | 0.70              |
| 1:F:789:MSE:HB3  | 1:G:789:MSE:HE3  | 1.72                     | 0.70              |
| 1:G:479:ILE:HD11 | 1:G:762:LEU:HD13 | 1.74                     | 0.70              |
| 1:D:479:ILE:HD11 | 1:D:762:LEU:CD1  | 2.22                     | 0.70              |
| 1:E:789:MSE:CE   | 1:H:789:MSE:CE   | 2.61                     | 0.70              |
| 1:F:796:ARG:O    | 1:F:800:GLN:HG3  | 1.92                     | 0.70              |
| 1:A:198:GLU:HA   | 1:A:198:GLU:OE1  | 1.91                     | 0.70              |
| 1:A:512:HIS:CE1  | 1:A:515:ASP:HB2  | 2.27                     | 0.70              |
| 1:A:432:THR:OG1  | 1:A:773:LYS:HE2  | 1.92                     | 0.70              |
| 1:F:59:GLN:HG3   | 1:F:60:THR:N     | 2.05                     | 0.70              |
| 1:F:83:PRO:CB    | 1:F:84:PRO:HD2   | 2.22                     | 0.70              |
| 1:F:140:GLU:N    | 1:F:141:PRO:HD2  | 2.06                     | 0.70              |
| 1:D:34:SER:O     | 1:D:37:GLU:HB2   | 1.91                     | 0.69              |
| 1:F:43:ILE:HG13  | 1:F:82:LEU:HA    | 1.74                     | 0.69              |
| 1:A:47:ASN:O     | 1:A:51:ALA:CB    | 2.39                     | 0.69              |
| 1:G:204:ASN:ND2  | 1:H:12:HIS:H     | 1.90                     | 0.69              |
| 1:B:45:GLN:CG    | 1:B:80:ILE:HG22  | 2.22                     | 0.69              |
| 1:B:80:ILE:HD11  | 1:B:87:ALA:CB    | 2.22                     | 0.69              |
| 1:E:36:VAL:HA    | 1:E:39:LYS:HB2   | 1.74                     | 0.69              |
| 1:E:226:TYR:CE2  | 1:E:240:ARG:HG2  | 2.27                     | 0.69              |
| 1:F:171:PHE:HD1  | 1:F:263:PRO:HD2  | 1.55                     | 0.69              |
| 1:D:414:ASN:O    | 1:D:418:GLY:HA3  | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:56:LEU:HG    | 1:A:70:PHE:CD1   | 2.27                     | 0.69              |
| 1:G:543:LEU:HA   | 1:G:545:LYS:HE3  | 1.73                     | 0.69              |
| 1:H:590:LEU:HB2  | 1:H:671:PRO:HG3  | 1.73                     | 0.69              |
| 1:B:46:GLN:HB2   | 1:B:50:ILE:HB    | 1.73                     | 0.69              |
| 1:D:131:GLY:CA   | 1:D:134:THR:HG23 | 2.22                     | 0.69              |
| 1:G:207:GLN:HE21 | 1:G:211:ARG:HE   | 1.37                     | 0.69              |
| 1:E:216:TYR:CD2  | 1:E:232:LYS:HE2  | 2.27                     | 0.69              |
| 1:B:146:ILE:HG23 | 1:B:147:PRO:HD2  | 1.75                     | 0.69              |
| 1:B:609:VAL:HG22 | 1:B:645:ILE:HB   | 1.75                     | 0.69              |
| 1:B:119:HIS:CE1  | 1:B:129:LYS:CB   | 2.76                     | 0.69              |
| 1:H:315:LEU:HB3  | 1:H:319:MSE:HE3  | 1.75                     | 0.69              |
| 1:B:75:SER:O     | 1:B:90:VAL:HG12  | 1.92                     | 0.69              |
| 1:H:32:LEU:HD22  | 1:H:35:ARG:NH1   | 2.07                     | 0.68              |
| 1:A:140:GLU:HB3  | 1:A:141:PRO:HD3  | 1.73                     | 0.68              |
| 1:D:54:GLU:HG3   | 1:D:55:ALA:H     | 1.59                     | 0.68              |
| 1:A:170:LEU:HD23 | 1:A:176:SER:OG   | 1.92                     | 0.68              |
| 1:E:670:GLN:O    | 1:E:670:GLN:HG3  | 1.93                     | 0.68              |
| 1:A:56:LEU:CB    | 1:A:57:PRO:HD3   | 2.23                     | 0.68              |
| 1:B:793:LEU:HD11 | 1:C:135:LEU:HD22 | 1.74                     | 0.68              |
| 1:C:681:VAL:HG12 | 1:C:685:MSE:HE2  | 1.73                     | 0.68              |
| 1:F:789:MSE:CB   | 1:G:789:MSE:HE3  | 2.24                     | 0.68              |
| 1:D:216:TYR:CD2  | 1:D:232:LYS:HG2  | 2.28                     | 0.68              |
| 1:D:173:ASP:HB3  | 1:D:176:SER:HB2  | 1.75                     | 0.68              |
| 1:E:315:LEU:HD12 | 1:E:759:SER:HB3  | 1.74                     | 0.68              |
| 1:A:52:GLU:HA    | 1:A:55:ALA:HB3   | 1.76                     | 0.68              |
| 1:G:146:ILE:HG23 | 1:G:147:PRO:HD2  | 1.74                     | 0.68              |
| 1:D:171:PHE:CD1  | 1:D:263:PRO:HD2  | 2.28                     | 0.68              |
| 1:H:124:LEU:HD23 | 1:H:124:LEU:O    | 1.93                     | 0.68              |
| 1:B:597:ASN:HB2  | 7:B:842:HOH:O    | 1.92                     | 0.68              |
| 1:H:276:PRO:HG3  | 1:H:326:GLN:HG3  | 1.74                     | 0.68              |
| 1:E:148:ARG:NH1  | 1:E:148:ARG:HG3  | 1.95                     | 0.68              |
| 1:B:583:ARG:CA   | 1:B:625:GLU:OE1  | 2.35                     | 0.68              |
| 1:A:373:LYS:N    | 1:A:373:LYS:CD   | 2.56                     | 0.68              |
| 1:B:756:GLN:CG   | 1:B:757:ILE:HD13 | 2.23                     | 0.68              |
| 1:B:220:LEU:HD22 | 1:B:224:THR:HG21 | 1.75                     | 0.68              |
| 1:B:101:ARG:CB   | 1:B:112:LEU:HD11 | 2.23                     | 0.68              |
| 1:F:649:MSE:HG3  | 7:F:897:HOH:O    | 1.92                     | 0.68              |
| 1:E:789:MSE:HE3  | 1:H:789:MSE:HG2  | 1.76                     | 0.67              |
| 1:H:757:ILE:HG22 | 1:H:761:ARG:HG2  | 1.75                     | 0.67              |
| 1:F:276:PRO:HG3  | 1:F:326:GLN:CG   | 2.24                     | 0.67              |
| 1:G:483:PHE:CE1  | 1:G:487:ALA:HB3  | 2.29                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:73:LEU:HD23  | 1:G:73:LEU:N     | 2.08                     | 0.67              |
| 1:E:315:LEU:HB3  | 1:E:319:MSE:HE3  | 1.76                     | 0.67              |
| 1:H:290:PHE:O    | 1:H:366:ARG:NH1  | 2.27                     | 0.67              |
| 1:A:207:GLN:HE21 | 1:A:211:ARG:NH1  | 1.92                     | 0.67              |
| 1:B:670:GLN:HG3  | 1:B:670:GLN:O    | 1.94                     | 0.67              |
| 1:D:538:GLU:OE1  | 1:D:541:ARG:HD3  | 1.94                     | 0.67              |
| 1:B:99:TYR:HE2   | 1:B:114:PRO:CG   | 2.04                     | 0.67              |
| 1:C:92:PRO:HD2   | 1:C:96:VAL:O     | 1.94                     | 0.67              |
| 1:F:52:GLU:O     | 1:F:55:ALA:N     | 2.28                     | 0.67              |
| 1:H:160:ASP:O    | 1:H:164:ARG:HG3  | 1.95                     | 0.67              |
| 1:B:189:HIS:ND1  | 1:B:330:ILE:HD13 | 2.10                     | 0.67              |
| 1:D:419:ASN:HB3  | 1:D:471:ALA:HB1  | 1.75                     | 0.67              |
| 1:A:195:MSE:HE3  | 1:A:242:TRP:CG   | 2.29                     | 0.67              |
| 1:E:45:GLN:HG3   | 1:E:124:LEU:CD2  | 2.24                     | 0.67              |
| 1:E:44:LEU:CA    | 1:E:124:LEU:HD11 | 2.25                     | 0.67              |
| 1:G:54:GLU:CG    | 1:G:55:ALA:N     | 2.58                     | 0.67              |
| 1:F:69:PHE:CD1   | 1:F:70:PHE:N     | 2.62                     | 0.67              |
| 1:B:29:VAL:HG13  | 1:B:30:LEU:CD1   | 2.25                     | 0.67              |
| 1:E:45:GLN:HG3   | 1:E:124:LEU:HD21 | 1.77                     | 0.66              |
| 1:A:83:PRO:CB    | 1:A:84:PRO:HD2   | 2.25                     | 0.66              |
| 1:E:458:LYS:HD2  | 1:E:459:TYR:CE2  | 2.28                     | 0.66              |
| 1:D:181:LEU:HD13 | 1:D:206:LEU:HD22 | 1.78                     | 0.66              |
| 1:E:216:TYR:HE1  | 1:E:220:LEU:HD21 | 1.60                     | 0.66              |
| 1:B:80:ILE:HG13  | 1:B:87:ALA:HB3   | 1.75                     | 0.66              |
| 1:H:668:PHE:HB2  | 1:H:689:LEU:HD23 | 1.77                     | 0.66              |
| 1:F:57:PRO:O     | 1:F:59:GLN:N     | 2.28                     | 0.66              |
| 1:G:82:LEU:N     | 1:G:83:PRO:CD    | 2.58                     | 0.66              |
| 1:A:45:GLN:HE22  | 1:A:80:ILE:CD1   | 2.06                     | 0.66              |
| 1:F:146:ILE:HG23 | 1:F:147:PRO:HD2  | 1.76                     | 0.66              |
| 1:F:414:ASN:ND2  | 1:F:438:HIS:NE2  | 2.43                     | 0.66              |
| 1:F:685:MSE:CE   | 1:F:745:GLY:HA2  | 2.25                     | 0.66              |
| 1:D:440:LEU:HD12 | 1:D:495:GLN:HB3  | 1.78                     | 0.66              |
| 1:B:225:LEU:HD23 | 1:B:225:LEU:N    | 2.09                     | 0.66              |
| 1:E:209:THR:HG23 | 1:E:236:ILE:HB   | 1.77                     | 0.66              |
| 1:H:625:GLU:O    | 1:H:629:MSE:HG2  | 1.96                     | 0.66              |
| 1:A:52:GLU:O     | 1:A:57:PRO:HD2   | 1.96                     | 0.66              |
| 1:B:80:ILE:HG12  | 1:B:87:ALA:HB3   | 1.77                     | 0.66              |
| 1:C:259:LEU:O    | 1:C:263:PRO:HG3  | 1.96                     | 0.66              |
| 1:E:315:LEU:CG   | 1:E:319:MSE:CE   | 2.71                     | 0.66              |
| 1:E:210:LEU:HD23 | 1:E:253:ILE:HG23 | 1.77                     | 0.66              |
| 1:H:30:LEU:HD13  | 1:H:62:LYS:O     | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:148:ARG:HD3  | 1:E:515:ASP:OD2  | 1.95                     | 0.66              |
| 1:A:176:SER:O    | 1:A:179:PRO:HD2  | 1.95                     | 0.66              |
| 1:G:81:VAL:HG12  | 1:G:86:VAL:HB    | 1.78                     | 0.66              |
| 1:F:789:MSE:SE   | 1:G:789:MSE:HE3  | 2.46                     | 0.65              |
| 1:G:48:GLN:NE2   | 1:G:48:GLN:CA    | 2.54                     | 0.65              |
| 1:A:524:VAL:HG12 | 1:A:758:TYR:CD2  | 2.31                     | 0.65              |
| 1:G:32:LEU:HD21  | 1:G:105:HIS:O    | 1.96                     | 0.65              |
| 1:H:34:SER:OG    | 1:H:55:ALA:HB1   | 1.96                     | 0.65              |
| 1:C:53:PHE:O     | 1:C:57:PRO:HG2   | 1.96                     | 0.65              |
| 1:A:124:LEU:HD23 | 1:A:124:LEU:C    | 2.16                     | 0.65              |
| 1:E:32:LEU:HD21  | 1:E:107:LEU:CB   | 2.26                     | 0.65              |
| 1:A:158:GLY:HA3  | 1:A:519:PRO:O    | 1.97                     | 0.65              |
| 1:E:315:LEU:O    | 1:E:319:MSE:HG3  | 1.96                     | 0.65              |
| 1:D:27:ASN:ND2   | 1:D:27:ASN:N     | 2.42                     | 0.65              |
| 1:G:667:ALA:CA   | 1:G:689:LEU:HD11 | 2.26                     | 0.65              |
| 1:A:264:ASP:OD1  | 1:A:267:THR:HB   | 1.96                     | 0.65              |
| 1:E:45:GLN:CG    | 1:E:80:ILE:HD13  | 2.27                     | 0.65              |
| 1:C:49:ILE:O     | 1:C:53:PHE:CB    | 2.45                     | 0.65              |
| 1:D:216:TYR:HE2  | 1:D:232:LYS:HG2  | 1.61                     | 0.65              |
| 1:B:86:VAL:O     | 1:B:101:ARG:HA   | 1.97                     | 0.65              |
| 1:A:181:LEU:HD13 | 1:A:206:LEU:HD22 | 1.78                     | 0.65              |
| 1:H:113:GLN:N    | 1:H:113:GLN:OE1  | 2.29                     | 0.65              |
| 1:B:33:LEU:O     | 1:B:36:VAL:HB    | 1.96                     | 0.65              |
| 1:A:145:SER:HB3  | 1:A:779:ASP:OD2  | 1.96                     | 0.65              |
| 1:D:102:VAL:HG23 | 1:D:109:VAL:CG2  | 2.26                     | 0.65              |
| 1:F:233:PHE:CD1  | 1:F:238:LEU:HD12 | 2.32                     | 0.65              |
| 1:G:48:GLN:HG2   | 7:G:877:HOH:O    | 1.96                     | 0.65              |
| 1:A:315:LEU:HG   | 1:A:319:MSE:HE2  | 1.77                     | 0.65              |
| 1:H:173:ASP:CB   | 1:H:176:SER:HB2  | 2.23                     | 0.65              |
| 1:C:552:GLU:O    | 1:C:556:SER:HB3  | 1.97                     | 0.65              |
| 1:G:486:ILE:HG22 | 1:G:516:VAL:HG22 | 1.79                     | 0.65              |
| 1:C:54:GLU:HG3   | 1:C:55:ALA:H     | 1.60                     | 0.65              |
| 1:H:95:GLY:HA3   | 1:H:517:PHE:HE2  | 1.61                     | 0.65              |
| 1:G:178:LEU:HB2  | 1:G:179:PRO:HD3  | 1.79                     | 0.65              |
| 1:G:66:GLY:HA2   | 1:G:71:ASP:OD2   | 1.96                     | 0.65              |
| 1:C:681:VAL:CG1  | 1:C:685:MSE:CE   | 2.67                     | 0.65              |
| 1:C:63:LYS:O     | 1:C:65:GLU:HG2   | 1.95                     | 0.65              |
| 1:B:460:HIS:NE2  | 1:B:802:VAL:HG13 | 2.12                     | 0.65              |
| 1:A:36:VAL:O     | 1:A:39:LYS:HG3   | 1.98                     | 0.64              |
| 1:G:31:ALA:HB3   | 1:G:35:ARG:HH21  | 1.60                     | 0.64              |
| 1:G:204:ASN:ND2  | 1:H:12:HIS:N     | 2.44                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:281:VAL:HG21 | 1:H:319:MSE:HE1  | 1.79                     | 0.64              |
| 1:C:80:ILE:HD11  | 1:C:121:LYS:HG3  | 1.80                     | 0.64              |
| 1:H:353:LEU:HD12 | 1:H:365:LEU:HD13 | 1.79                     | 0.64              |
| 1:H:169:LYS:HG2  | 1:H:176:SER:OG   | 1.98                     | 0.64              |
| 1:B:442:LYS:HD2  | 1:B:449:ASP:HB3  | 1.78                     | 0.64              |
| 1:E:564:LEU:HD22 | 1:E:613:ARG:NH2  | 2.11                     | 0.64              |
| 1:B:178:LEU:HB2  | 1:B:179:PRO:HD3  | 1.79                     | 0.64              |
| 1:F:37:GLU:OE1   | 1:F:59:GLN:HB2   | 1.97                     | 0.64              |
| 1:C:131:GLY:CA   | 1:C:134:THR:HG23 | 2.27                     | 0.64              |
| 1:E:36:VAL:HA    | 1:E:39:LYS:HB3   | 1.77                     | 0.64              |
| 1:E:282:VAL:HG13 | 1:E:337:LEU:HD23 | 1.80                     | 0.64              |
| 1:B:552:GLU:O    | 1:B:556:SER:HB3  | 1.97                     | 0.64              |
| 1:B:146:ILE:HG22 | 1:B:147:PRO:HD2  | 1.78                     | 0.64              |
| 1:F:91:ARG:HD2   | 1:F:97:TRP:CZ2   | 2.33                     | 0.64              |
| 1:C:69:PHE:CD1   | 1:C:70:PHE:N     | 2.66                     | 0.64              |
| 1:C:224:THR:HG23 | 1:C:228:GLU:HG3  | 1.79                     | 0.64              |
| 1:B:54:GLU:HG3   | 1:B:55:ALA:H     | 1.62                     | 0.64              |
| 1:B:668:PHE:HB2  | 1:B:689:LEU:CD2  | 2.27                     | 0.64              |
| 1:D:131:GLY:HA3  | 1:D:134:THR:HG23 | 1.79                     | 0.64              |
| 1:F:486:ILE:HG22 | 1:F:516:VAL:HG22 | 1.79                     | 0.64              |
| 1:E:675:GLU:O    | 1:E:697:GLY:HA3  | 1.97                     | 0.64              |
| 1:E:321:GLN:O    | 1:E:325:GLN:HG3  | 1.98                     | 0.64              |
| 1:E:333:ARG:HH11 | 1:E:333:ARG:HG2  | 1.63                     | 0.64              |
| 1:F:315:LEU:HB3  | 1:F:319:MSE:HE2  | 1.78                     | 0.64              |
| 1:F:171:PHE:CD1  | 1:F:263:PRO:HD2  | 2.33                     | 0.64              |
| 1:H:139:PHE:CE1  | 1:H:787:LEU:HD21 | 2.33                     | 0.64              |
| 1:B:748:ARG:NH1  | 1:B:752:LYS:HD2  | 2.13                     | 0.64              |
| 1:E:105:HIS:O    | 1:E:106:ALA:HB3  | 1.96                     | 0.64              |
| 1:H:171:PHE:CD1  | 1:H:263:PRO:HD2  | 2.33                     | 0.64              |
| 1:A:367:VAL:HG22 | 1:A:399:GLU:HG3  | 1.79                     | 0.64              |
| 1:E:45:GLN:CB    | 1:E:80:ILE:HA    | 2.17                     | 0.63              |
| 1:B:224:THR:HG23 | 1:B:228:GLU:HG3  | 1.80                     | 0.63              |
| 1:G:667:ALA:HA   | 1:G:689:LEU:CD1  | 2.27                     | 0.63              |
| 1:F:158:GLY:HA3  | 1:F:519:PRO:O    | 1.98                     | 0.63              |
| 1:C:207:GLN:HE21 | 1:C:211:ARG:HH21 | 1.46                     | 0.63              |
| 1:B:190:GLN:HA   | 1:B:190:GLN:OE1  | 1.97                     | 0.63              |
| 1:A:149:PRO:HB3  | 1:A:161:PHE:CE1  | 2.32                     | 0.63              |
| 1:E:243:GLY:HA2  | 1:E:326:GLN:HA   | 1.80                     | 0.63              |
| 1:F:59:GLN:HG3   | 1:F:60:THR:H     | 1.62                     | 0.63              |
| 1:G:31:ALA:HB3   | 1:G:35:ARG:NH2   | 2.13                     | 0.63              |
| 1:A:647:SER:HB2  | 1:A:649:MSE:HE3  | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:212:LYS:HE3  | 1:G:232:LYS:HZ2  | 1.64                     | 0.63              |
| 1:G:538:GLU:OE1  | 1:G:541:ARG:HD3  | 1.97                     | 0.63              |
| 1:B:250:LEU:O    | 1:B:254:ARG:HG3  | 1.98                     | 0.63              |
| 1:G:83:PRO:CB    | 1:G:84:PRO:HD2   | 2.27                     | 0.63              |
| 1:E:789:MSE:HG2  | 1:H:789:MSE:CE   | 2.27                     | 0.63              |
| 1:A:70:PHE:C     | 1:A:70:PHE:CD2   | 2.71                     | 0.63              |
| 1:C:796:ARG:O    | 1:C:800:GLN:HG3  | 1.98                     | 0.63              |
| 1:E:400:LEU:C    | 1:E:400:LEU:HD12 | 2.19                     | 0.63              |
| 1:B:366:ARG:HD3  | 7:B:837:HOH:O    | 1.97                     | 0.63              |
| 1:H:35:ARG:O     | 1:H:104:LEU:HD22 | 1.99                     | 0.63              |
| 1:C:224:THR:CG2  | 1:C:228:GLU:HG3  | 2.28                     | 0.63              |
| 1:A:90:VAL:HG23  | 1:A:98:GLU:O     | 1.98                     | 0.63              |
| 1:E:315:LEU:CD1  | 1:E:762:LEU:HD23 | 2.27                     | 0.63              |
| 1:G:692:PHE:CD2  | 1:G:724:LEU:HD23 | 2.34                     | 0.63              |
| 1:E:588:SER:HB3  | 1:E:625:GLU:OE2  | 1.99                     | 0.63              |
| 1:D:561:LYS:HD2  | 1:D:613:ARG:O    | 1.99                     | 0.63              |
| 1:G:477:PHE:HA   | 1:G:520:LYS:HB2  | 1.81                     | 0.63              |
| 1:H:211:ARG:HD2  | 7:H:867:HOH:O    | 1.98                     | 0.63              |
| 1:G:156:GLY:O    | 1:G:522:ASN:HA   | 1.98                     | 0.63              |
| 1:F:387:PRO:HD3  | 1:F:802:VAL:HB   | 1.81                     | 0.63              |
| 1:C:173:ASP:HB3  | 1:C:176:SER:HB3  | 1.81                     | 0.63              |
| 1:G:304:GLN:CB   | 3:G:902:FRU:H11  | 2.26                     | 0.63              |
| 1:G:596:LYS:HG2  | 1:G:636:TYR:HE1  | 1.59                     | 0.63              |
| 1:C:207:GLN:NE2  | 1:C:211:ARG:HH21 | 1.95                     | 0.63              |
| 1:C:371:THR:OG1  | 1:C:373:LYS:HG3  | 1.99                     | 0.63              |
| 1:B:348:THR:O    | 1:B:351:GLU:HG2  | 1.99                     | 0.63              |
| 1:E:61:ARG:HG3   | 1:E:61:ARG:NH1   | 1.98                     | 0.62              |
| 1:E:85:TRP:N     | 1:E:85:TRP:CD1   | 2.64                     | 0.62              |
| 1:H:90:VAL:N     | 1:H:98:GLU:O     | 2.32                     | 0.62              |
| 1:E:146:ILE:HD11 | 1:E:772:TRP:CZ2  | 2.34                     | 0.62              |
| 1:D:195:MSE:HE1  | 1:D:241:GLY:HA3  | 1.81                     | 0.62              |
| 1:E:230:GLU:OE1  | 1:E:240:ARG:NH1  | 2.32                     | 0.62              |
| 1:B:142:PHE:HB3  | 1:B:783:ALA:HB2  | 1.79                     | 0.62              |
| 1:A:420:LEU:C    | 1:A:420:LEU:HD13 | 2.20                     | 0.62              |
| 1:H:17:ARG:NH2   | 1:H:72:LEU:CB    | 2.52                     | 0.62              |
| 1:C:217:LEU:HD11 | 1:C:249:VAL:HG12 | 1.81                     | 0.62              |
| 1:F:65:GLU:HG3   | 1:F:70:PHE:CB    | 2.28                     | 0.62              |
| 1:H:719:GLN:HG3  | 4:H:913:SO4:O4   | 1.98                     | 0.62              |
| 1:H:552:GLU:O    | 1:H:556:SER:HB3  | 1.98                     | 0.62              |
| 1:D:298:TYR:CE1  | 1:D:649:MSE:CE   | 2.79                     | 0.62              |
| 1:H:140:GLU:N    | 1:H:141:PRO:HD2  | 2.14                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:772:TRP:CZ2  | 1:C:776:SER:HB3  | 2.34                     | 0.62              |
| 1:A:52:GLU:CG    | 1:A:56:LEU:HB2   | 2.28                     | 0.62              |
| 1:D:105:HIS:O    | 1:D:106:ALA:CB   | 2.46                     | 0.62              |
| 1:H:784:ARG:O    | 1:H:788:GLU:HG3  | 1.98                     | 0.62              |
| 1:A:682:VAL:HG13 | 1:A:749:ILE:HD12 | 1.81                     | 0.62              |
| 1:D:56:LEU:HB3   | 1:D:57:PRO:CD    | 2.30                     | 0.62              |
| 1:H:82:LEU:HD12  | 1:H:84:PRO:CG    | 2.29                     | 0.62              |
| 1:E:45:GLN:HG2   | 1:E:80:ILE:HD12  | 1.82                     | 0.62              |
| 1:A:400:LEU:HD12 | 1:A:401:SER:N    | 2.15                     | 0.62              |
| 1:H:281:VAL:HG21 | 1:H:319:MSE:CE   | 2.30                     | 0.62              |
| 1:E:756:GLN:HG2  | 1:E:757:ILE:N    | 2.15                     | 0.62              |
| 1:G:702:ILE:HA   | 1:G:753:TYR:OH   | 2.00                     | 0.62              |
| 1:E:159:VAL:HG13 | 1:E:160:ASP:N    | 2.15                     | 0.62              |
| 1:D:536:TYR:CE1  | 1:D:537:THR:HG23 | 2.34                     | 0.62              |
| 1:E:789:MSE:HE1  | 1:H:789:MSE:CB   | 2.30                     | 0.62              |
| 1:D:146:ILE:CD1  | 1:D:772:TRP:CZ2  | 2.82                     | 0.62              |
| 1:B:50:ILE:O     | 1:B:54:GLU:HB2   | 2.00                     | 0.62              |
| 1:A:178:LEU:HB2  | 1:A:179:PRO:HD3  | 1.82                     | 0.62              |
| 1:G:230:GLU:O    | 1:G:234:GLU:HG3  | 2.00                     | 0.62              |
| 1:G:65:GLU:CB    | 1:G:70:PHE:CD1   | 2.71                     | 0.62              |
| 1:E:61:ARG:CG    | 1:E:61:ARG:NH1   | 2.55                     | 0.62              |
| 1:D:340:LEU:HB2  | 1:D:366:ARG:HB3  | 1.82                     | 0.62              |
| 1:G:53:PHE:O     | 1:G:57:PRO:HD2   | 2.00                     | 0.61              |
| 1:A:51:ALA:O     | 1:A:53:PHE:N     | 2.33                     | 0.61              |
| 1:A:83:PRO:CB    | 1:A:84:PRO:CD    | 2.77                     | 0.61              |
| 1:A:84:PRO:O     | 1:A:104:LEU:N    | 2.25                     | 0.61              |
| 1:A:46:GLN:OE1   | 1:A:46:GLN:HA    | 1.99                     | 0.61              |
| 1:D:231:ALA:O    | 1:D:235:GLU:HG2  | 2.00                     | 0.61              |
| 1:C:54:GLU:CG    | 1:C:55:ALA:N     | 2.55                     | 0.61              |
| 1:A:140:GLU:HB3  | 1:A:141:PRO:CD   | 2.30                     | 0.61              |
| 1:A:255:LEU:HD23 | 1:A:267:THR:HG23 | 1.82                     | 0.61              |
| 1:A:483:PHE:CE1  | 1:A:487:ALA:HB3  | 2.34                     | 0.61              |
| 1:B:293:ASP:HB2  | 7:B:847:HOH:O    | 2.00                     | 0.61              |
| 1:C:354:GLU:OE1  | 1:C:366:ARG:NH2  | 2.34                     | 0.61              |
| 1:G:146:ILE:HD11 | 1:G:772:TRP:CZ2  | 2.35                     | 0.61              |
| 1:E:321:GLN:HE21 | 1:E:325:GLN:NE2  | 1.99                     | 0.61              |
| 1:B:230:GLU:O    | 1:B:234:GLU:HG3  | 2.00                     | 0.61              |
| 1:H:46:GLN:O     | 1:H:78:GLU:HA    | 2.00                     | 0.61              |
| 1:C:748:ARG:NH1  | 1:C:752:LYS:HG3  | 2.14                     | 0.61              |
| 1:G:39:LYS:HZ3   | 1:G:105:HIS:CD2  | 2.19                     | 0.61              |
| 1:D:590:LEU:HB2  | 1:D:671:PRO:HG3  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:789:MSE:HE1  | 1:H:790:PHE:N    | 2.16                     | 0.61              |
| 1:B:308:ILE:O    | 1:B:312:VAL:HG22 | 2.00                     | 0.61              |
| 1:G:245:ASN:O    | 1:G:249:VAL:HG23 | 2.00                     | 0.61              |
| 1:C:414:ASN:O    | 1:C:418:GLY:HA3  | 2.01                     | 0.61              |
| 1:D:327:GLY:O    | 1:D:328:LEU:HD23 | 2.00                     | 0.61              |
| 1:C:119:HIS:CE1  | 1:C:509:ARG:NH1  | 2.68                     | 0.61              |
| 1:G:414:ASN:O    | 1:G:418:GLY:HA3  | 2.01                     | 0.61              |
| 1:E:43:ILE:HG12  | 1:E:44:LEU:H     | 1.66                     | 0.61              |
| 1:D:216:TYR:CE1  | 1:D:220:LEU:HD11 | 2.35                     | 0.61              |
| 1:F:69:PHE:C     | 1:F:69:PHE:CD1   | 2.72                     | 0.61              |
| 1:F:685:MSE:HE3  | 1:F:745:GLY:HA2  | 1.81                     | 0.61              |
| 1:B:163:ASN:HD21 | 1:B:269:GLU:HG3  | 1.66                     | 0.61              |
| 1:F:65:GLU:HG3   | 1:F:70:PHE:HB2   | 1.81                     | 0.61              |
| 1:B:333:ARG:NH1  | 1:B:333:ARG:HG2  | 2.15                     | 0.61              |
| 1:F:420:LEU:HD13 | 1:F:420:LEU:C    | 2.21                     | 0.61              |
| 1:D:211:ARG:HG3  | 1:D:211:ARG:HH11 | 1.66                     | 0.61              |
| 1:H:46:GLN:CB    | 1:H:79:ALA:HB3   | 2.27                     | 0.61              |
| 1:C:33:LEU:O     | 1:C:36:VAL:HB    | 2.01                     | 0.61              |
| 1:F:547:HIS:O    | 1:F:551:GLU:HG2  | 2.00                     | 0.61              |
| 1:E:60:THR:HG23  | 1:E:62:LYS:H     | 1.65                     | 0.61              |
| 1:A:30:LEU:HD12  | 1:A:62:LYS:O     | 2.01                     | 0.61              |
| 1:D:524:VAL:HG12 | 1:D:758:TYR:CD2  | 2.36                     | 0.61              |
| 1:G:70:PHE:HD2   | 1:G:70:PHE:C     | 2.04                     | 0.60              |
| 1:C:483:PHE:CE1  | 1:C:487:ALA:HB3  | 2.35                     | 0.60              |
| 1:F:675:GLU:O    | 1:F:697:GLY:HA3  | 2.01                     | 0.60              |
| 1:E:60:THR:O     | 1:E:63:LYS:HG3   | 2.01                     | 0.60              |
| 1:F:82:LEU:HD13  | 1:F:83:PRO:HG3   | 1.82                     | 0.60              |
| 1:G:419:ASN:HB3  | 1:G:471:ALA:CB   | 2.31                     | 0.60              |
| 1:A:164:ARG:HD2  | 1:B:262:ALA:HB1  | 1.83                     | 0.60              |
| 1:H:419:ASN:OD1  | 1:H:435:THR:HB   | 2.01                     | 0.60              |
| 1:A:39:LYS:NZ    | 1:A:105:HIS:HD2  | 1.99                     | 0.60              |
| 1:F:789:MSE:HG2  | 1:G:789:MSE:HE3  | 1.81                     | 0.60              |
| 1:B:43:ILE:HG23  | 1:B:43:ILE:O     | 2.00                     | 0.60              |
| 1:A:373:LYS:H    | 1:A:373:LYS:CD   | 2.13                     | 0.60              |
| 1:H:89:ALA:HB1   | 1:H:99:TYR:CD1   | 2.35                     | 0.60              |
| 1:C:83:PRO:O     | 1:C:104:LEU:HD12 | 2.01                     | 0.60              |
| 1:D:43:ILE:HG23  | 1:D:124:LEU:HD12 | 1.82                     | 0.60              |
| 1:B:245:ASN:O    | 1:B:249:VAL:HG23 | 2.02                     | 0.60              |
| 1:H:259:LEU:O    | 1:H:263:PRO:HG3  | 2.02                     | 0.60              |
| 1:D:411:ILE:HG13 | 1:D:431:VAL:HG11 | 1.82                     | 0.60              |
| 1:D:750:GLU:HA   | 1:D:750:GLU:OE2  | 2.00                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:158:GLY:HA3  | 1:H:519:PRO:O    | 2.01                     | 0.60              |
| 1:D:32:LEU:O     | 1:D:36:VAL:HG23  | 2.01                     | 0.60              |
| 1:C:586:ASN:HB3  | 1:C:671:PRO:O    | 2.01                     | 0.60              |
| 1:C:60:THR:C     | 1:C:62:LYS:N     | 2.54                     | 0.60              |
| 1:C:80:ILE:HD11  | 1:C:121:LYS:CG   | 2.30                     | 0.60              |
| 1:D:564:LEU:HG   | 1:D:613:ARG:NH2  | 2.16                     | 0.60              |
| 1:A:794:LYS:O    | 1:A:797:PRO:HD2  | 2.02                     | 0.60              |
| 1:C:597:ASN:O    | 1:C:601:ARG:HG3  | 2.02                     | 0.60              |
| 1:A:37:GLU:HG3   | 1:A:59:GLN:HE22  | 1.65                     | 0.60              |
| 1:F:668:PHE:HB2  | 1:F:689:LEU:HD23 | 1.83                     | 0.60              |
| 1:C:534:PHE:HB2  | 1:C:535:PRO:CD   | 2.31                     | 0.60              |
| 1:D:116:GLU:O    | 1:D:119:HIS:HB2  | 2.02                     | 0.60              |
| 1:C:140:GLU:N    | 1:C:141:PRO:HD2  | 2.15                     | 0.60              |
| 1:F:43:ILE:HG23  | 1:F:44:LEU:H     | 1.66                     | 0.60              |
| 1:H:145:SER:HB3  | 1:H:779:ASP:CG   | 2.21                     | 0.60              |
| 1:E:547:HIS:O    | 1:E:551:GLU:HG3  | 2.00                     | 0.60              |
| 1:G:158:GLY:HA3  | 1:G:519:PRO:O    | 2.01                     | 0.60              |
| 1:B:441:GLU:OE1  | 1:B:441:GLU:HA   | 2.01                     | 0.60              |
| 1:G:56:LEU:HB3   | 1:G:57:PRO:CD    | 2.30                     | 0.60              |
| 1:D:43:ILE:O     | 1:D:44:LEU:HB2   | 2.01                     | 0.60              |
| 1:B:32:LEU:O     | 1:B:36:VAL:HG23  | 2.02                     | 0.60              |
| 1:C:217:LEU:CD1  | 1:C:249:VAL:HG12 | 2.32                     | 0.60              |
| 1:B:716:HIS:HB3  | 4:B:913:SO4:O4   | 2.02                     | 0.60              |
| 1:B:659:ARG:O    | 1:B:662:CYS:HB2  | 2.02                     | 0.60              |
| 1:H:545:LYS:HD3  | 1:H:545:LYS:H    | 1.66                     | 0.60              |
| 1:B:131:GLY:CA   | 1:B:134:THR:HG21 | 2.29                     | 0.60              |
| 1:D:629:MSE:CE   | 1:D:629:MSE:HA   | 2.29                     | 0.60              |
| 1:F:647:SER:HB2  | 1:F:649:MSE:HE2  | 1.84                     | 0.60              |
| 1:H:668:PHE:HB2  | 1:H:689:LEU:CD2  | 2.31                     | 0.60              |
| 1:H:17:ARG:HH21  | 1:H:72:LEU:CB    | 2.11                     | 0.60              |
| 1:D:54:GLU:HG3   | 1:D:55:ALA:N     | 2.16                     | 0.60              |
| 1:F:629:MSE:HE2  | 1:F:629:MSE:HA   | 1.84                     | 0.60              |
| 1:B:210:LEU:CD2  | 1:B:253:ILE:HG23 | 2.31                     | 0.60              |
| 1:H:564:LEU:HD22 | 1:H:613:ARG:NH2  | 2.17                     | 0.60              |
| 1:C:83:PRO:HG2   | 1:C:84:PRO:CD    | 2.15                     | 0.59              |
| 1:E:789:MSE:HB3  | 1:H:789:MSE:HE2  | 1.84                     | 0.59              |
| 1:G:597:ASN:O    | 1:G:601:ARG:HG3  | 2.02                     | 0.59              |
| 1:D:137:LEU:HD12 | 1:D:510:VAL:HG22 | 1.84                     | 0.59              |
| 1:F:789:MSE:CE   | 1:G:790:PHE:N    | 2.65                     | 0.59              |
| 1:D:195:MSE:HE1  | 1:D:241:GLY:CA   | 2.32                     | 0.59              |
| 1:F:155:ILE:HD13 | 1:F:516:VAL:CG1  | 2.32                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:73:LEU:N     | 1:A:73:LEU:HD23  | 2.16                     | 0.59              |
| 1:A:193:ASN:HB3  | 1:A:239:GLU:HG3  | 1.84                     | 0.59              |
| 1:H:670:GLN:O    | 1:H:670:GLN:HG3  | 2.02                     | 0.59              |
| 1:C:56:LEU:HB3   | 1:C:57:PRO:HD3   | 1.84                     | 0.59              |
| 1:C:170:LEU:HD22 | 1:C:177:LEU:HD23 | 1.83                     | 0.59              |
| 1:D:146:ILE:CG2  | 1:D:147:PRO:CD   | 2.79                     | 0.59              |
| 1:G:48:GLN:HE21  | 1:G:48:GLN:C     | 2.05                     | 0.59              |
| 1:C:290:PHE:O    | 1:C:366:ARG:NH1  | 2.35                     | 0.59              |
| 1:E:210:LEU:HD22 | 1:E:253:ILE:HG23 | 1.82                     | 0.59              |
| 1:G:146:ILE:CG2  | 1:G:147:PRO:HD2  | 2.33                     | 0.59              |
| 1:G:419:ASN:HB3  | 1:G:471:ALA:HB1  | 1.84                     | 0.59              |
| 1:A:739:ASP:O    | 1:A:743:LYS:HG2  | 2.02                     | 0.59              |
| 1:C:622:GLU:O    | 1:C:626:MSE:HG3  | 2.03                     | 0.59              |
| 1:F:82:LEU:HD12  | 1:F:83:PRO:HG3   | 1.81                     | 0.59              |
| 1:E:65:GLU:HB3   | 1:E:70:PHE:HD1   | 1.67                     | 0.59              |
| 1:D:187:HIS:HD2  | 1:D:194:LEU:HB2  | 1.67                     | 0.59              |
| 1:D:48:GLN:HE22  | 1:D:492:THR:HG22 | 1.66                     | 0.59              |
| 1:E:67:GLY:O     | 1:E:71:ASP:HB2   | 2.03                     | 0.59              |
| 1:A:56:LEU:HG    | 1:A:70:PHE:HD1   | 1.66                     | 0.59              |
| 1:H:82:LEU:CD1   | 1:H:84:PRO:HG2   | 2.31                     | 0.59              |
| 1:A:146:ILE:CG2  | 1:A:147:PRO:HD2  | 2.33                     | 0.59              |
| 1:F:668:PHE:HB2  | 1:F:689:LEU:CD2  | 2.32                     | 0.59              |
| 1:E:586:ASN:HB3  | 1:E:671:PRO:O    | 2.03                     | 0.59              |
| 1:A:65:GLU:HA    | 1:A:65:GLU:OE2   | 2.03                     | 0.59              |
| 1:B:30:LEU:N     | 1:B:30:LEU:CD1   | 2.66                     | 0.59              |
| 1:F:65:GLU:HA    | 1:F:65:GLU:OE2   | 2.03                     | 0.59              |
| 1:A:249:VAL:O    | 1:A:253:ILE:HG13 | 2.02                     | 0.59              |
| 1:B:209:THR:HG23 | 1:B:236:ILE:HB   | 1.83                     | 0.59              |
| 1:B:518:ASP:OD1  | 1:B:519:PRO:HD2  | 2.03                     | 0.59              |
| 1:F:54:GLU:HG3   | 1:F:55:ALA:N     | 2.17                     | 0.59              |
| 1:E:83:PRO:O     | 1:E:85:TRP:N     | 2.36                     | 0.59              |
| 1:H:187:HIS:HD2  | 1:H:195:MSE:HG2  | 1.68                     | 0.59              |
| 1:H:564:LEU:HD22 | 1:H:613:ARG:CZ   | 2.33                     | 0.59              |
| 1:C:378:LYS:HD3  | 1:C:805:ALA:HB1  | 1.84                     | 0.59              |
| 1:G:675:GLU:O    | 1:G:697:GLY:HA3  | 2.03                     | 0.59              |
| 1:D:248:ARG:HB3  | 1:D:248:ARG:HH11 | 1.67                     | 0.59              |
| 1:A:80:ILE:N     | 1:A:87:ALA:O     | 2.34                     | 0.59              |
| 1:F:647:SER:HB2  | 1:F:649:MSE:CE   | 2.33                     | 0.59              |
| 1:F:316:GLU:HA   | 1:F:319:MSE:CE   | 2.20                     | 0.59              |
| 1:B:43:ILE:HD13  | 1:B:43:ILE:O     | 2.03                     | 0.59              |
| 1:B:249:VAL:O    | 1:B:253:ILE:HG12 | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:39:LYS:HZ2   | 1:D:39:LYS:HB2   | 1.66                     | 0.59              |
| 1:B:217:LEU:HD11 | 1:B:233:PHE:HZ   | 1.67                     | 0.59              |
| 1:E:60:THR:HG23  | 1:E:62:LYS:CB    | 2.33                     | 0.58              |
| 1:A:195:MSE:HE3  | 1:A:242:TRP:CE2  | 2.38                     | 0.58              |
| 1:F:81:VAL:HG23  | 1:F:81:VAL:O     | 2.03                     | 0.58              |
| 1:C:146:ILE:HG23 | 1:C:147:PRO:HD2  | 1.85                     | 0.58              |
| 1:H:171:PHE:HD1  | 1:H:263:PRO:HD2  | 1.68                     | 0.58              |
| 1:A:547:HIS:O    | 1:A:551:GLU:HG3  | 2.03                     | 0.58              |
| 1:C:564:LEU:HG   | 1:C:613:ARG:NH2  | 2.17                     | 0.58              |
| 1:G:83:PRO:HB2   | 1:G:84:PRO:HD2   | 1.85                     | 0.58              |
| 1:B:146:ILE:HD11 | 1:B:772:TRP:CZ2  | 2.38                     | 0.58              |
| 1:A:772:TRP:CZ2  | 1:A:776:SER:HB3  | 2.38                     | 0.58              |
| 1:H:131:GLY:CA   | 1:H:134:THR:HG23 | 2.33                     | 0.58              |
| 1:D:102:VAL:HG23 | 1:D:109:VAL:HG23 | 1.85                     | 0.58              |
| 1:F:545:LYS:CD   | 1:F:545:LYS:H    | 2.16                     | 0.58              |
| 1:E:100:LEU:O    | 1:E:100:LEU:HD12 | 2.03                     | 0.58              |
| 1:D:41:LYS:N     | 7:D:868:HOH:O    | 2.36                     | 0.58              |
| 1:A:81:VAL:HA    | 1:A:86:VAL:HG23  | 1.85                     | 0.58              |
| 1:F:284:LEU:O    | 1:F:414:ASN:HB2  | 2.04                     | 0.58              |
| 1:A:435:THR:HG23 | 1:A:475:THR:HB   | 1.84                     | 0.58              |
| 1:G:586:ASN:HB3  | 1:G:671:PRO:O    | 2.03                     | 0.58              |
| 1:B:83:PRO:C     | 1:B:85:TRP:N     | 2.57                     | 0.58              |
| 1:A:789:MSE:HE2  | 1:D:789:MSE:CG   | 2.33                     | 0.58              |
| 1:G:170:LEU:HD13 | 1:G:177:LEU:HD23 | 1.85                     | 0.58              |
| 1:C:121:LYS:O    | 1:C:124:LEU:HB3  | 2.02                     | 0.58              |
| 1:D:187:HIS:CD2  | 1:D:194:LEU:HB2  | 2.39                     | 0.58              |
| 1:D:387:PRO:HD3  | 1:D:802:VAL:HB   | 1.85                     | 0.58              |
| 1:F:582:ASP:HB2  | 1:F:621:GLU:OE1  | 2.04                     | 0.58              |
| 1:C:156:GLY:O    | 1:C:522:ASN:HA   | 2.03                     | 0.58              |
| 1:G:56:LEU:HD13  | 1:G:63:LYS:HG2   | 1.85                     | 0.58              |
| 1:C:50:ILE:CD1   | 1:C:54:GLU:CB    | 2.75                     | 0.58              |
| 1:F:162:LEU:HD11 | 1:F:772:TRP:CD2  | 2.38                     | 0.58              |
| 1:H:82:LEU:HD12  | 1:H:84:PRO:HD2   | 1.85                     | 0.58              |
| 1:G:698:GLY:N    | 1:G:699:PRO:CD   | 2.67                     | 0.58              |
| 1:E:593:TRP:HB3  | 1:E:721:ALA:HB2  | 1.84                     | 0.58              |
| 1:B:796:ARG:HB2  | 1:B:797:PRO:HD3  | 1.85                     | 0.58              |
| 1:C:221:LYS:HE3  | 1:C:223:GLU:OE2  | 2.04                     | 0.58              |
| 1:E:207:GLN:HE21 | 1:E:211:ARG:NH2  | 2.01                     | 0.58              |
| 1:E:148:ARG:NH1  | 1:E:148:ARG:CG   | 2.57                     | 0.58              |
| 1:G:131:GLY:HA3  | 1:G:134:THR:HG23 | 1.84                     | 0.58              |
| 1:D:39:LYS:HZ2   | 1:D:39:LYS:CB    | 2.17                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:80:ILE:CD1   | 1:C:121:LYS:HG3  | 2.34                     | 0.58              |
| 1:G:249:VAL:O    | 1:G:253:ILE:HG12 | 2.03                     | 0.58              |
| 1:G:591:VAL:HG12 | 1:G:632:LEU:HD13 | 1.86                     | 0.58              |
| 1:G:479:ILE:HD11 | 1:G:762:LEU:CD1  | 2.34                     | 0.58              |
| 1:D:48:GLN:HA    | 1:D:51:ALA:HB3   | 1.84                     | 0.58              |
| 1:F:244:ASP:OD2  | 1:F:248:ARG:HD2  | 2.04                     | 0.58              |
| 1:H:681:VAL:HG12 | 1:H:685:MSE:SE   | 2.54                     | 0.58              |
| 1:G:407:LYS:HB2  | 1:G:408:PRO:CD   | 2.33                     | 0.58              |
| 1:G:65:GLU:CG    | 1:G:70:PHE:HB2   | 2.34                     | 0.58              |
| 1:G:338:THR:HG23 | 1:G:366:ARG:HG2  | 1.84                     | 0.58              |
| 1:E:65:GLU:CG    | 1:E:70:PHE:HB2   | 2.33                     | 0.58              |
| 1:H:113:GLN:N    | 1:H:113:GLN:CD   | 2.57                     | 0.58              |
| 1:E:207:GLN:HE21 | 1:E:211:ARG:HH22 | 1.52                     | 0.58              |
| 1:A:796:ARG:O    | 1:A:800:GLN:HG3  | 2.03                     | 0.58              |
| 1:D:27:ASN:HD22  | 1:D:27:ASN:N     | 2.01                     | 0.57              |
| 1:H:217:LEU:HD23 | 1:H:220:LEU:HD12 | 1.85                     | 0.57              |
| 1:F:173:ASP:HB3  | 1:F:176:SER:CB   | 2.33                     | 0.57              |
| 1:C:564:LEU:HG   | 1:C:613:ARG:HH22 | 1.70                     | 0.57              |
| 1:B:259:LEU:HD21 | 1:B:268:LEU:HA   | 1.85                     | 0.57              |
| 1:E:53:PHE:O     | 1:E:57:PRO:CG    | 2.50                     | 0.57              |
| 1:C:772:TRP:CH2  | 1:C:776:SER:HB3  | 2.39                     | 0.57              |
| 1:H:143:ASN:HB3  | 1:H:148:ARG:HH12 | 1.69                     | 0.57              |
| 1:E:158:GLY:HA3  | 1:E:519:PRO:O    | 2.04                     | 0.57              |
| 1:B:160:ASP:O    | 1:B:164:ARG:HG3  | 2.03                     | 0.57              |
| 1:E:156:GLY:O    | 1:E:522:ASN:HA   | 2.03                     | 0.57              |
| 1:F:65:GLU:CG    | 1:F:70:PHE:HB2   | 2.34                     | 0.57              |
| 1:F:70:PHE:CG    | 1:F:71:ASP:N     | 2.72                     | 0.57              |
| 1:B:338:THR:HG23 | 1:B:366:ARG:HG2  | 1.84                     | 0.57              |
| 1:B:622:GLU:HG2  | 1:B:626:MSE:HE3  | 1.86                     | 0.57              |
| 1:D:83:PRO:CG    | 1:D:84:PRO:CD    | 2.82                     | 0.57              |
| 1:B:278:VAL:HG12 | 1:B:319:MSE:HE3  | 1.87                     | 0.57              |
| 1:F:633:ILE:HA   | 1:F:638:LEU:HD12 | 1.86                     | 0.57              |
| 1:G:659:ARG:O    | 1:G:662:CYS:HB2  | 2.04                     | 0.57              |
| 1:F:145:SER:HB2  | 1:F:779:ASP:OD2  | 2.04                     | 0.57              |
| 1:G:124:LEU:O    | 1:G:124:LEU:HD23 | 2.05                     | 0.57              |
| 1:A:789:MSE:HE1  | 1:D:790:PHE:N    | 2.19                     | 0.57              |
| 1:H:131:GLY:N    | 1:H:134:THR:HG23 | 2.19                     | 0.57              |
| 1:E:756:GLN:HG2  | 1:E:757:ILE:H    | 1.69                     | 0.57              |
| 1:A:407:LYS:HB2  | 1:A:408:PRO:HD2  | 1.87                     | 0.57              |
| 1:E:442:LYS:HD2  | 1:E:449:ASP:HB3  | 1.85                     | 0.57              |
| 1:C:39:LYS:CB    | 1:C:104:LEU:HD13 | 2.29                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:37:GLU:HG3   | 1:D:59:GLN:HE21  | 1.68                     | 0.57              |
| 1:C:217:LEU:HD11 | 1:C:249:VAL:CG1  | 2.34                     | 0.57              |
| 1:B:140:GLU:N    | 1:B:141:PRO:HD2  | 2.19                     | 0.57              |
| 1:C:407:LYS:HB2  | 1:C:408:PRO:CD   | 2.35                     | 0.57              |
| 1:F:315:LEU:O    | 1:F:319:MSE:HG3  | 2.05                     | 0.57              |
| 1:B:52:GLU:O     | 1:B:57:PRO:HD2   | 2.04                     | 0.57              |
| 1:C:566:VAL:HG12 | 1:C:567:LEU:N    | 2.19                     | 0.57              |
| 1:B:17:ARG:CB    | 1:B:72:LEU:HD21  | 2.34                     | 0.57              |
| 1:F:52:GLU:CG    | 1:F:53:PHE:N     | 2.66                     | 0.57              |
| 1:H:95:GLY:HA3   | 1:H:517:PHE:CE2  | 2.38                     | 0.57              |
| 1:C:80:ILE:CD1   | 1:C:121:LYS:CG   | 2.83                     | 0.57              |
| 1:E:73:LEU:CD2   | 1:E:73:LEU:N     | 2.67                     | 0.57              |
| 1:F:56:LEU:N     | 1:F:57:PRO:CD    | 2.68                     | 0.57              |
| 1:F:59:GLN:CG    | 1:F:60:THR:H     | 2.17                     | 0.57              |
| 1:G:784:ARG:O    | 1:G:788:GLU:HG3  | 2.04                     | 0.57              |
| 1:G:32:LEU:O     | 1:G:32:LEU:HD13  | 2.05                     | 0.56              |
| 1:G:119:HIS:CE1  | 1:G:129:LYS:CB   | 2.88                     | 0.56              |
| 1:F:726:ASP:O    | 1:F:730:LYS:HG3  | 2.04                     | 0.56              |
| 1:D:322:ARG:HD2  | 1:D:763:LEU:HD12 | 1.86                     | 0.56              |
| 1:G:472:MSE:SE   | 1:G:514:ILE:HB   | 2.55                     | 0.56              |
| 1:F:628:LYS:CA   | 1:F:628:LYS:HE2  | 2.35                     | 0.56              |
| 1:F:479:ILE:CD1  | 1:F:762:LEU:HD13 | 2.35                     | 0.56              |
| 1:E:44:LEU:O     | 1:E:81:VAL:HG12  | 2.04                     | 0.56              |
| 1:F:82:LEU:HD12  | 1:F:82:LEU:H     | 1.71                     | 0.56              |
| 1:E:173:ASP:HB3  | 1:E:176:SER:HB2  | 1.87                     | 0.56              |
| 1:C:70:PHE:O     | 1:C:71:ASP:CB    | 2.52                     | 0.56              |
| 1:A:784:ARG:O    | 1:A:788:GLU:HG3  | 2.05                     | 0.56              |
| 1:A:668:PHE:HB2  | 1:A:689:LEU:HD23 | 1.87                     | 0.56              |
| 1:F:83:PRO:HG2   | 1:F:85:TRP:HB2   | 1.88                     | 0.56              |
| 1:D:166:LEU:O    | 1:D:170:LEU:HB2  | 2.05                     | 0.56              |
| 1:D:259:LEU:O    | 1:D:263:PRO:HG3  | 2.06                     | 0.56              |
| 1:G:54:GLU:OE2   | 1:G:55:ALA:HA    | 2.05                     | 0.56              |
| 1:C:119:HIS:HE1  | 1:C:509:ARG:HH12 | 1.50                     | 0.56              |
| 1:C:171:PHE:CD1  | 1:C:263:PRO:HD2  | 2.40                     | 0.56              |
| 1:E:565:CYS:C    | 1:E:566:VAL:CG2  | 2.73                     | 0.56              |
| 1:G:565:CYS:HB2  | 1:G:642:PHE:O    | 2.05                     | 0.56              |
| 1:A:470:PHE:CE1  | 1:A:791:TYR:HB2  | 2.40                     | 0.56              |
| 1:H:407:LYS:HB2  | 1:H:408:PRO:HD2  | 1.86                     | 0.56              |
| 1:G:625:GLU:O    | 1:G:629:MSE:HG2  | 2.05                     | 0.56              |
| 1:C:348:THR:O    | 1:C:351:GLU:HG2  | 2.05                     | 0.56              |
| 1:G:657:LEU:O    | 1:G:661:ILE:HG12 | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:682:VAL:HG13 | 1:B:749:ILE:HD12 | 1.87                     | 0.56              |
| 1:D:491:GLU:CD   | 1:D:491:GLU:H    | 2.09                     | 0.56              |
| 1:E:447:ASP:HB3  | 1:E:451:TYR:CD2  | 2.40                     | 0.56              |
| 1:F:56:LEU:N     | 1:F:57:PRO:HD2   | 2.20                     | 0.56              |
| 1:A:195:MSE:HE1  | 1:A:242:TRP:CA   | 2.31                     | 0.56              |
| 1:D:44:LEU:HA    | 1:D:124:LEU:HD11 | 1.87                     | 0.56              |
| 1:E:565:CYS:C    | 1:E:566:VAL:HG23 | 2.26                     | 0.56              |
| 1:F:534:PHE:HB2  | 1:F:535:PRO:CD   | 2.36                     | 0.56              |
| 1:E:435:THR:HG23 | 1:E:475:THR:CB   | 2.36                     | 0.56              |
| 1:B:63:LYS:HG3   | 1:B:64:LEU:H     | 1.70                     | 0.56              |
| 1:C:670:GLN:O    | 1:C:670:GLN:HG3  | 2.05                     | 0.56              |
| 1:B:83:PRO:C     | 1:B:85:TRP:H     | 2.08                     | 0.56              |
| 1:B:206:LEU:HD11 | 1:B:210:LEU:HD11 | 1.87                     | 0.56              |
| 1:D:39:LYS:NZ    | 1:D:39:LYS:CB    | 2.68                     | 0.56              |
| 1:A:72:LEU:C     | 1:A:73:LEU:HD23  | 2.26                     | 0.56              |
| 1:E:156:GLY:HA3  | 1:E:523:ILE:HG13 | 1.86                     | 0.56              |
| 1:F:189:HIS:ND1  | 1:F:330:ILE:HD13 | 2.21                     | 0.56              |
| 1:B:407:LYS:HB2  | 1:B:408:PRO:HD2  | 1.86                     | 0.56              |
| 1:F:717:GLY:O    | 1:F:720:ALA:HB3  | 2.05                     | 0.56              |
| 1:B:102:VAL:HA   | 1:B:109:VAL:HA   | 1.88                     | 0.56              |
| 1:D:400:LEU:HD12 | 1:D:400:LEU:C    | 2.25                     | 0.56              |
| 1:H:56:LEU:O     | 1:H:63:LYS:HD2   | 2.06                     | 0.56              |
| 1:H:63:LYS:O     | 1:H:65:GLU:HG2   | 2.05                     | 0.56              |
| 1:B:420:LEU:HD13 | 1:B:420:LEU:C    | 2.25                     | 0.56              |
| 1:F:51:ALA:O     | 1:F:52:GLU:HB3   | 2.05                     | 0.56              |
| 1:F:469:ILE:CD1  | 1:F:472:MSE:HE1  | 2.19                     | 0.56              |
| 1:E:217:LEU:HD23 | 1:E:220:LEU:CD1  | 2.36                     | 0.56              |
| 1:B:56:LEU:CB    | 1:B:57:PRO:HD3   | 2.32                     | 0.56              |
| 1:D:532:ILE:HD12 | 1:D:652:VAL:HG22 | 1.88                     | 0.56              |
| 1:A:338:THR:HG23 | 1:A:366:ARG:HG2  | 1.88                     | 0.56              |
| 1:E:659:ARG:O    | 1:E:662:CYS:HB2  | 2.05                     | 0.56              |
| 1:E:224:THR:HG23 | 1:E:228:GLU:HG3  | 1.87                     | 0.56              |
| 1:E:44:LEU:HA    | 1:E:124:LEU:HD21 | 1.88                     | 0.56              |
| 1:G:390:GLU:HG3  | 1:G:791:TYR:OH   | 2.06                     | 0.56              |
| 1:D:131:GLY:C    | 1:D:134:THR:HG23 | 2.26                     | 0.56              |
| 1:D:181:LEU:HD12 | 1:D:196:LEU:HD12 | 1.86                     | 0.56              |
| 1:E:101:ARG:H    | 1:E:112:LEU:HD21 | 1.70                     | 0.56              |
| 1:B:794:LYS:O    | 1:B:798:LEU:HD12 | 2.05                     | 0.56              |
| 1:A:789:MSE:HE2  | 1:D:789:MSE:SE   | 2.56                     | 0.56              |
| 1:E:789:MSE:HE1  | 1:H:789:MSE:C    | 2.26                     | 0.56              |
| 1:C:172:HIS:CD2  | 1:D:147:PRO:HB2  | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:193:ASN:HB3  | 1:E:239:GLU:HG3  | 1.88                     | 0.56              |
| 1:A:536:TYR:CE1  | 1:A:537:THR:HG23 | 2.41                     | 0.56              |
| 1:G:65:GLU:HG2   | 1:G:70:PHE:HB2   | 1.88                     | 0.56              |
| 1:F:315:LEU:HD11 | 1:F:762:LEU:HD23 | 1.87                     | 0.56              |
| 1:E:83:PRO:CB    | 1:E:84:PRO:CD    | 2.84                     | 0.56              |
| 1:G:131:GLY:H    | 1:G:134:THR:CG2  | 2.18                     | 0.56              |
| 1:B:449:ASP:O    | 1:B:504:LEU:HD22 | 2.06                     | 0.56              |
| 1:B:63:LYS:CG    | 1:B:64:LEU:H     | 2.19                     | 0.56              |
| 1:A:232:LYS:HE3  | 1:A:236:ILE:HD13 | 1.87                     | 0.56              |
| 1:B:232:LYS:O    | 1:B:235:GLU:HB2  | 2.06                     | 0.56              |
| 1:E:116:GLU:O    | 1:E:119:HIS:HB2  | 2.05                     | 0.56              |
| 1:D:216:TYR:C    | 1:D:216:TYR:CD1  | 2.80                     | 0.56              |
| 1:G:670:GLN:O    | 1:G:670:GLN:HG3  | 2.06                     | 0.56              |
| 1:B:99:TYR:CZ    | 1:B:114:PRO:HG3  | 2.40                     | 0.55              |
| 1:A:153:LYS:HD3  | 1:A:154:TYR:CE2  | 2.41                     | 0.55              |
| 1:C:623:LYS:HA   | 1:C:626:MSE:HE2  | 1.87                     | 0.55              |
| 1:F:778:LEU:HD12 | 1:F:779:ASP:H    | 1.70                     | 0.55              |
| 1:A:146:ILE:HG22 | 1:A:147:PRO:O    | 2.06                     | 0.55              |
| 1:A:170:LEU:HD22 | 1:A:177:LEU:HD23 | 1.88                     | 0.55              |
| 1:C:278:VAL:HG21 | 1:C:763:LEU:HD23 | 1.87                     | 0.55              |
| 1:B:146:ILE:HG22 | 1:B:147:PRO:CD   | 2.35                     | 0.55              |
| 1:F:591:VAL:CG2  | 1:F:629:MSE:HE1  | 2.35                     | 0.55              |
| 1:C:146:ILE:HD11 | 1:C:162:LEU:HD13 | 1.87                     | 0.55              |
| 1:A:135:LEU:HD22 | 1:D:793:LEU:HD11 | 1.88                     | 0.55              |
| 1:E:125:VAL:HG22 | 1:E:126:ASP:OD2  | 2.05                     | 0.55              |
| 1:E:414:ASN:O    | 1:E:418:GLY:HA3  | 2.07                     | 0.55              |
| 1:C:665:LYS:HD3  | 1:C:665:LYS:N    | 2.21                     | 0.55              |
| 1:D:223:GLU:HG3  | 1:D:223:GLU:O    | 2.05                     | 0.55              |
| 1:F:82:LEU:HD12  | 1:F:83:PRO:CG    | 2.36                     | 0.55              |
| 1:D:146:ILE:HG22 | 1:D:147:PRO:N    | 2.21                     | 0.55              |
| 1:A:681:VAL:O    | 1:A:685:MSE:HG3  | 2.06                     | 0.55              |
| 1:F:68:PRO:O     | 1:F:70:PHE:N     | 2.39                     | 0.55              |
| 1:E:48:GLN:HB3   | 7:E:875:HOH:O    | 2.06                     | 0.55              |
| 1:F:137:LEU:HD12 | 1:F:510:VAL:HG22 | 1.89                     | 0.55              |
| 1:C:52:GLU:OE2   | 1:C:53:PHE:N     | 2.39                     | 0.55              |
| 1:F:210:LEU:CD2  | 1:F:253:ILE:HG23 | 2.35                     | 0.55              |
| 1:E:249:VAL:O    | 1:E:253:ILE:HG12 | 2.05                     | 0.55              |
| 1:F:70:PHE:CD2   | 1:F:71:ASP:HB2   | 2.41                     | 0.55              |
| 1:E:680:THR:HG23 | 2:E:901:UDP:O1A  | 2.07                     | 0.55              |
| 1:F:250:LEU:HG   | 1:F:254:ARG:NH1  | 2.22                     | 0.55              |
| 1:D:222:SER:HB3  | 1:D:247:GLU:HB2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:789:MSE:HE2  | 1:G:789:MSE:HE3  | 1.89                     | 0.55              |
| 1:D:106:ALA:CB   | 1:D:108:VAL:HG23 | 2.32                     | 0.55              |
| 1:D:131:GLY:O    | 1:D:134:THR:HG23 | 2.06                     | 0.55              |
| 1:D:532:ILE:HG13 | 1:D:651:ARG:HD2  | 1.88                     | 0.55              |
| 1:A:156:GLY:HA3  | 1:A:523:ILE:HG13 | 1.89                     | 0.55              |
| 1:F:419:ASN:HB3  | 1:F:471:ALA:HB1  | 1.89                     | 0.55              |
| 1:H:216:TYR:CD1  | 1:H:220:LEU:HD11 | 2.40                     | 0.55              |
| 1:F:32:LEU:O     | 1:F:35:ARG:HB3   | 2.07                     | 0.55              |
| 1:F:629:MSE:HE3  | 1:F:629:MSE:HA   | 1.88                     | 0.55              |
| 1:H:143:ASN:HB3  | 1:H:148:ARG:NH1  | 2.22                     | 0.55              |
| 1:B:318:GLU:HG3  | 1:B:322:ARG:HD2  | 1.89                     | 0.55              |
| 1:F:81:VAL:HG12  | 1:F:86:VAL:CA    | 2.35                     | 0.55              |
| 1:F:35:ARG:CD    | 1:F:104:LEU:HA   | 2.32                     | 0.55              |
| 1:F:233:PHE:CE1  | 1:F:238:LEU:HD12 | 2.42                     | 0.55              |
| 1:C:298:TYR:CE1  | 1:C:649:MSE:HE1  | 2.42                     | 0.55              |
| 1:E:367:VAL:HG22 | 1:E:399:GLU:HG3  | 1.88                     | 0.55              |
| 1:E:333:ARG:HG2  | 1:E:333:ARG:NH1  | 2.22                     | 0.55              |
| 1:A:789:MSE:CE   | 1:D:789:MSE:CG   | 2.84                     | 0.55              |
| 1:A:82:LEU:HB3   | 1:A:83:PRO:CD    | 2.35                     | 0.55              |
| 1:A:230:GLU:OE1  | 1:A:240:ARG:NH1  | 2.40                     | 0.55              |
| 1:H:33:LEU:HA    | 1:H:36:VAL:CB    | 2.37                     | 0.54              |
| 1:F:141:PRO:HB2  | 1:G:782:GLU:HG3  | 1.90                     | 0.54              |
| 1:A:140:GLU:N    | 1:A:141:PRO:HD2  | 2.21                     | 0.54              |
| 1:H:91:ARG:HD2   | 1:H:97:TRP:CZ2   | 2.42                     | 0.54              |
| 1:H:400:LEU:C    | 1:H:400:LEU:HD12 | 2.27                     | 0.54              |
| 1:A:316:GLU:CA   | 1:A:319:MSE:HE3  | 2.32                     | 0.54              |
| 1:A:56:LEU:HB3   | 1:A:57:PRO:CD    | 2.34                     | 0.54              |
| 1:F:216:TYR:CE2  | 1:F:232:LYS:HG2  | 2.41                     | 0.54              |
| 1:A:154:TYR:OH   | 1:B:262:ALA:HB3  | 2.06                     | 0.54              |
| 1:A:419:ASN:HB3  | 1:A:471:ALA:HB1  | 1.89                     | 0.54              |
| 1:F:793:LEU:HB3  | 1:G:793:LEU:HB3  | 1.89                     | 0.54              |
| 1:A:458:LYS:HE2  | 1:A:459:TYR:CZ   | 2.42                     | 0.54              |
| 1:A:786:TYR:CE1  | 1:D:789:MSE:HE3  | 2.41                     | 0.54              |
| 1:D:56:LEU:CD1   | 1:D:57:PRO:CD    | 2.84                     | 0.54              |
| 1:H:210:LEU:CD2  | 1:H:253:ILE:HG23 | 2.34                     | 0.54              |
| 1:F:428:LYS:HG2  | 1:F:429:LEU:HD23 | 1.90                     | 0.54              |
| 1:C:692:PHE:CG   | 1:C:724:LEU:HD21 | 2.42                     | 0.54              |
| 1:C:757:ILE:N    | 1:C:757:ILE:HD13 | 2.23                     | 0.54              |
| 1:C:681:VAL:HG13 | 1:C:691:THR:HG21 | 1.89                     | 0.54              |
| 1:D:41:LYS:HE3   | 1:D:54:GLU:CG    | 2.37                     | 0.54              |
| 1:C:63:LYS:O     | 1:C:65:GLU:CG    | 2.55                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:225:LEU:O    | 1:B:228:GLU:HG2  | 2.08                     | 0.54              |
| 1:B:354:GLU:OE1  | 1:B:366:ARG:NH2  | 2.40                     | 0.54              |
| 1:B:777:ASN:OD1  | 1:B:778:LEU:HD23 | 2.08                     | 0.54              |
| 1:D:518:ASP:OD1  | 1:D:520:LYS:HG2  | 2.07                     | 0.54              |
| 1:F:434:CYS:SG   | 1:F:479:ILE:HG13 | 2.47                     | 0.54              |
| 1:H:39:LYS:O     | 1:H:39:LYS:HD3   | 2.08                     | 0.54              |
| 1:B:41:LYS:HD2   | 1:B:46:GLN:HE22  | 1.73                     | 0.54              |
| 1:G:315:LEU:HD21 | 1:G:762:LEU:CD2  | 2.36                     | 0.54              |
| 1:A:245:ASN:O    | 1:A:249:VAL:HG23 | 2.07                     | 0.54              |
| 1:G:73:LEU:N     | 1:G:73:LEU:CD2   | 2.70                     | 0.54              |
| 1:D:210:LEU:HD22 | 1:D:253:ILE:HG23 | 1.89                     | 0.54              |
| 1:A:232:LYS:O    | 1:A:235:GLU:HB2  | 2.07                     | 0.54              |
| 1:A:793:LEU:HB3  | 1:D:793:LEU:HB3  | 1.88                     | 0.54              |
| 1:E:534:PHE:HB2  | 1:E:535:PRO:CD   | 2.37                     | 0.54              |
| 1:H:657:LEU:O    | 1:H:661:ILE:HG12 | 2.08                     | 0.54              |
| 1:C:158:GLY:HA3  | 1:C:519:PRO:O    | 2.07                     | 0.54              |
| 1:B:534:PHE:HB2  | 1:B:535:PRO:CD   | 2.38                     | 0.54              |
| 1:E:790:PHE:O    | 1:E:794:LYS:HB3  | 2.07                     | 0.54              |
| 1:H:82:LEU:HD11  | 1:H:85:TRP:HB2   | 1.89                     | 0.54              |
| 1:C:483:PHE:CZ   | 1:C:487:ALA:HB3  | 2.43                     | 0.54              |
| 1:C:607:VAL:HG22 | 1:C:643:ARG:HB3  | 1.89                     | 0.54              |
| 1:E:189:HIS:ND1  | 1:E:330:ILE:HD13 | 2.22                     | 0.54              |
| 1:G:164:ARG:HD2  | 1:H:262:ALA:HB1  | 1.89                     | 0.54              |
| 1:G:259:LEU:HD21 | 1:G:267:THR:HG22 | 1.89                     | 0.54              |
| 1:C:87:ALA:O     | 1:C:88:LEU:HD23  | 2.08                     | 0.54              |
| 1:E:137:LEU:HD11 | 1:E:790:PHE:CE1  | 2.42                     | 0.54              |
| 1:A:195:MSE:CE   | 1:A:242:TRP:HA   | 2.32                     | 0.54              |
| 1:C:692:PHE:CE2  | 1:C:724:LEU:HD23 | 2.42                     | 0.54              |
| 1:G:278:VAL:HG12 | 1:G:319:MSE:HE3  | 1.89                     | 0.54              |
| 1:F:716:HIS:HB3  | 4:F:913:SO4:O2   | 2.08                     | 0.54              |
| 1:A:609:VAL:HG22 | 1:A:645:ILE:HB   | 1.90                     | 0.54              |
| 1:B:131:GLY:CA   | 1:B:134:THR:CG2  | 2.76                     | 0.54              |
| 1:D:176:SER:O    | 1:D:179:PRO:HD2  | 2.08                     | 0.54              |
| 1:E:65:GLU:CG    | 1:E:70:PHE:CB    | 2.83                     | 0.54              |
| 1:H:33:LEU:HD23  | 1:H:33:LEU:H     | 1.72                     | 0.54              |
| 1:D:112:LEU:CD2  | 1:D:116:GLU:HB3  | 2.38                     | 0.54              |
| 1:D:131:GLY:HA3  | 1:D:134:THR:CG2  | 2.37                     | 0.54              |
| 1:H:407:LYS:HB2  | 1:H:408:PRO:CD   | 2.38                     | 0.54              |
| 1:B:322:ARG:CD   | 1:B:763:LEU:HD13 | 2.37                     | 0.54              |
| 1:H:308:ILE:O    | 1:H:312:VAL:HG22 | 2.08                     | 0.54              |
| 1:H:94:PRO:HB3   | 1:H:487:ALA:HB1  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:443:THR:HG21 | 1:G:495:GLN:HA   | 1.88                     | 0.54              |
| 1:D:770:GLY:O    | 1:D:773:LYS:HG2  | 2.08                     | 0.54              |
| 1:B:672:ALA:O    | 1:B:714:PRO:HG3  | 2.07                     | 0.54              |
| 1:F:315:LEU:C    | 1:F:319:MSE:HE2  | 2.28                     | 0.54              |
| 1:D:298:TYR:HE1  | 1:D:649:MSE:HE1  | 1.62                     | 0.54              |
| 1:A:685:MSE:HE3  | 1:A:745:GLY:CA   | 2.36                     | 0.54              |
| 1:C:216:TYR:HE2  | 1:C:232:LYS:CD   | 2.21                     | 0.54              |
| 1:A:354:GLU:OE1  | 1:A:366:ARG:NH2  | 2.41                     | 0.54              |
| 1:C:86:VAL:HB    | 1:C:104:LEU:HD21 | 1.90                     | 0.54              |
| 1:F:181:LEU:HD13 | 1:F:206:LEU:HD22 | 1.90                     | 0.54              |
| 1:G:27:ASN:C     | 1:G:30:LEU:HD12  | 2.29                     | 0.54              |
| 1:H:163:ASN:ND2  | 1:H:269:GLU:HB2  | 2.23                     | 0.54              |
| 1:B:633:ILE:HA   | 1:B:638:LEU:HD12 | 1.90                     | 0.54              |
| 1:H:553:LEU:CD2  | 1:H:645:ILE:HD13 | 2.38                     | 0.54              |
| 1:A:116:GLU:O    | 1:A:119:HIS:HB2  | 2.08                     | 0.54              |
| 1:A:35:ARG:O     | 1:A:39:LYS:HG3   | 2.08                     | 0.53              |
| 1:F:789:MSE:CE   | 1:G:789:MSE:C    | 2.77                     | 0.53              |
| 1:B:43:ILE:N     | 1:B:81:VAL:CB    | 2.71                     | 0.53              |
| 1:B:30:LEU:CG    | 1:B:62:LYS:O     | 2.56                     | 0.53              |
| 1:B:153:LYS:HG2  | 1:B:154:TYR:CD2  | 2.43                     | 0.53              |
| 1:G:146:ILE:HG22 | 1:G:147:PRO:O    | 2.08                     | 0.53              |
| 1:C:207:GLN:NE2  | 1:C:211:ARG:NH2  | 2.56                     | 0.53              |
| 1:C:242:TRP:HB2  | 1:C:249:VAL:HG22 | 1.91                     | 0.53              |
| 1:B:259:LEU:O    | 1:B:263:PRO:HG3  | 2.07                     | 0.53              |
| 1:C:243:GLY:HA2  | 1:C:326:GLN:HA   | 1.89                     | 0.53              |
| 1:D:140:GLU:N    | 1:D:141:PRO:HD2  | 2.22                     | 0.53              |
| 1:F:789:MSE:SE   | 1:G:789:MSE:CE   | 3.06                     | 0.53              |
| 1:B:91:ARG:HD2   | 1:B:97:TRP:CZ2   | 2.43                     | 0.53              |
| 1:E:35:ARG:CG    | 1:E:35:ARG:HH11  | 2.19                     | 0.53              |
| 1:B:789:MSE:HE2  | 1:C:135:LEU:HD21 | 1.90                     | 0.53              |
| 1:G:126:ASP:C    | 1:G:128:VAL:H    | 2.10                     | 0.53              |
| 1:E:140:GLU:N    | 1:E:141:PRO:HD2  | 2.23                     | 0.53              |
| 1:G:49:ILE:HD12  | 1:G:49:ILE:N     | 2.23                     | 0.53              |
| 1:F:53:PHE:O     | 1:F:57:PRO:HB2   | 2.08                     | 0.53              |
| 1:G:692:PHE:CD2  | 1:G:724:LEU:CD2  | 2.91                     | 0.53              |
| 1:H:131:GLY:N    | 1:H:134:THR:CG2  | 2.72                     | 0.53              |
| 1:G:117:PHE:O    | 1:G:120:PHE:HB2  | 2.08                     | 0.53              |
| 1:F:88:LEU:HB2   | 1:F:100:LEU:HD12 | 1.89                     | 0.53              |
| 1:E:35:ARG:HG2   | 1:E:35:ARG:HH11  | 1.73                     | 0.53              |
| 1:E:105:HIS:O    | 1:E:106:ALA:CB   | 2.57                     | 0.53              |
| 1:E:178:LEU:N    | 1:E:179:PRO:HD2  | 2.22                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:443:THR:HG21 | 1:C:495:GLN:HA   | 1.89                     | 0.53              |
| 1:C:222:SER:HB3  | 1:C:247:GLU:HB2  | 1.91                     | 0.53              |
| 1:G:458:LYS:HD3  | 1:G:459:TYR:CE2  | 2.43                     | 0.53              |
| 1:E:441:GLU:HA   | 1:E:441:GLU:OE1  | 2.08                     | 0.53              |
| 1:F:178:LEU:HB2  | 1:F:179:PRO:HD3  | 1.89                     | 0.53              |
| 1:G:131:GLY:N    | 1:G:134:THR:CG2  | 2.71                     | 0.53              |
| 1:E:178:LEU:HB2  | 1:E:179:PRO:HD3  | 1.89                     | 0.53              |
| 1:C:420:LEU:C    | 1:C:420:LEU:HD13 | 2.29                     | 0.53              |
| 1:H:486:ILE:HG22 | 1:H:516:VAL:HG22 | 1.90                     | 0.53              |
| 1:G:137:LEU:HD11 | 1:G:790:PHE:CE1  | 2.43                     | 0.53              |
| 1:B:45:GLN:HG3   | 1:B:80:ILE:HG22  | 1.89                     | 0.53              |
| 1:E:181:LEU:HD13 | 1:E:206:LEU:HD22 | 1.91                     | 0.53              |
| 1:B:793:LEU:HB3  | 1:C:793:LEU:HB3  | 1.89                     | 0.53              |
| 1:C:195:MSE:HE1  | 1:C:241:GLY:HA3  | 1.90                     | 0.53              |
| 1:F:277:MSE:HE1  | 1:F:767:GLY:HA2  | 1.89                     | 0.53              |
| 1:F:789:MSE:CE   | 1:G:789:MSE:CE   | 2.86                     | 0.53              |
| 1:D:48:GLN:NE2   | 1:D:492:THR:HG22 | 2.24                     | 0.53              |
| 1:E:536:TYR:CE1  | 1:E:537:THR:HG23 | 2.44                     | 0.53              |
| 1:F:59:GLN:CG    | 1:F:60:THR:N     | 2.70                     | 0.53              |
| 1:A:36:VAL:HA    | 1:A:39:LYS:CD    | 2.38                     | 0.53              |
| 1:G:27:ASN:HA    | 1:G:30:LEU:HD12  | 1.90                     | 0.53              |
| 1:H:43:ILE:HG22  | 1:H:43:ILE:O     | 2.09                     | 0.53              |
| 1:G:534:PHE:HB2  | 1:G:535:PRO:CD   | 2.39                     | 0.53              |
| 1:G:131:GLY:N    | 1:G:134:THR:HG21 | 2.22                     | 0.53              |
| 1:H:12:HIS:CE1   | 1:H:150:THR:HG21 | 2.43                     | 0.53              |
| 1:D:102:VAL:HG23 | 1:D:109:VAL:HG22 | 1.91                     | 0.53              |
| 1:D:354:GLU:OE1  | 1:D:366:ARG:NH2  | 2.41                     | 0.53              |
| 1:A:290:PHE:O    | 1:A:366:ARG:NH1  | 2.40                     | 0.53              |
| 1:G:91:ARG:NH2   | 1:G:94:PRO:HA    | 2.23                     | 0.53              |
| 1:C:565:CYS:HB2  | 1:C:642:PHE:O    | 2.07                     | 0.53              |
| 1:H:72:LEU:CA    | 1:H:75:SER:HB3   | 2.33                     | 0.53              |
| 1:E:217:LEU:HD23 | 1:E:220:LEU:HD12 | 1.91                     | 0.53              |
| 1:H:82:LEU:HD12  | 1:H:84:PRO:CD    | 2.39                     | 0.53              |
| 1:D:248:ARG:NH1  | 1:D:248:ARG:HB3  | 2.24                     | 0.53              |
| 1:E:629:MSE:HG2  | 1:E:644:TRP:CZ2  | 2.44                     | 0.53              |
| 1:C:394:GLU:OE1  | 1:C:428:LYS:HE3  | 2.09                     | 0.53              |
| 1:E:394:GLU:OE2  | 1:H:132:ASN:OD1  | 2.27                     | 0.53              |
| 1:F:160:ASP:O    | 1:F:164:ARG:HG3  | 2.08                     | 0.53              |
| 1:G:298:TYR:CE1  | 1:G:649:MSE:CE   | 2.92                     | 0.52              |
| 1:F:35:ARG:HG2   | 1:F:104:LEU:O    | 2.09                     | 0.52              |
| 1:H:84:PRO:O     | 1:H:85:TRP:HD1   | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:37:GLU:HG2   | 1:G:54:GLU:OE2   | 2.09                     | 0.52              |
| 1:B:792:ALA:HA   | 1:B:796:ARG:HG3  | 1.91                     | 0.52              |
| 1:D:685:MSE:HE1  | 1:D:748:ARG:HG2  | 1.91                     | 0.52              |
| 1:F:46:GLN:HB3   | 1:F:50:ILE:HB    | 1.91                     | 0.52              |
| 1:B:59:GLN:CG    | 1:B:60:THR:H     | 2.22                     | 0.52              |
| 1:E:170:LEU:HD23 | 1:E:176:SER:HB3  | 1.90                     | 0.52              |
| 1:D:131:GLY:CA   | 1:D:134:THR:CG2  | 2.87                     | 0.52              |
| 1:C:69:PHE:C     | 1:C:69:PHE:CD1   | 2.82                     | 0.52              |
| 1:A:171:PHE:CD1  | 1:A:263:PRO:HD2  | 2.44                     | 0.52              |
| 1:A:451:TYR:HB3  | 1:A:454:LYS:HE2  | 1.91                     | 0.52              |
| 1:G:150:THR:N    | 1:H:261:GLU:OE1  | 2.40                     | 0.52              |
| 1:C:451:TYR:HB3  | 1:C:454:LYS:HE2  | 1.90                     | 0.52              |
| 1:G:761:ARG:HD2  | 7:G:835:HOH:O    | 2.07                     | 0.52              |
| 1:A:83:PRO:O     | 1:A:85:TRP:N     | 2.42                     | 0.52              |
| 1:F:155:ILE:HB   | 1:F:483:PHE:HE2  | 1.73                     | 0.52              |
| 1:D:607:VAL:HG22 | 1:D:643:ARG:HB3  | 1.91                     | 0.52              |
| 1:B:173:ASP:HB3  | 1:B:176:SER:HB3  | 1.90                     | 0.52              |
| 1:F:116:GLU:O    | 1:F:119:HIS:HB2  | 2.08                     | 0.52              |
| 1:G:580:ARG:HD3  | 2:G:901:UDP:O3B  | 2.08                     | 0.52              |
| 1:G:82:LEU:CG    | 1:G:83:PRO:HD3   | 2.39                     | 0.52              |
| 1:G:49:ILE:O     | 1:G:53:PHE:CB    | 2.58                     | 0.52              |
| 1:E:44:LEU:HA    | 1:E:124:LEU:CD1  | 2.33                     | 0.52              |
| 1:F:789:MSE:HE2  | 1:G:789:MSE:HE2  | 1.89                     | 0.52              |
| 1:G:48:GLN:O     | 1:G:48:GLN:NE2   | 2.43                     | 0.52              |
| 1:F:547:HIS:O    | 1:F:551:GLU:CG   | 2.56                     | 0.52              |
| 1:D:472:MSE:SE   | 1:D:514:ILE:HB   | 2.60                     | 0.52              |
| 1:H:411:ILE:HG13 | 1:H:431:VAL:HG11 | 1.91                     | 0.52              |
| 1:A:49:ILE:HG22  | 1:A:50:ILE:N     | 2.25                     | 0.52              |
| 1:E:94:PRO:HB3   | 1:E:487:ALA:HB1  | 1.91                     | 0.52              |
| 1:F:83:PRO:CB    | 1:F:84:PRO:CD    | 2.88                     | 0.52              |
| 1:A:340:LEU:HB2  | 1:A:366:ARG:HB3  | 1.92                     | 0.52              |
| 1:D:56:LEU:HD12  | 1:D:57:PRO:CD    | 2.21                     | 0.52              |
| 1:A:103:ASN:CB   | 1:A:106:ALA:CB   | 2.74                     | 0.52              |
| 1:B:100:LEU:C    | 1:B:112:LEU:HD12 | 2.30                     | 0.52              |
| 1:F:414:ASN:O    | 1:F:418:GLY:HA3  | 2.09                     | 0.52              |
| 1:A:143:ASN:HA   | 1:A:780:ARG:HH12 | 1.73                     | 0.52              |
| 1:G:407:LYS:HB2  | 1:G:408:PRO:HD2  | 1.91                     | 0.52              |
| 1:G:609:VAL:HG22 | 1:G:645:ILE:HB   | 1.91                     | 0.52              |
| 1:C:538:GLU:OE1  | 1:C:541:ARG:HD3  | 2.10                     | 0.52              |
| 1:F:190:GLN:OE1  | 1:F:190:GLN:HA   | 2.09                     | 0.52              |
| 1:C:545:LYS:CD   | 1:C:545:LYS:H    | 2.22                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:675:GLU:O    | 1:H:697:GLY:HA3  | 2.09                     | 0.52              |
| 1:B:92:PRO:HD2   | 1:B:96:VAL:O     | 2.10                     | 0.52              |
| 1:F:81:VAL:CG1   | 1:F:86:VAL:CG2   | 2.85                     | 0.52              |
| 1:D:86:VAL:CG1   | 1:D:102:VAL:HG12 | 2.39                     | 0.52              |
| 1:F:145:SER:HB2  | 1:F:779:ASP:CG   | 2.31                     | 0.52              |
| 1:E:72:LEU:C     | 1:E:73:LEU:HD22  | 2.29                     | 0.52              |
| 1:C:479:ILE:CD1  | 1:C:762:LEU:HD13 | 2.39                     | 0.52              |
| 1:B:723:THR:O    | 1:B:726:ASP:HB2  | 2.09                     | 0.52              |
| 1:C:536:TYR:HH   | 1:C:738:TRP:HZ3  | 1.58                     | 0.52              |
| 1:F:407:LYS:HB2  | 1:F:408:PRO:CD   | 2.40                     | 0.52              |
| 1:E:35:ARG:HG2   | 1:E:104:LEU:HA   | 1.90                     | 0.52              |
| 1:D:400:LEU:HD12 | 1:D:401:SER:N    | 2.25                     | 0.52              |
| 1:G:259:LEU:O    | 1:G:263:PRO:HG3  | 2.10                     | 0.52              |
| 1:C:645:ILE:HG22 | 1:C:648:GLN:HE21 | 1.75                     | 0.52              |
| 1:A:716:HIS:HB3  | 4:A:913:SO4:O2   | 2.09                     | 0.52              |
| 1:A:434:CYS:HB2  | 1:A:477:PHE:CZ   | 2.45                     | 0.52              |
| 1:G:83:PRO:HB2   | 1:G:84:PRO:CD    | 2.40                     | 0.52              |
| 1:B:162:LEU:HD11 | 1:B:772:TRP:CD2  | 2.45                     | 0.52              |
| 1:H:33:LEU:HA    | 1:H:36:VAL:CG2   | 2.39                     | 0.52              |
| 1:B:153:LYS:CG   | 1:B:154:TYR:CD2  | 2.93                     | 0.52              |
| 1:D:682:VAL:HG13 | 1:D:749:ILE:HD12 | 1.91                     | 0.52              |
| 1:C:226:TYR:HA   | 1:C:229:PHE:CZ   | 2.45                     | 0.52              |
| 1:C:784:ARG:O    | 1:C:788:GLU:HG3  | 2.10                     | 0.52              |
| 1:B:291:ALA:HB3  | 1:B:295:VAL:HG11 | 1.91                     | 0.52              |
| 1:C:195:MSE:HE2  | 1:C:195:MSE:H    | 1.73                     | 0.52              |
| 1:F:524:VAL:HG12 | 1:F:758:TYR:CD2  | 2.45                     | 0.52              |
| 1:A:105:HIS:O    | 1:A:106:ALA:HB2  | 2.10                     | 0.51              |
| 1:A:28:GLU:O     | 1:A:32:LEU:CG    | 2.53                     | 0.51              |
| 1:G:31:ALA:CB    | 1:G:35:ARG:NH2   | 2.64                     | 0.51              |
| 1:F:207:GLN:NE2  | 1:F:211:ARG:NH2  | 2.56                     | 0.51              |
| 1:B:315:LEU:O    | 1:B:319:MSE:HG3  | 2.09                     | 0.51              |
| 1:A:607:VAL:HG22 | 1:A:643:ARG:HB3  | 1.91                     | 0.51              |
| 1:C:437:ALA:C    | 1:C:439:ALA:H    | 2.13                     | 0.51              |
| 1:A:386:TRP:N    | 1:A:387:PRO:HD2  | 2.25                     | 0.51              |
| 1:B:284:LEU:HD13 | 1:B:337:LEU:HB2  | 1.92                     | 0.51              |
| 1:B:90:VAL:HG23  | 1:B:98:GLU:CB    | 2.40                     | 0.51              |
| 1:E:32:LEU:CD2   | 1:E:107:LEU:CB   | 2.87                     | 0.51              |
| 1:A:264:ASP:OD1  | 1:A:267:THR:CB   | 2.58                     | 0.51              |
| 1:A:435:THR:HG23 | 1:A:475:THR:CB   | 2.40                     | 0.51              |
| 1:E:737:HIS:HE1  | 5:E:921:MLA:O3A  | 1.93                     | 0.51              |
| 1:C:197:SER:OG   | 1:C:237:GLY:HA2  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:518:ASP:OD1  | 1:E:520:LYS:HG2  | 2.10                     | 0.51              |
| 1:F:479:ILE:HD11 | 1:F:762:LEU:HD13 | 1.92                     | 0.51              |
| 1:E:319:MSE:HE1  | 1:E:334:ILE:CD1  | 2.41                     | 0.51              |
| 1:B:44:LEU:O     | 1:B:80:ILE:HA    | 2.10                     | 0.51              |
| 1:C:32:LEU:HD11  | 1:C:105:HIS:HA   | 1.92                     | 0.51              |
| 1:G:470:PHE:CE1  | 1:G:791:TYR:HB2  | 2.46                     | 0.51              |
| 1:B:793:LEU:HD11 | 1:C:135:LEU:CD2  | 2.40                     | 0.51              |
| 1:E:43:ILE:HG23  | 1:E:44:LEU:N     | 2.24                     | 0.51              |
| 1:H:146:ILE:HG21 | 1:H:519:PRO:HG2  | 1.90                     | 0.51              |
| 1:A:608:VAL:HG11 | 1:A:629:MSE:HE1  | 1.91                     | 0.51              |
| 1:A:284:LEU:HD13 | 1:A:337:LEU:HB2  | 1.91                     | 0.51              |
| 1:E:784:ARG:O    | 1:E:788:GLU:HG3  | 2.10                     | 0.51              |
| 1:C:105:HIS:O    | 1:C:106:ALA:CB   | 2.55                     | 0.51              |
| 1:H:145:SER:HB3  | 1:H:779:ASP:OD1  | 2.11                     | 0.51              |
| 1:F:230:GLU:OE1  | 1:F:240:ARG:NH1  | 2.44                     | 0.51              |
| 1:E:789:MSE:CG   | 1:H:789:MSE:HE2  | 2.41                     | 0.51              |
| 1:D:625:GLU:O    | 1:D:629:MSE:HG2  | 2.10                     | 0.51              |
| 1:G:31:ALA:O     | 1:G:35:ARG:HB2   | 2.10                     | 0.51              |
| 1:G:72:LEU:C     | 1:G:73:LEU:HD23  | 2.31                     | 0.51              |
| 1:H:545:LYS:CD   | 1:H:545:LYS:H    | 2.21                     | 0.51              |
| 1:F:112:LEU:HD22 | 1:F:116:GLU:HB3  | 1.92                     | 0.51              |
| 1:H:105:HIS:CG   | 1:H:106:ALA:H    | 2.28                     | 0.51              |
| 1:G:703:ILE:HG22 | 1:G:703:ILE:O    | 2.10                     | 0.51              |
| 1:G:63:LYS:O     | 1:G:64:LEU:C     | 2.48                     | 0.51              |
| 1:H:146:ILE:HG12 | 1:H:147:PRO:CD   | 2.22                     | 0.51              |
| 1:D:647:SER:HB2  | 1:D:649:MSE:HE3  | 1.92                     | 0.51              |
| 1:E:65:GLU:HG3   | 1:E:70:PHE:HB2   | 1.86                     | 0.51              |
| 1:B:224:THR:CG2  | 1:B:228:GLU:HG3  | 2.41                     | 0.51              |
| 1:G:692:PHE:CG   | 1:G:724:LEU:HD21 | 2.46                     | 0.51              |
| 1:D:479:ILE:CD1  | 1:D:762:LEU:CD1  | 2.88                     | 0.51              |
| 1:D:577:THR:HG21 | 1:D:590:LEU:HD23 | 1.92                     | 0.51              |
| 1:A:248:ARG:NH2  | 7:A:836:HOH:O    | 2.44                     | 0.51              |
| 1:H:170:LEU:HD22 | 1:H:177:LEU:HD23 | 1.93                     | 0.51              |
| 1:B:566:VAL:CG1  | 1:B:567:LEU:N    | 2.74                     | 0.51              |
| 1:G:148:ARG:CG   | 1:G:148:ARG:NH1  | 2.51                     | 0.51              |
| 1:B:113:GLN:O    | 1:B:116:GLU:HB2  | 2.11                     | 0.51              |
| 1:C:261:GLU:OE1  | 1:D:150:THR:N    | 2.44                     | 0.51              |
| 1:B:789:MSE:HG3  | 1:B:793:LEU:HD12 | 1.91                     | 0.51              |
| 1:G:135:LEU:HD12 | 1:G:136:GLU:N    | 2.25                     | 0.51              |
| 1:B:198:GLU:O    | 1:B:201:GLN:NE2  | 2.44                     | 0.51              |
| 1:D:54:GLU:CG    | 1:D:55:ALA:N     | 2.73                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:789:MSE:HE2  | 1:G:789:MSE:HG2  | 1.92                     | 0.51              |
| 1:C:32:LEU:CD1   | 1:C:105:HIS:HA   | 2.40                     | 0.51              |
| 1:H:483:PHE:CZ   | 1:H:487:ALA:HB3  | 2.46                     | 0.51              |
| 1:H:224:THR:HG23 | 1:H:228:GLU:HG3  | 1.93                     | 0.51              |
| 1:A:670:GLN:HG3  | 1:A:670:GLN:O    | 2.10                     | 0.51              |
| 1:G:52:GLU:OE1   | 1:G:53:PHE:HA    | 2.10                     | 0.51              |
| 1:B:54:GLU:O     | 1:B:56:LEU:N     | 2.44                     | 0.51              |
| 1:G:689:LEU:HD12 | 1:G:690:PRO:HD2  | 1.91                     | 0.51              |
| 1:B:290:PHE:O    | 1:B:366:ARG:NH1  | 2.44                     | 0.51              |
| 1:B:415:TYR:CG   | 1:B:416:SER:N    | 2.80                     | 0.51              |
| 1:D:30:LEU:HD22  | 1:D:30:LEU:N     | 2.25                     | 0.50              |
| 1:G:172:HIS:CD2  | 1:H:147:PRO:HB2  | 2.46                     | 0.50              |
| 1:C:56:LEU:HD13  | 1:C:63:LYS:HG2   | 1.94                     | 0.50              |
| 1:H:217:LEU:HB2  | 1:H:250:LEU:HD13 | 1.92                     | 0.50              |
| 1:H:56:LEU:HG    | 1:H:70:PHE:HE1   | 1.75                     | 0.50              |
| 1:B:322:ARG:HD3  | 1:B:763:LEU:HD13 | 1.93                     | 0.50              |
| 1:E:730:LYS:NZ   | 5:E:921:MLA:C2   | 2.74                     | 0.50              |
| 1:G:140:GLU:N    | 1:G:141:PRO:HD2  | 2.26                     | 0.50              |
| 1:F:242:TRP:O    | 1:F:252:MSE:HG3  | 2.10                     | 0.50              |
| 1:C:287:HIS:HD2  | 1:C:300:ASP:HB3  | 1.75                     | 0.50              |
| 1:F:477:PHE:HA   | 1:F:520:LYS:HB2  | 1.91                     | 0.50              |
| 1:D:444:LYS:O    | 1:D:446:PRO:HD3  | 2.11                     | 0.50              |
| 1:H:193:ASN:ND2  | 1:H:197:SER:HA   | 2.25                     | 0.50              |
| 1:H:72:LEU:HD12  | 1:H:72:LEU:C     | 2.31                     | 0.50              |
| 1:B:56:LEU:HB3   | 1:B:57:PRO:CD    | 2.39                     | 0.50              |
| 1:C:216:TYR:CE2  | 1:C:232:LYS:HD3  | 2.46                     | 0.50              |
| 1:C:294:ASN:C    | 1:C:649:MSE:SE   | 3.00                     | 0.50              |
| 1:C:692:PHE:CD2  | 1:C:724:LEU:CD2  | 2.94                     | 0.50              |
| 1:C:342:PRO:HD2  | 1:C:377:ARG:O    | 2.10                     | 0.50              |
| 1:B:195:MSE:HE1  | 1:B:252:MSE:CE   | 2.41                     | 0.50              |
| 1:D:670:GLN:O    | 1:D:670:GLN:HG3  | 2.11                     | 0.50              |
| 1:E:82:LEU:C     | 1:E:83:PRO:O     | 2.49                     | 0.50              |
| 1:H:53:PHE:O     | 1:H:57:PRO:HG2   | 2.11                     | 0.50              |
| 1:A:794:LYS:C    | 1:A:797:PRO:HD2  | 2.32                     | 0.50              |
| 1:C:692:PHE:HZ   | 1:C:727:PHE:CG   | 2.30                     | 0.50              |
| 1:C:394:GLU:O    | 1:C:398:VAL:HG23 | 2.12                     | 0.50              |
| 1:C:673:LEU:HD23 | 1:C:714:PRO:HB2  | 1.94                     | 0.50              |
| 1:A:564:LEU:HD22 | 1:A:613:ARG:NH2  | 2.25                     | 0.50              |
| 1:C:387:PRO:HD3  | 1:C:802:VAL:HB   | 1.93                     | 0.50              |
| 1:C:190:GLN:HG3  | 1:C:190:GLN:O    | 2.11                     | 0.50              |
| 1:C:532:ILE:HD13 | 1:C:532:ILE:N    | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:52:GLU:CD    | 1:G:53:PHE:N     | 2.65                     | 0.50              |
| 1:B:92:PRO:CG    | 1:B:96:VAL:HG23  | 2.30                     | 0.50              |
| 1:E:190:GLN:NE2  | 1:E:405:ASN:HB3  | 2.26                     | 0.50              |
| 1:E:160:ASP:O    | 1:E:164:ARG:HG3  | 2.10                     | 0.50              |
| 1:F:483:PHE:CZ   | 1:F:487:ALA:HB3  | 2.46                     | 0.50              |
| 1:C:420:LEU:HD23 | 1:C:467:ALA:CB   | 2.41                     | 0.50              |
| 1:B:173:ASP:HB3  | 1:B:176:SER:CB   | 2.40                     | 0.50              |
| 1:F:609:VAL:HG22 | 1:F:645:ILE:HB   | 1.92                     | 0.50              |
| 1:F:784:ARG:O    | 1:F:788:GLU:HG3  | 2.11                     | 0.50              |
| 1:E:319:MSE:CE   | 1:E:334:ILE:CD1  | 2.87                     | 0.50              |
| 1:D:56:LEU:O     | 1:D:59:GLN:N     | 2.41                     | 0.50              |
| 1:E:143:ASN:HB3  | 1:E:148:ARG:CZ   | 2.41                     | 0.50              |
| 1:E:790:PHE:N    | 1:H:789:MSE:HE1  | 2.27                     | 0.50              |
| 1:G:154:TYR:CD1  | 1:G:161:PHE:HB2  | 2.46                     | 0.50              |
| 1:B:789:MSE:HG2  | 1:C:789:MSE:SE   | 2.61                     | 0.50              |
| 1:H:43:ILE:HG23  | 1:H:124:LEU:HD21 | 1.93                     | 0.50              |
| 1:G:81:VAL:O     | 1:G:81:VAL:HG23  | 2.12                     | 0.50              |
| 1:H:211:ARG:NE   | 7:H:867:HOH:O    | 2.44                     | 0.50              |
| 1:E:150:THR:N    | 1:F:261:GLU:OE1  | 2.42                     | 0.50              |
| 1:D:56:LEU:O     | 1:D:58:GLU:N     | 2.44                     | 0.50              |
| 1:D:146:ILE:HG22 | 1:D:147:PRO:O    | 2.12                     | 0.50              |
| 1:F:80:ILE:N     | 1:F:80:ILE:HD12  | 2.27                     | 0.50              |
| 1:E:70:PHE:HD2   | 1:E:70:PHE:C     | 2.12                     | 0.50              |
| 1:H:338:THR:HG23 | 1:H:366:ARG:HG2  | 1.94                     | 0.50              |
| 1:E:178:LEU:N    | 1:E:179:PRO:CD   | 2.75                     | 0.50              |
| 1:C:195:MSE:CE   | 1:C:241:GLY:HA3  | 2.42                     | 0.50              |
| 1:F:119:HIS:HD2  | 1:F:129:LYS:CB   | 2.24                     | 0.50              |
| 1:G:685:MSE:HE1  | 1:G:748:ARG:HG2  | 1.93                     | 0.50              |
| 1:G:185:ARG:HD2  | 1:G:198:GLU:OE2  | 2.12                     | 0.50              |
| 1:G:188:SER:HB2  | 1:G:192:LYS:O    | 2.12                     | 0.50              |
| 1:A:367:VAL:CG2  | 1:A:399:GLU:HG3  | 2.42                     | 0.50              |
| 1:H:211:ARG:CD   | 7:H:867:HOH:O    | 2.59                     | 0.50              |
| 1:A:113:GLN:HB2  | 1:A:116:GLU:OE1  | 2.11                     | 0.50              |
| 1:E:37:GLU:OE1   | 1:E:59:GLN:NE2   | 2.45                     | 0.50              |
| 1:G:242:TRP:O    | 1:G:252:MSE:HG3  | 2.11                     | 0.50              |
| 1:D:483:PHE:CZ   | 1:D:487:ALA:HB3  | 2.47                     | 0.50              |
| 1:E:437:ALA:O    | 1:E:438:HIS:HB2  | 2.11                     | 0.50              |
| 1:F:146:ILE:HD11 | 1:F:772:TRP:CZ2  | 2.47                     | 0.50              |
| 1:D:259:LEU:HD21 | 1:D:267:THR:HG22 | 1.94                     | 0.50              |
| 1:F:206:LEU:HD11 | 1:F:210:LEU:HD11 | 1.94                     | 0.50              |
| 1:H:366:ARG:HD3  | 7:H:857:HOH:O    | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:65:GLU:O     | 1:H:70:PHE:HB2   | 2.11                     | 0.50              |
| 1:F:564:LEU:HD22 | 1:F:613:ARG:NH2  | 2.26                     | 0.50              |
| 1:D:779:ASP:N    | 1:D:779:ASP:OD1  | 2.44                     | 0.50              |
| 1:F:146:ILE:HG22 | 1:F:147:PRO:N    | 2.27                     | 0.49              |
| 1:E:162:LEU:HD11 | 1:E:772:TRP:CD2  | 2.46                     | 0.49              |
| 1:A:210:LEU:CD2  | 1:A:253:ILE:HG23 | 2.41                     | 0.49              |
| 1:B:552:GLU:O    | 1:B:556:SER:CB   | 2.59                     | 0.49              |
| 1:C:283:ILE:HG23 | 1:C:414:ASN:HD21 | 1.76                     | 0.49              |
| 1:H:145:SER:HB3  | 1:H:779:ASP:OD2  | 2.12                     | 0.49              |
| 1:H:155:ILE:HB   | 1:H:483:PHE:HE2  | 1.76                     | 0.49              |
| 1:B:415:TYR:HA   | 1:B:437:ALA:O    | 2.12                     | 0.49              |
| 1:H:596:LYS:HE3  | 1:H:636:TYR:OH   | 2.12                     | 0.49              |
| 1:A:552:GLU:O    | 1:A:556:SER:HB3  | 2.12                     | 0.49              |
| 1:E:82:LEU:CB    | 1:E:83:PRO:HD2   | 2.35                     | 0.49              |
| 1:C:702:ILE:HA   | 1:C:753:TYR:OH   | 2.13                     | 0.49              |
| 1:B:613:ARG:NH1  | 1:B:613:ARG:HG3  | 2.24                     | 0.49              |
| 1:H:315:LEU:HG   | 1:H:319:MSE:CE   | 2.42                     | 0.49              |
| 1:F:420:LEU:HD13 | 1:F:420:LEU:O    | 2.11                     | 0.49              |
| 1:G:282:VAL:HG21 | 1:G:400:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:100:LEU:HD23 | 1:A:111:GLU:HA   | 1.93                     | 0.49              |
| 1:C:46:GLN:HB2   | 1:C:50:ILE:HG23  | 1.93                     | 0.49              |
| 1:A:56:LEU:HG    | 1:A:70:PHE:CE1   | 2.47                     | 0.49              |
| 1:B:226:TYR:CE2  | 1:B:240:ARG:HG2  | 2.47                     | 0.49              |
| 1:G:437:ALA:O    | 1:G:438:HIS:HB2  | 2.12                     | 0.49              |
| 1:D:57:PRO:HA    | 1:D:63:LYS:HE3   | 1.93                     | 0.49              |
| 1:E:56:LEU:HB3   | 1:E:57:PRO:HD3   | 1.94                     | 0.49              |
| 1:H:82:LEU:CG    | 1:H:85:TRP:O     | 2.57                     | 0.49              |
| 1:E:28:GLU:O     | 1:E:32:LEU:HD23  | 2.13                     | 0.49              |
| 1:G:575:LEU:HD21 | 1:G:724:LEU:HD13 | 1.93                     | 0.49              |
| 1:D:462:SER:HB2  | 1:D:507:LEU:HD21 | 1.93                     | 0.49              |
| 1:F:665:LYS:HD2  | 1:F:738:TRP:CD2  | 2.47                     | 0.49              |
| 1:E:137:LEU:HD11 | 1:E:790:PHE:CZ   | 2.48                     | 0.49              |
| 1:D:121:LYS:O    | 1:D:124:LEU:HB3  | 2.12                     | 0.49              |
| 1:H:99:TYR:HB2   | 1:H:112:LEU:O    | 2.11                     | 0.49              |
| 1:D:479:ILE:HD11 | 1:D:762:LEU:HD12 | 1.94                     | 0.49              |
| 1:F:414:ASN:HD22 | 1:F:438:HIS:CD2  | 2.30                     | 0.49              |
| 1:C:772:TRP:CZ2  | 1:C:776:SER:CB   | 2.95                     | 0.49              |
| 1:A:37:GLU:HG3   | 1:A:59:GLN:NE2   | 2.27                     | 0.49              |
| 1:E:419:ASN:HB3  | 1:E:471:ALA:CB   | 2.43                     | 0.49              |
| 1:B:437:ALA:C    | 1:B:439:ALA:H    | 2.15                     | 0.49              |
| 1:D:578:MSE:HE3  | 2:D:901:UDP:O2'  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:65:GLU:HB3   | 1:D:70:PHE:HB2   | 1.94                     | 0.49              |
| 1:B:657:LEU:O    | 1:B:661:ILE:HG12 | 2.13                     | 0.49              |
| 1:H:162:LEU:HD21 | 1:H:772:TRP:CG   | 2.47                     | 0.49              |
| 1:D:407:LYS:HB2  | 1:D:408:PRO:CD   | 2.42                     | 0.49              |
| 1:E:242:TRP:O    | 1:E:252:MSE:HG3  | 2.13                     | 0.49              |
| 1:C:48:GLN:HA    | 1:C:51:ALA:HB3   | 1.93                     | 0.49              |
| 1:D:195:MSE:HE2  | 1:D:241:GLY:HA3  | 1.93                     | 0.49              |
| 1:D:419:ASN:HB3  | 1:D:471:ALA:CB   | 2.42                     | 0.49              |
| 1:C:567:LEU:HD21 | 1:C:643:ARG:HB2  | 1.94                     | 0.49              |
| 1:A:331:LYS:NZ   | 1:F:61:ARG:HH12  | 2.11                     | 0.49              |
| 1:D:79:ALA:HA    | 1:D:87:ALA:O     | 2.13                     | 0.49              |
| 1:C:312:VAL:HG12 | 1:C:334:ILE:HG21 | 1.93                     | 0.49              |
| 1:F:659:ARG:O    | 1:F:662:CYS:HB2  | 2.12                     | 0.49              |
| 1:D:512:HIS:CE1  | 1:D:515:ASP:HB2  | 2.47                     | 0.49              |
| 1:H:387:PRO:HD3  | 1:H:802:VAL:HB   | 1.93                     | 0.49              |
| 1:A:63:LYS:O     | 1:A:65:GLU:N     | 2.46                     | 0.49              |
| 1:F:80:ILE:H     | 1:F:80:ILE:HD12  | 1.78                     | 0.49              |
| 1:D:264:ASP:OD1  | 1:D:267:THR:CB   | 2.57                     | 0.49              |
| 1:A:207:GLN:HE21 | 1:A:211:ARG:HH12 | 1.59                     | 0.49              |
| 1:D:535:PRO:O    | 1:D:538:GLU:HG3  | 2.12                     | 0.49              |
| 1:E:432:THR:OG1  | 1:E:773:LYS:HE3  | 2.13                     | 0.49              |
| 1:C:185:ARG:HD2  | 1:C:198:GLU:OE1  | 2.13                     | 0.49              |
| 1:E:375:ILE:O    | 1:E:375:ILE:HG13 | 2.11                     | 0.49              |
| 1:C:34:SER:CA    | 1:C:59:GLN:HE22  | 2.17                     | 0.49              |
| 1:B:52:GLU:O     | 1:B:57:PRO:CD    | 2.60                     | 0.49              |
| 1:A:124:LEU:CD2  | 1:A:124:LEU:C    | 2.81                     | 0.49              |
| 1:E:35:ARG:NH1   | 1:E:35:ARG:CB    | 2.74                     | 0.49              |
| 1:C:173:ASP:OD2  | 1:C:176:SER:HB2  | 2.12                     | 0.49              |
| 1:B:313:ARG:HD3  | 1:B:357:TYR:O    | 2.12                     | 0.49              |
| 1:D:166:LEU:HD21 | 1:D:772:TRP:CE3  | 2.47                     | 0.49              |
| 1:F:102:VAL:HA   | 1:F:108:VAL:O    | 2.12                     | 0.49              |
| 1:E:32:LEU:O     | 1:E:36:VAL:HG23  | 2.13                     | 0.49              |
| 1:D:82:LEU:O     | 1:D:85:TRP:O     | 2.31                     | 0.49              |
| 1:B:21:THR:C     | 1:B:23:VAL:H     | 2.15                     | 0.49              |
| 1:E:216:TYR:CD1  | 1:E:216:TYR:C    | 2.85                     | 0.49              |
| 1:B:55:ALA:O     | 1:B:59:GLN:CB    | 2.50                     | 0.49              |
| 1:B:30:LEU:N     | 1:B:30:LEU:HD12  | 2.28                     | 0.49              |
| 1:E:303:GLY:HA3  | 2:E:901:UDP:O2B  | 2.12                     | 0.48              |
| 1:E:141:PRO:HB2  | 1:H:782:GLU:HG3  | 1.94                     | 0.48              |
| 1:F:367:VAL:HG22 | 1:F:399:GLU:HG3  | 1.94                     | 0.48              |
| 1:C:474:HIS:HB2  | 1:C:787:LEU:HD13 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:210:LEU:HD22 | 1:C:253:ILE:HG23 | 1.95                     | 0.48              |
| 1:B:739:ASP:O    | 1:B:743:LYS:HG2  | 2.12                     | 0.48              |
| 1:G:178:LEU:N    | 1:G:179:PRO:CD   | 2.76                     | 0.48              |
| 1:F:420:LEU:C    | 1:F:420:LEU:CD1  | 2.80                     | 0.48              |
| 1:H:561:LYS:HD3  | 1:H:613:ARG:O    | 2.13                     | 0.48              |
| 1:C:226:TYR:CE2  | 1:C:240:ARG:HG2  | 2.48                     | 0.48              |
| 1:D:599:ARG:O    | 1:D:603:LEU:HD12 | 2.13                     | 0.48              |
| 1:G:137:LEU:HD11 | 1:G:790:PHE:CZ   | 2.48                     | 0.48              |
| 1:B:44:LEU:O     | 1:B:81:VAL:N     | 2.46                     | 0.48              |
| 1:B:41:LYS:HD2   | 1:B:46:GLN:NE2   | 2.28                     | 0.48              |
| 1:C:69:PHE:HD1   | 1:C:70:PHE:N     | 2.10                     | 0.48              |
| 1:C:617:SER:O    | 1:C:623:LYS:HD3  | 2.14                     | 0.48              |
| 1:A:417:ASP:OD1  | 1:A:418:GLY:N    | 2.45                     | 0.48              |
| 1:D:319:MSE:HE2  | 1:D:332:PRO:CB   | 2.43                     | 0.48              |
| 1:C:160:ASP:O    | 1:C:164:ARG:HG3  | 2.13                     | 0.48              |
| 1:F:223:GLU:N    | 1:F:223:GLU:OE2  | 2.46                     | 0.48              |
| 1:A:789:MSE:HE3  | 1:D:789:MSE:C    | 2.33                     | 0.48              |
| 1:D:146:ILE:CD1  | 1:D:772:TRP:CH2  | 2.95                     | 0.48              |
| 1:G:685:MSE:HE1  | 1:G:748:ARG:CG   | 2.43                     | 0.48              |
| 1:E:34:SER:O     | 1:E:37:GLU:HB3   | 2.12                     | 0.48              |
| 1:C:573:PRO:HD2  | 1:C:603:LEU:O    | 2.13                     | 0.48              |
| 1:E:447:ASP:HB3  | 1:E:451:TYR:HD2  | 1.78                     | 0.48              |
| 1:A:48:GLN:O     | 1:A:51:ALA:HB3   | 2.14                     | 0.48              |
| 1:B:59:GLN:HG2   | 1:B:60:THR:H     | 1.79                     | 0.48              |
| 1:D:83:PRO:HG2   | 1:D:84:PRO:HD2   | 1.93                     | 0.48              |
| 1:E:52:GLU:C     | 1:E:52:GLU:CD    | 2.72                     | 0.48              |
| 1:E:146:ILE:HG12 | 1:E:772:TRP:CH2  | 2.48                     | 0.48              |
| 1:B:250:LEU:HG   | 1:B:254:ARG:NH1  | 2.29                     | 0.48              |
| 1:D:211:ARG:NH1  | 1:D:211:ARG:HG3  | 2.29                     | 0.48              |
| 1:H:143:ASN:HD22 | 1:H:148:ARG:HH22 | 1.60                     | 0.48              |
| 1:A:312:VAL:HG23 | 1:A:313:ARG:N    | 2.28                     | 0.48              |
| 1:D:493:VAL:CG2  | 1:D:494:GLY:N    | 2.77                     | 0.48              |
| 1:H:367:VAL:HG13 | 1:H:368:PRO:HD2  | 1.94                     | 0.48              |
| 1:F:72:LEU:C     | 1:F:73:LEU:HD12  | 2.34                     | 0.48              |
| 1:B:177:LEU:HD13 | 1:B:260:LEU:HD23 | 1.95                     | 0.48              |
| 1:G:354:GLU:OE1  | 1:G:366:ARG:NH2  | 2.47                     | 0.48              |
| 1:F:74:LYS:CA    | 7:F:891:HOH:O    | 2.54                     | 0.48              |
| 1:G:81:VAL:CG1   | 1:G:86:VAL:HB    | 2.43                     | 0.48              |
| 1:H:65:GLU:C     | 1:H:67:GLY:H     | 2.17                     | 0.48              |
| 1:D:140:GLU:HB3  | 1:D:141:PRO:CD   | 2.42                     | 0.48              |
| 1:H:197:SER:HB3  | 1:H:239:GLU:OE1  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:574:ILE:HG23 | 1:B:607:VAL:HG23 | 1.96                     | 0.48              |
| 1:G:566:VAL:O    | 1:G:640:GLY:HA2  | 2.13                     | 0.48              |
| 1:H:791:TYR:CE1  | 1:H:795:TYR:CD2  | 3.01                     | 0.48              |
| 1:G:45:GLN:HA    | 1:G:45:GLN:NE2   | 2.28                     | 0.48              |
| 1:D:466:THR:HG23 | 1:D:790:PHE:CZ   | 2.49                     | 0.48              |
| 1:B:20:GLU:CD    | 1:B:72:LEU:HD23  | 2.34                     | 0.48              |
| 1:E:789:MSE:CB   | 1:H:789:MSE:HE1  | 2.36                     | 0.48              |
| 1:A:259:LEU:O    | 1:A:263:PRO:HG3  | 2.14                     | 0.48              |
| 1:E:387:PRO:HD3  | 1:E:802:VAL:HB   | 1.94                     | 0.48              |
| 1:E:647:SER:HB2  | 1:E:649:MSE:HE3  | 1.95                     | 0.48              |
| 1:A:449:ASP:OD1  | 1:A:450:ILE:N    | 2.46                     | 0.48              |
| 1:G:387:PRO:HD3  | 1:G:802:VAL:HB   | 1.95                     | 0.48              |
| 1:B:483:PHE:CZ   | 1:B:487:ALA:HB3  | 2.48                     | 0.48              |
| 1:C:360:GLU:HB2  | 1:C:361:TYR:CD2  | 2.49                     | 0.48              |
| 1:B:83:PRO:CG    | 1:B:85:TRP:HB2   | 2.13                     | 0.48              |
| 1:E:42:GLY:O     | 1:E:81:VAL:CG1   | 2.62                     | 0.48              |
| 1:E:789:MSE:HE2  | 1:H:789:MSE:HB3  | 1.94                     | 0.48              |
| 1:F:786:TYR:O    | 1:G:789:MSE:HE1  | 2.13                     | 0.48              |
| 1:F:333:ARG:NH1  | 1:F:403:GLU:HB3  | 2.21                     | 0.48              |
| 1:D:86:VAL:HG13  | 1:D:102:VAL:HG12 | 1.95                     | 0.48              |
| 1:C:534:PHE:HB2  | 1:C:535:PRO:HD2  | 1.96                     | 0.48              |
| 1:B:233:PHE:HB3  | 1:B:238:LEU:HB2  | 1.95                     | 0.48              |
| 1:A:419:ASN:HB3  | 1:A:471:ALA:CB   | 2.43                     | 0.48              |
| 1:B:242:TRP:O    | 1:B:252:MSE:HG3  | 2.14                     | 0.48              |
| 1:F:354:GLU:OE1  | 1:F:366:ARG:NH2  | 2.46                     | 0.48              |
| 1:F:293:ASP:HB2  | 7:F:849:HOH:O    | 2.14                     | 0.48              |
| 1:C:355:ARG:HD2  | 1:C:359:SER:O    | 2.13                     | 0.48              |
| 1:H:196:LEU:HD22 | 1:H:200:ILE:HD12 | 1.94                     | 0.48              |
| 1:A:206:LEU:HD11 | 1:A:210:LEU:HD11 | 1.96                     | 0.48              |
| 1:F:143:ASN:HA   | 1:F:780:ARG:NH1  | 2.25                     | 0.48              |
| 1:F:282:VAL:HG13 | 1:F:337:LEU:HD23 | 1.96                     | 0.48              |
| 1:D:577:THR:HG21 | 1:D:590:LEU:CD2  | 2.44                     | 0.48              |
| 1:E:419:ASN:HB3  | 1:E:471:ALA:HB1  | 1.94                     | 0.48              |
| 1:G:553:LEU:HG   | 1:G:645:ILE:HD13 | 1.96                     | 0.48              |
| 1:B:139:PHE:CE1  | 1:B:787:LEU:HD21 | 2.49                     | 0.48              |
| 1:G:348:THR:O    | 1:G:351:GLU:HG2  | 2.14                     | 0.48              |
| 1:C:82:LEU:O     | 1:C:85:TRP:O     | 2.32                     | 0.48              |
| 1:C:338:THR:OG1  | 1:C:339:ARG:N    | 2.47                     | 0.48              |
| 1:H:433:GLN:O    | 1:H:476:ASP:HB2  | 2.14                     | 0.48              |
| 1:D:86:VAL:CG1   | 1:D:102:VAL:CG1  | 2.92                     | 0.47              |
| 1:A:414:ASN:O    | 1:A:418:GLY:HA3  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:437:ALA:C    | 1:F:439:ALA:H    | 2.17                     | 0.47              |
| 1:B:779:ASP:OD1  | 1:B:779:ASP:N    | 2.48                     | 0.47              |
| 1:G:83:PRO:CB    | 1:G:85:TRP:H     | 2.17                     | 0.47              |
| 1:G:290:PHE:O    | 1:G:366:ARG:NH1  | 2.47                     | 0.47              |
| 1:G:160:ASP:O    | 1:G:164:ARG:HG3  | 2.14                     | 0.47              |
| 1:B:145:SER:HB3  | 7:B:877:HOH:O    | 2.13                     | 0.47              |
| 1:G:484:GLN:HG2  | 1:G:488:GLY:HA2  | 1.94                     | 0.47              |
| 1:D:284:LEU:HD22 | 1:D:284:LEU:N    | 2.29                     | 0.47              |
| 1:D:449:ASP:OD1  | 1:D:450:ILE:N    | 2.46                     | 0.47              |
| 1:D:479:ILE:CD1  | 1:D:762:LEU:HD13 | 2.44                     | 0.47              |
| 1:H:354:GLU:OE1  | 1:H:366:ARG:NH2  | 2.46                     | 0.47              |
| 1:H:34:SER:OG    | 1:H:55:ALA:CB    | 2.61                     | 0.47              |
| 1:B:462:SER:HB2  | 1:B:798:LEU:HD22 | 1.96                     | 0.47              |
| 1:H:553:LEU:HD21 | 1:H:645:ILE:HG21 | 1.96                     | 0.47              |
| 1:D:140:GLU:HB3  | 1:D:141:PRO:HD3  | 1.95                     | 0.47              |
| 1:C:195:MSE:HE1  | 1:C:241:GLY:C    | 2.35                     | 0.47              |
| 1:C:82:LEU:O     | 1:C:85:TRP:N     | 2.47                     | 0.47              |
| 1:F:444:LYS:O    | 1:F:446:PRO:HD3  | 2.14                     | 0.47              |
| 1:F:415:TYR:CG   | 1:F:416:SER:N    | 2.82                     | 0.47              |
| 1:E:794:LYS:O    | 1:E:794:LYS:HD3  | 2.15                     | 0.47              |
| 1:D:166:LEU:HD21 | 1:D:772:TRP:HE3  | 1.79                     | 0.47              |
| 1:D:781:LEU:O    | 1:D:784:ARG:HB3  | 2.14                     | 0.47              |
| 1:G:162:LEU:HD11 | 1:G:772:TRP:CD2  | 2.50                     | 0.47              |
| 1:G:483:PHE:CZ   | 1:G:487:ALA:HB3  | 2.49                     | 0.47              |
| 1:D:319:MSE:HE2  | 1:D:332:PRO:HB2  | 1.95                     | 0.47              |
| 1:H:23:VAL:C     | 1:H:25:GLU:N     | 2.68                     | 0.47              |
| 1:G:82:LEU:HG    | 1:G:83:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:789:MSE:CE   | 1:D:790:PHE:N    | 2.78                     | 0.47              |
| 1:G:276:PRO:HG3  | 1:G:326:GLN:CB   | 2.45                     | 0.47              |
| 1:F:276:PRO:HG3  | 1:F:326:GLN:CB   | 2.44                     | 0.47              |
| 1:C:796:ARG:HB2  | 1:C:797:PRO:CD   | 2.39                     | 0.47              |
| 1:C:319:MSE:HE2  | 1:C:332:PRO:HB3  | 1.95                     | 0.47              |
| 1:H:315:LEU:HD21 | 1:H:762:LEU:HD23 | 1.95                     | 0.47              |
| 1:G:178:LEU:N    | 1:G:179:PRO:HD2  | 2.29                     | 0.47              |
| 1:G:212:LYS:NZ   | 1:G:232:LYS:HZ1  | 2.13                     | 0.47              |
| 1:B:483:PHE:CE1  | 1:B:487:ALA:HB3  | 2.49                     | 0.47              |
| 1:D:282:VAL:HG13 | 1:D:337:LEU:HD23 | 1.97                     | 0.47              |
| 1:B:126:ASP:HB2  | 1:B:128:VAL:O    | 2.14                     | 0.47              |
| 1:D:657:LEU:O    | 1:D:661:ILE:HG12 | 2.14                     | 0.47              |
| 1:D:484:GLN:HG2  | 1:D:488:GLY:HA2  | 1.97                     | 0.47              |
| 1:H:390:GLU:OE2  | 1:H:796:ARG:NH1  | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:704:VAL:HA   | 4:E:912:SO4:O3   | 2.13                     | 0.47              |
| 1:F:290:PHE:HD2  | 7:F:894:HOH:O    | 1.96                     | 0.47              |
| 1:E:474:HIS:HA   | 1:E:787:LEU:HD13 | 1.97                     | 0.47              |
| 1:C:367:VAL:HG13 | 1:C:368:PRO:HD2  | 1.96                     | 0.47              |
| 1:A:673:LEU:HD23 | 1:A:714:PRO:HB2  | 1.97                     | 0.47              |
| 1:A:219:GLU:HA   | 1:A:219:GLU:OE1  | 2.15                     | 0.47              |
| 1:B:90:VAL:N     | 1:B:98:GLU:O     | 2.40                     | 0.47              |
| 1:C:172:HIS:CD2  | 1:D:147:PRO:CB   | 2.97                     | 0.47              |
| 1:E:159:VAL:CG1  | 1:E:160:ASP:N    | 2.77                     | 0.47              |
| 1:E:588:SER:CB   | 1:E:625:GLU:OE2  | 2.63                     | 0.47              |
| 1:A:143:ASN:O    | 1:A:145:SER:N    | 2.48                     | 0.47              |
| 1:A:189:HIS:ND1  | 1:A:330:ILE:HD13 | 2.30                     | 0.47              |
| 1:E:46:GLN:HA    | 1:E:50:ILE:HD12  | 1.97                     | 0.47              |
| 1:F:52:GLU:O     | 1:F:57:PRO:CD    | 2.52                     | 0.47              |
| 1:C:50:ILE:C     | 1:C:52:GLU:N     | 2.67                     | 0.47              |
| 1:B:91:ARG:HD2   | 1:B:97:TRP:CH2   | 2.50                     | 0.47              |
| 1:F:35:ARG:O     | 1:F:38:ALA:N     | 2.47                     | 0.47              |
| 1:D:125:VAL:HG13 | 1:D:126:ASP:H    | 1.80                     | 0.47              |
| 1:B:30:LEU:CD2   | 7:B:863:HOH:O    | 2.63                     | 0.47              |
| 1:A:772:TRP:CH2  | 1:A:776:SER:HB3  | 2.49                     | 0.47              |
| 1:B:561:LYS:HD3  | 1:B:613:ARG:O    | 2.15                     | 0.47              |
| 1:H:319:MSE:O    | 1:H:323:ILE:HG13 | 2.14                     | 0.47              |
| 1:E:212:LYS:HD2  | 1:E:236:ILE:HG21 | 1.96                     | 0.47              |
| 1:G:81:VAL:HG12  | 1:G:86:VAL:CB    | 2.43                     | 0.47              |
| 1:G:39:LYS:NZ    | 1:G:105:HIS:CD2  | 2.83                     | 0.47              |
| 1:H:415:TYR:CG   | 1:H:416:SER:N    | 2.81                     | 0.47              |
| 1:C:566:VAL:CG1  | 1:C:567:LEU:N    | 2.78                     | 0.47              |
| 1:E:680:THR:HG22 | 2:E:901:UDP:H3'  | 1.96                     | 0.47              |
| 1:H:105:HIS:CG   | 1:H:106:ALA:N    | 2.82                     | 0.47              |
| 1:E:665:LYS:HD3  | 1:E:665:LYS:HA   | 1.70                     | 0.47              |
| 1:H:355:ARG:HD2  | 1:H:359:SER:O    | 2.15                     | 0.47              |
| 1:E:572:LYS:HE2  | 1:E:602:GLU:O    | 2.15                     | 0.47              |
| 1:H:437:ALA:C    | 1:H:439:ALA:H    | 2.18                     | 0.47              |
| 1:B:479:ILE:CD1  | 1:B:762:LEU:HD13 | 2.45                     | 0.47              |
| 1:H:626:MSE:O    | 1:H:630:TYR:HD2  | 1.97                     | 0.47              |
| 1:G:573:PRO:HD2  | 1:G:603:LEU:O    | 2.14                     | 0.47              |
| 1:G:82:LEU:HD12  | 1:G:83:PRO:HD3   | 1.92                     | 0.47              |
| 1:A:137:LEU:CD2  | 1:D:789:MSE:HE2  | 2.45                     | 0.47              |
| 1:E:315:LEU:CB   | 1:E:319:MSE:HE3  | 2.44                     | 0.47              |
| 1:A:81:VAL:HA    | 1:A:86:VAL:HG22  | 1.95                     | 0.47              |
| 1:G:35:ARG:HH12  | 1:G:107:LEU:CB   | 2.27                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:662:CYS:SG   | 1:C:689:LEU:HB2  | 2.54                     | 0.47              |
| 1:H:245:ASN:O    | 1:H:249:VAL:HG23 | 2.14                     | 0.47              |
| 1:G:633:ILE:HA   | 1:G:638:LEU:HD12 | 1.97                     | 0.47              |
| 1:C:56:LEU:HB3   | 1:C:57:PRO:CD    | 2.45                     | 0.47              |
| 1:C:216:TYR:C    | 1:C:216:TYR:HD1  | 2.18                     | 0.47              |
| 1:G:590:LEU:HB2  | 1:G:671:PRO:HG3  | 1.97                     | 0.47              |
| 1:G:319:MSE:O    | 1:G:323:ILE:HG13 | 2.15                     | 0.47              |
| 1:C:440:LEU:HD12 | 1:C:495:GLN:HB3  | 1.97                     | 0.47              |
| 1:C:420:LEU:CD1  | 1:C:420:LEU:C    | 2.83                     | 0.47              |
| 1:F:159:VAL:HB   | 1:F:765:LEU:CD2  | 2.45                     | 0.47              |
| 1:C:389:LEU:HD11 | 1:C:417:ASP:CB   | 2.45                     | 0.47              |
| 1:H:153:LYS:HG3  | 1:H:154:TYR:CD2  | 2.50                     | 0.47              |
| 1:D:681:VAL:HG13 | 1:D:691:THR:HG21 | 1.96                     | 0.47              |
| 1:C:419:ASN:HB3  | 1:C:471:ALA:CB   | 2.45                     | 0.47              |
| 1:F:53:PHE:O     | 1:F:57:PRO:HG2   | 2.13                     | 0.47              |
| 1:C:130:ASN:HB3  | 1:C:134:THR:OG1  | 2.15                     | 0.47              |
| 1:A:68:PRO:O     | 1:A:72:LEU:HD12  | 2.14                     | 0.47              |
| 1:B:472:MSE:HG2  | 1:B:496:TYR:HE1  | 1.80                     | 0.47              |
| 1:G:78:GLU:OE2   | 1:G:121:LYS:CE   | 2.63                     | 0.47              |
| 1:E:552:GLU:O    | 1:E:556:SER:HB2  | 2.15                     | 0.47              |
| 1:F:209:THR:CG2  | 1:F:236:ILE:HG13 | 2.45                     | 0.47              |
| 1:C:434:CYS:HB2  | 1:C:477:PHE:CZ   | 2.50                     | 0.47              |
| 1:E:582:ASP:C    | 1:E:582:ASP:OD1  | 2.52                     | 0.47              |
| 1:A:490:LYS:HE3  | 1:A:490:LYS:HB2  | 1.72                     | 0.47              |
| 1:C:48:GLN:HB2   | 1:C:77:GLN:O     | 2.15                     | 0.46              |
| 1:H:76:THR:O     | 1:H:77:GLN:CB    | 2.63                     | 0.46              |
| 1:C:99:TYR:C     | 1:C:100:LEU:HD23 | 2.36                     | 0.46              |
| 1:D:690:PRO:HA   | 7:D:866:HOH:O    | 2.14                     | 0.46              |
| 1:H:32:LEU:CD2   | 1:H:35:ARG:NH1   | 2.75                     | 0.46              |
| 1:F:79:ALA:HB2   | 1:F:88:LEU:CD2   | 2.44                     | 0.46              |
| 1:D:433:GLN:O    | 1:D:476:ASP:HB2  | 2.14                     | 0.46              |
| 1:A:339:ARG:HD2  | 1:A:369:PHE:CE2  | 2.51                     | 0.46              |
| 1:B:292:GLN:HE22 | 1:B:356:VAL:HA   | 1.80                     | 0.46              |
| 1:H:210:LEU:HD11 | 1:H:256:LEU:HD23 | 1.97                     | 0.46              |
| 1:F:125:VAL:HG21 | 1:F:450:ILE:O    | 2.14                     | 0.46              |
| 1:H:90:VAL:O     | 1:H:98:GLU:N     | 2.45                     | 0.46              |
| 1:C:146:ILE:HD11 | 1:C:162:LEU:CD1  | 2.45                     | 0.46              |
| 1:G:54:GLU:OE2   | 1:G:55:ALA:CA    | 2.62                     | 0.46              |
| 1:H:139:PHE:HE1  | 1:H:787:LEU:HD21 | 1.78                     | 0.46              |
| 1:C:94:PRO:HB3   | 1:C:487:ALA:HB1  | 1.97                     | 0.46              |
| 1:E:566:VAL:O    | 1:E:567:LEU:HD23 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:193:ASN:O    | 1:E:194:LEU:HD23 | 2.15                     | 0.46              |
| 1:C:717:GLY:O    | 1:C:720:ALA:HB3  | 2.15                     | 0.46              |
| 1:F:142:PHE:CE2  | 1:F:786:TYR:CD2  | 3.04                     | 0.46              |
| 1:D:146:ILE:CG1  | 1:D:772:TRP:CZ2  | 2.99                     | 0.46              |
| 1:D:216:TYR:C    | 1:D:216:TYR:HD1  | 2.17                     | 0.46              |
| 1:B:387:PRO:HD3  | 1:B:802:VAL:HB   | 1.97                     | 0.46              |
| 1:A:770:GLY:O    | 1:A:773:LYS:HB2  | 2.15                     | 0.46              |
| 1:B:798:LEU:O    | 1:B:801:ALA:HB3  | 2.16                     | 0.46              |
| 1:C:575:LEU:HD21 | 1:C:724:LEU:HD13 | 1.96                     | 0.46              |
| 1:C:692:PHE:CD2  | 1:C:724:LEU:HD23 | 2.51                     | 0.46              |
| 1:G:171:PHE:CD1  | 1:G:263:PRO:HD2  | 2.51                     | 0.46              |
| 1:A:259:LEU:HD21 | 1:A:268:LEU:HA   | 1.98                     | 0.46              |
| 1:F:73:LEU:N     | 1:F:73:LEU:CD1   | 2.78                     | 0.46              |
| 1:B:292:GLN:NE2  | 1:B:356:VAL:HA   | 2.30                     | 0.46              |
| 1:C:563:HIS:HA   | 1:C:644:TRP:O    | 2.16                     | 0.46              |
| 1:H:449:ASP:O    | 1:H:504:LEU:HD22 | 2.16                     | 0.46              |
| 1:E:92:PRO:HD2   | 1:E:96:VAL:O     | 2.16                     | 0.46              |
| 1:G:65:GLU:HG3   | 1:G:70:PHE:CB    | 2.45                     | 0.46              |
| 1:H:52:GLU:OE1   | 1:H:53:PHE:HA    | 2.15                     | 0.46              |
| 1:G:39:LYS:O     | 1:G:39:LYS:HG2   | 2.15                     | 0.46              |
| 1:E:73:LEU:HD22  | 1:E:73:LEU:N     | 2.30                     | 0.46              |
| 1:B:414:ASN:O    | 1:B:418:GLY:HA3  | 2.16                     | 0.46              |
| 1:D:796:ARG:HB2  | 1:D:797:PRO:HD3  | 1.96                     | 0.46              |
| 1:A:479:ILE:HD11 | 1:A:762:LEU:HD13 | 1.97                     | 0.46              |
| 1:C:284:LEU:N    | 1:C:284:LEU:CD2  | 2.79                     | 0.46              |
| 1:G:49:ILE:CD1   | 1:G:49:ILE:N     | 2.79                     | 0.46              |
| 1:C:319:MSE:HE2  | 1:C:332:PRO:CB   | 2.45                     | 0.46              |
| 1:C:216:TYR:C    | 1:C:216:TYR:CD1  | 2.88                     | 0.46              |
| 1:G:204:ASN:HD21 | 1:H:12:HIS:N     | 2.12                     | 0.46              |
| 1:B:789:MSE:HE3  | 1:B:789:MSE:HB2  | 1.81                     | 0.46              |
| 1:B:789:MSE:SE   | 1:C:789:MSE:HG2  | 2.66                     | 0.46              |
| 1:A:189:HIS:CD2  | 1:A:279:PHE:HD2  | 2.33                     | 0.46              |
| 1:C:151:LEU:N    | 1:D:261:GLU:OE1  | 2.49                     | 0.46              |
| 1:C:137:LEU:HD11 | 1:C:790:PHE:CZ   | 2.51                     | 0.46              |
| 1:F:580:ARG:HG3  | 7:F:839:HOH:O    | 2.15                     | 0.46              |
| 1:B:781:LEU:HD12 | 1:B:781:LEU:HA   | 1.74                     | 0.46              |
| 1:G:56:LEU:CB    | 1:G:57:PRO:HD3   | 2.33                     | 0.46              |
| 1:G:190:GLN:HG2  | 1:G:405:ASN:HD22 | 1.80                     | 0.46              |
| 1:F:789:MSE:CE   | 1:G:789:MSE:HE3  | 2.45                     | 0.46              |
| 1:A:195:MSE:HE2  | 1:A:252:MSE:CE   | 2.45                     | 0.46              |
| 1:F:169:LYS:HG2  | 1:F:176:SER:OG   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:38:ALA:O     | 1:F:41:LYS:HB2   | 2.16                     | 0.46              |
| 1:E:146:ILE:CG2  | 1:E:147:PRO:HD2  | 2.45                     | 0.46              |
| 1:D:195:MSE:HE1  | 1:D:241:GLY:O    | 2.14                     | 0.46              |
| 1:F:675:GLU:HA   | 1:F:675:GLU:OE2  | 2.15                     | 0.46              |
| 1:F:545:LYS:H    | 1:F:545:LYS:HD3  | 1.80                     | 0.46              |
| 1:B:581:LEU:HD13 | 1:B:587:LEU:HD12 | 1.98                     | 0.46              |
| 1:F:163:ASN:ND2  | 1:F:269:GLU:HB2  | 2.31                     | 0.46              |
| 1:C:400:LEU:HD12 | 1:C:400:LEU:C    | 2.36                     | 0.46              |
| 1:C:657:LEU:O    | 1:C:661:ILE:HG12 | 2.16                     | 0.46              |
| 1:H:466:THR:HG23 | 1:H:790:PHE:CZ   | 2.50                     | 0.46              |
| 1:D:43:ILE:CG2   | 1:D:124:LEU:HD12 | 2.45                     | 0.46              |
| 1:F:81:VAL:HG12  | 1:F:86:VAL:CB    | 2.45                     | 0.46              |
| 1:G:756:GLN:HG2  | 1:G:757:ILE:H    | 1.80                     | 0.46              |
| 1:G:757:ILE:HD13 | 1:G:757:ILE:HA   | 1.59                     | 0.46              |
| 1:H:49:ILE:O     | 1:H:53:PHE:CB    | 2.64                     | 0.46              |
| 1:C:155:ILE:CG2  | 1:C:483:PHE:CE2  | 2.98                     | 0.46              |
| 1:A:366:ARG:HD3  | 7:A:898:HOH:O    | 2.14                     | 0.46              |
| 1:C:278:VAL:HG21 | 1:C:763:LEU:CD2  | 2.45                     | 0.46              |
| 1:B:704:VAL:HA   | 4:B:912:SO4:O1   | 2.16                     | 0.46              |
| 1:F:435:THR:HG23 | 1:F:475:THR:CB   | 2.46                     | 0.46              |
| 1:D:698:GLY:N    | 1:D:699:PRO:CD   | 2.79                     | 0.46              |
| 1:B:193:ASN:ND2  | 1:B:197:SER:HA   | 2.30                     | 0.46              |
| 1:C:540:LYS:HG3  | 1:C:540:LYS:H    | 1.54                     | 0.46              |
| 1:E:45:GLN:CB    | 1:E:80:ILE:HD13  | 2.46                     | 0.46              |
| 1:D:37:GLU:HG3   | 1:D:59:GLN:NE2   | 2.31                     | 0.46              |
| 1:A:45:GLN:NE2   | 1:A:80:ILE:HD13  | 2.13                     | 0.46              |
| 1:D:146:ILE:CG1  | 1:D:772:TRP:CH2  | 2.99                     | 0.46              |
| 1:E:348:THR:O    | 1:E:351:GLU:HG2  | 2.16                     | 0.46              |
| 1:F:176:SER:O    | 1:F:179:PRO:HD2  | 2.16                     | 0.46              |
| 1:H:33:LEU:N     | 1:H:33:LEU:HD23  | 2.29                     | 0.46              |
| 1:F:400:LEU:HD12 | 1:F:401:SER:N    | 2.31                     | 0.46              |
| 1:C:80:ILE:CD1   | 1:C:121:LYS:HG2  | 2.45                     | 0.46              |
| 1:F:244:ASP:OD2  | 1:F:248:ARG:CD   | 2.63                     | 0.46              |
| 1:C:400:LEU:HD12 | 1:C:401:SER:N    | 2.31                     | 0.46              |
| 1:G:163:ASN:ND2  | 1:G:269:GLU:OE1  | 2.49                     | 0.46              |
| 1:G:452:TRP:CD1  | 1:G:504:LEU:HB3  | 2.51                     | 0.46              |
| 1:E:85:TRP:H     | 1:E:85:TRP:HD1   | 1.62                     | 0.46              |
| 1:F:538:GLU:O    | 1:F:542:ARG:HG2  | 2.15                     | 0.46              |
| 1:C:220:LEU:N    | 1:C:220:LEU:HD12 | 2.31                     | 0.46              |
| 1:A:155:ILE:HB   | 1:A:483:PHE:CE2  | 2.51                     | 0.46              |
| 1:C:360:GLU:HB2  | 1:C:361:TYR:CE2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:706:GLY:HA2  | 1:C:710:PHE:CE2  | 2.51                     | 0.46              |
| 1:B:452:TRP:CG   | 1:B:453:LYS:N    | 2.83                     | 0.46              |
| 1:H:508:TYR:HD2  | 1:H:794:LYS:HE3  | 1.81                     | 0.45              |
| 1:E:83:PRO:CB    | 1:E:84:PRO:HD2   | 2.38                     | 0.45              |
| 1:A:63:LYS:O     | 1:A:65:GLU:HG2   | 2.15                     | 0.45              |
| 1:B:223:GLU:O    | 1:B:225:LEU:HD23 | 2.16                     | 0.45              |
| 1:D:86:VAL:HG12  | 1:D:102:VAL:CG1  | 2.46                     | 0.45              |
| 1:A:155:ILE:HB   | 1:A:483:PHE:HE2  | 1.81                     | 0.45              |
| 1:B:140:GLU:O    | 1:B:143:ASN:HB2  | 2.16                     | 0.45              |
| 1:F:277:MSE:CE   | 1:F:767:GLY:HA2  | 2.47                     | 0.45              |
| 1:F:128:VAL:HG22 | 1:F:129:LYS:N    | 2.31                     | 0.45              |
| 1:G:140:GLU:HB3  | 1:G:141:PRO:HD3  | 1.97                     | 0.45              |
| 1:H:438:HIS:O    | 1:H:439:ALA:HB2  | 2.16                     | 0.45              |
| 1:E:552:GLU:O    | 1:E:556:SER:CB   | 2.64                     | 0.45              |
| 1:E:434:CYS:HB2  | 1:E:477:PHE:CZ   | 2.51                     | 0.45              |
| 1:D:675:GLU:O    | 1:D:697:GLY:HA3  | 2.16                     | 0.45              |
| 1:C:194:LEU:HD22 | 1:C:328:LEU:HD11 | 1.98                     | 0.45              |
| 1:F:56:LEU:HD22  | 1:F:56:LEU:HA    | 1.69                     | 0.45              |
| 1:F:59:GLN:C     | 1:F:60:THR:CG2   | 2.84                     | 0.45              |
| 1:B:54:GLU:HG3   | 1:B:55:ALA:N     | 2.30                     | 0.45              |
| 1:B:146:ILE:CG2  | 1:B:147:PRO:CD   | 2.87                     | 0.45              |
| 1:E:154:TYR:OH   | 1:F:262:ALA:HB3  | 2.16                     | 0.45              |
| 1:G:101:ARG:HB3  | 1:G:112:LEU:HD11 | 1.99                     | 0.45              |
| 1:A:794:LYS:HD2  | 1:A:798:LEU:HD11 | 1.97                     | 0.45              |
| 1:C:692:PHE:CD2  | 1:C:724:LEU:HD21 | 2.51                     | 0.45              |
| 1:B:437:ALA:O    | 1:B:438:HIS:HB2  | 2.16                     | 0.45              |
| 1:E:133:PHE:HB3  | 1:H:791:TYR:HE2  | 1.79                     | 0.45              |
| 1:C:99:TYR:O     | 1:C:100:LEU:HD23 | 2.16                     | 0.45              |
| 1:H:230:GLU:O    | 1:H:234:GLU:HG3  | 2.15                     | 0.45              |
| 1:C:572:LYS:HE3  | 1:C:605:ASN:OD1  | 2.17                     | 0.45              |
| 1:E:124:LEU:HD12 | 1:E:124:LEU:O    | 2.16                     | 0.45              |
| 1:D:55:ALA:O     | 1:D:56:LEU:CB    | 2.64                     | 0.45              |
| 1:H:28:GLU:HG2   | 1:H:32:LEU:HD23  | 1.98                     | 0.45              |
| 1:B:93:ARG:HB2   | 1:B:96:VAL:CG2   | 2.46                     | 0.45              |
| 1:B:76:THR:CA    | 1:B:89:ALA:O     | 2.51                     | 0.45              |
| 1:F:628:LYS:HA   | 1:F:628:LYS:CE   | 2.42                     | 0.45              |
| 1:F:628:LYS:HA   | 1:F:628:LYS:HD2  | 1.86                     | 0.45              |
| 1:H:60:THR:O     | 1:H:63:LYS:HD3   | 2.16                     | 0.45              |
| 1:E:534:PHE:HB2  | 1:E:535:PRO:HD2  | 1.98                     | 0.45              |
| 1:H:224:THR:CG2  | 1:H:228:GLU:HG3  | 2.46                     | 0.45              |
| 1:A:287:HIS:C    | 1:A:287:HIS:CD2  | 2.89                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:566:VAL:O    | 1:D:640:GLY:HA2  | 2.16                     | 0.45              |
| 1:D:667:ALA:CA   | 1:D:689:LEU:HD11 | 2.47                     | 0.45              |
| 1:B:334:ILE:HD12 | 1:B:362:CYS:SG   | 2.55                     | 0.45              |
| 1:A:275:VAL:O    | 1:A:277:MSE:HG3  | 2.16                     | 0.45              |
| 1:G:261:GLU:HG2  | 1:H:151:LEU:HD12 | 1.98                     | 0.45              |
| 1:D:178:LEU:N    | 1:D:179:PRO:CD   | 2.80                     | 0.45              |
| 1:D:130:ASN:HB3  | 1:D:134:THR:OG1  | 2.16                     | 0.45              |
| 1:A:407:LYS:HB2  | 1:A:408:PRO:CD   | 2.45                     | 0.45              |
| 1:C:420:LEU:HD23 | 1:C:467:ALA:HB1  | 1.97                     | 0.45              |
| 1:G:140:GLU:HB3  | 1:G:141:PRO:CD   | 2.46                     | 0.45              |
| 1:G:672:ALA:O    | 1:G:714:PRO:HG3  | 2.16                     | 0.45              |
| 1:G:291:ALA:HB3  | 1:G:295:VAL:HG11 | 1.99                     | 0.45              |
| 1:G:221:LYS:HE2  | 1:G:221:LYS:HB3  | 1.62                     | 0.45              |
| 1:C:491:GLU:CD   | 1:C:491:GLU:H    | 2.19                     | 0.45              |
| 1:E:80:ILE:HG23  | 1:E:124:LEU:HD22 | 1.99                     | 0.45              |
| 1:E:42:GLY:O     | 1:E:81:VAL:HG13  | 2.16                     | 0.45              |
| 1:E:135:LEU:CD1  | 1:H:789:MSE:HG3  | 2.42                     | 0.45              |
| 1:E:82:LEU:CB    | 1:E:83:PRO:CD    | 2.87                     | 0.45              |
| 1:E:85:TRP:HB2   | 1:E:102:VAL:O    | 2.17                     | 0.45              |
| 1:D:146:ILE:CG2  | 1:D:147:PRO:N    | 2.78                     | 0.45              |
| 1:D:216:TYR:O    | 1:D:216:TYR:HD1  | 2.00                     | 0.45              |
| 1:E:52:GLU:CD    | 1:E:53:PHE:N     | 2.70                     | 0.45              |
| 1:F:70:PHE:CD2   | 1:F:71:ASP:CA    | 3.00                     | 0.45              |
| 1:H:187:HIS:NE2  | 1:H:276:PRO:O    | 2.48                     | 0.45              |
| 1:C:609:VAL:HG22 | 1:C:645:ILE:HB   | 1.98                     | 0.45              |
| 1:E:55:ALA:O     | 1:E:59:GLN:HB2   | 2.16                     | 0.45              |
| 1:A:150:THR:N    | 1:B:261:GLU:OE1  | 2.47                     | 0.45              |
| 1:C:442:LYS:HG3  | 1:C:465:PHE:CZ   | 2.51                     | 0.45              |
| 1:C:178:LEU:N    | 1:C:179:PRO:CD   | 2.80                     | 0.45              |
| 1:C:50:ILE:C     | 1:C:52:GLU:H     | 2.20                     | 0.45              |
| 1:G:169:LYS:HG2  | 1:G:169:LYS:O    | 2.17                     | 0.45              |
| 1:H:29:VAL:O     | 1:H:33:LEU:HD21  | 2.17                     | 0.45              |
| 1:H:140:GLU:HB2  | 1:H:512:HIS:CD2  | 2.51                     | 0.45              |
| 1:B:508:TYR:CD2  | 1:B:794:LYS:HE2  | 2.52                     | 0.45              |
| 1:G:550:ILE:O    | 1:G:553:LEU:HB3  | 2.16                     | 0.45              |
| 1:E:187:HIS:NE2  | 1:E:276:PRO:O    | 2.50                     | 0.45              |
| 1:A:302:GLY:N    | 3:A:902:FRU:O1   | 2.50                     | 0.45              |
| 1:E:315:LEU:CD2  | 1:E:319:MSE:HE2  | 2.46                     | 0.45              |
| 1:E:319:MSE:HE1  | 1:E:334:ILE:HD11 | 1.94                     | 0.45              |
| 1:C:143:ASN:HB3  | 1:C:148:ARG:HH22 | 1.79                     | 0.45              |
| 1:H:794:LYS:HA   | 1:H:794:LYS:HD3  | 1.62                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:43:ILE:HG23  | 1:A:82:LEU:HD23  | 1.99                     | 0.45              |
| 1:D:103:ASN:CB   | 1:D:106:ALA:CB   | 2.89                     | 0.45              |
| 1:B:206:LEU:HD11 | 1:B:210:LEU:CD1  | 2.47                     | 0.45              |
| 1:H:33:LEU:CA    | 1:H:36:VAL:HB    | 2.45                     | 0.45              |
| 1:C:216:TYR:O    | 1:C:216:TYR:HD1  | 2.00                     | 0.45              |
| 1:H:243:GLY:HA2  | 1:H:326:GLN:HA   | 1.99                     | 0.45              |
| 1:A:518:ASP:OD1  | 1:A:519:PRO:HD2  | 2.17                     | 0.45              |
| 1:B:407:LYS:HB2  | 1:B:408:PRO:CD   | 2.46                     | 0.45              |
| 1:F:435:THR:HG23 | 1:F:475:THR:OG1  | 2.17                     | 0.45              |
| 1:F:673:LEU:HD23 | 1:F:714:PRO:HB2  | 1.98                     | 0.45              |
| 1:H:698:GLY:N    | 1:H:699:PRO:CD   | 2.79                     | 0.45              |
| 1:H:453:LYS:HB2  | 1:H:453:LYS:HE2  | 1.76                     | 0.45              |
| 1:E:407:LYS:HB2  | 1:E:408:PRO:HD2  | 1.97                     | 0.45              |
| 1:A:566:VAL:O    | 1:A:640:GLY:HA2  | 2.17                     | 0.45              |
| 1:H:146:ILE:CG1  | 1:H:147:PRO:HD2  | 2.24                     | 0.45              |
| 1:C:53:PHE:O     | 1:C:57:PRO:CG    | 2.64                     | 0.45              |
| 1:A:30:LEU:HA    | 1:A:33:LEU:HD12  | 1.98                     | 0.45              |
| 1:A:56:LEU:CB    | 1:A:57:PRO:CD    | 2.92                     | 0.45              |
| 1:B:114:PRO:O    | 1:B:115:ALA:HB3  | 2.16                     | 0.45              |
| 1:E:35:ARG:NH1   | 1:E:35:ARG:CG    | 2.77                     | 0.45              |
| 1:C:216:TYR:HE2  | 1:C:232:LYS:HE2  | 1.81                     | 0.45              |
| 1:D:181:LEU:HD12 | 1:D:196:LEU:CD1  | 2.47                     | 0.45              |
| 1:E:730:LYS:CE   | 5:E:921:MLA:HC22 | 2.46                     | 0.45              |
| 1:A:189:HIS:CD2  | 1:A:279:PHE:CD2  | 3.05                     | 0.45              |
| 1:A:472:MSE:HG2  | 1:A:514:ILE:HD13 | 1.99                     | 0.45              |
| 1:A:452:TRP:CG   | 1:A:453:LYS:N    | 2.84                     | 0.45              |
| 1:D:437:ALA:C    | 1:D:439:ALA:H    | 2.20                     | 0.45              |
| 1:G:581:LEU:CD2  | 1:G:626:MSE:HG3  | 2.46                     | 0.45              |
| 1:C:628:LYS:HA   | 1:C:628:LYS:HD2  | 1.80                     | 0.45              |
| 1:C:681:VAL:CG1  | 1:C:685:MSE:HE2  | 2.42                     | 0.45              |
| 1:A:41:LYS:HD2   | 1:A:41:LYS:HA    | 1.56                     | 0.45              |
| 1:F:146:ILE:CG2  | 1:F:147:PRO:HD2  | 2.46                     | 0.45              |
| 1:E:153:LYS:HD3  | 1:E:154:TYR:CE2  | 2.52                     | 0.45              |
| 1:G:78:GLU:OE2   | 1:G:121:LYS:HE3  | 2.17                     | 0.45              |
| 1:C:137:LEU:HD11 | 1:C:790:PHE:CE1  | 2.52                     | 0.45              |
| 1:E:723:THR:O    | 1:E:726:ASP:HB2  | 2.17                     | 0.45              |
| 1:D:135:LEU:HD12 | 1:D:136:GLU:N    | 2.32                     | 0.45              |
| 1:F:587:LEU:HD13 | 1:F:608:VAL:HG13 | 1.98                     | 0.45              |
| 1:H:28:GLU:CG    | 1:H:32:LEU:HD23  | 2.47                     | 0.45              |
| 1:G:596:LYS:CG   | 1:G:636:TYR:CE1  | 2.92                     | 0.45              |
| 1:F:63:LYS:C     | 1:F:65:GLU:N     | 2.68                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:565:CYS:O    | 1:E:566:VAL:HG22 | 2.17                     | 0.45              |
| 1:F:338:THR:HG23 | 1:F:366:ARG:HG2  | 1.98                     | 0.45              |
| 1:A:261:GLU:HG2  | 1:B:151:LEU:HB2  | 1.98                     | 0.45              |
| 1:C:321:GLN:HG2  | 1:C:325:GLN:NE2  | 2.32                     | 0.45              |
| 1:A:217:LEU:CD2  | 1:A:220:LEU:HD12 | 2.47                     | 0.45              |
| 1:H:538:GLU:O    | 1:H:542:ARG:HG2  | 2.16                     | 0.45              |
| 1:G:425:LEU:HD23 | 1:G:425:LEU:HA   | 1.79                     | 0.45              |
| 1:E:44:LEU:HD11  | 1:E:451:TYR:OH   | 2.17                     | 0.44              |
| 1:C:148:ARG:CG   | 1:C:148:ARG:NH1  | 2.44                     | 0.44              |
| 1:B:45:GLN:CB    | 1:B:80:ILE:HG22  | 2.47                     | 0.44              |
| 1:B:449:ASP:OD1  | 1:B:450:ILE:HG22 | 2.17                     | 0.44              |
| 1:G:212:LYS:HE3  | 1:G:232:LYS:NZ   | 2.32                     | 0.44              |
| 1:D:290:PHE:O    | 1:D:366:ARG:NH1  | 2.38                     | 0.44              |
| 1:F:135:LEU:HD12 | 1:F:136:GLU:N    | 2.32                     | 0.44              |
| 1:C:420:LEU:O    | 1:C:420:LEU:HD13 | 2.16                     | 0.44              |
| 1:C:419:ASN:HB3  | 1:C:471:ALA:HB1  | 1.99                     | 0.44              |
| 1:A:217:LEU:HD23 | 1:A:220:LEU:HD12 | 1.98                     | 0.44              |
| 1:H:748:ARG:NH1  | 1:H:752:LYS:HG3  | 2.32                     | 0.44              |
| 1:F:566:VAL:CG1  | 1:F:567:LEU:N    | 2.80                     | 0.44              |
| 1:F:313:ARG:O    | 1:F:317:ILE:HG13 | 2.17                     | 0.44              |
| 1:C:490:LYS:O    | 1:C:490:LYS:HD2  | 2.17                     | 0.44              |
| 1:D:73:LEU:N     | 1:D:73:LEU:CD1   | 2.79                     | 0.44              |
| 1:E:117:PHE:C    | 1:E:117:PHE:CD1  | 2.90                     | 0.44              |
| 1:F:53:PHE:O     | 1:F:57:PRO:CB    | 2.64                     | 0.44              |
| 1:B:93:ARG:O     | 1:B:96:VAL:CG2   | 2.62                     | 0.44              |
| 1:F:207:GLN:NE2  | 1:F:211:ARG:HH22 | 2.07                     | 0.44              |
| 1:F:796:ARG:N    | 1:F:797:PRO:CD   | 2.79                     | 0.44              |
| 1:F:172:HIS:CE1  | 1:F:261:GLU:O    | 2.71                     | 0.44              |
| 1:G:437:ALA:C    | 1:G:439:ALA:H    | 2.20                     | 0.44              |
| 1:F:73:LEU:HD12  | 1:F:73:LEU:N     | 2.33                     | 0.44              |
| 1:A:125:VAL:HG21 | 1:A:450:ILE:HG12 | 1.99                     | 0.44              |
| 1:G:770:GLY:O    | 1:G:773:LYS:HB2  | 2.17                     | 0.44              |
| 1:A:534:PHE:HB2  | 1:A:535:PRO:CD   | 2.46                     | 0.44              |
| 1:B:340:LEU:HD23 | 1:B:368:PRO:HB3  | 1.99                     | 0.44              |
| 1:D:415:TYR:CG   | 1:D:416:SER:N    | 2.85                     | 0.44              |
| 1:C:252:MSE:O    | 1:C:255:LEU:HB2  | 2.17                     | 0.44              |
| 1:D:497:GLU:HB2  | 1:D:516:VAL:HG11 | 1.99                     | 0.44              |
| 1:D:242:TRP:O    | 1:D:252:MSE:HG3  | 2.17                     | 0.44              |
| 3:C:902:FRU:H61  | 7:C:841:HOH:O    | 2.16                     | 0.44              |
| 1:D:33:LEU:O     | 1:D:37:GLU:CG    | 2.66                     | 0.44              |
| 1:H:790:PHE:O    | 1:H:794:LYS:HB3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:76:THR:C     | 1:B:77:GLN:HG2   | 2.38                     | 0.44              |
| 1:F:80:ILE:HD11  | 1:F:117:PHE:CZ   | 2.52                     | 0.44              |
| 1:G:796:ARG:N    | 1:G:797:PRO:CD   | 2.81                     | 0.44              |
| 1:H:43:ILE:HA    | 1:H:81:VAL:O     | 2.17                     | 0.44              |
| 1:G:43:ILE:HA    | 1:G:81:VAL:O     | 2.17                     | 0.44              |
| 1:E:400:LEU:HD12 | 1:E:401:SER:N    | 2.31                     | 0.44              |
| 1:A:153:LYS:HG3  | 1:A:154:TYR:N    | 2.31                     | 0.44              |
| 1:E:419:ASN:OD1  | 1:E:435:THR:HB   | 2.18                     | 0.44              |
| 1:H:481:SER:O    | 1:H:482:THR:CG2  | 2.66                     | 0.44              |
| 1:H:149:PRO:HB3  | 1:H:161:PHE:CE1  | 2.52                     | 0.44              |
| 1:H:534:PHE:HB2  | 1:H:535:PRO:CD   | 2.48                     | 0.44              |
| 1:C:404:LEU:HD23 | 1:C:404:LEU:HA   | 1.79                     | 0.44              |
| 1:H:178:LEU:HA   | 1:H:178:LEU:HD22 | 1.70                     | 0.44              |
| 1:G:41:LYS:HB3   | 1:G:41:LYS:HE2   | 1.77                     | 0.44              |
| 1:D:56:LEU:CB    | 1:D:57:PRO:CD    | 2.96                     | 0.44              |
| 1:F:82:LEU:CD1   | 1:F:83:PRO:CG    | 2.91                     | 0.44              |
| 1:A:56:LEU:HD22  | 1:A:56:LEU:HA    | 1.78                     | 0.44              |
| 1:G:32:LEU:O     | 1:G:36:VAL:HG23  | 2.17                     | 0.44              |
| 1:D:327:GLY:C    | 1:D:328:LEU:HD23 | 2.37                     | 0.44              |
| 1:C:692:PHE:N    | 1:C:692:PHE:CD1  | 2.86                     | 0.44              |
| 1:A:417:ASP:O    | 1:A:421:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:178:LEU:HB2  | 1:C:179:PRO:HD3  | 2.00                     | 0.44              |
| 1:H:481:SER:HB2  | 1:H:677:PHE:CD2  | 2.52                     | 0.44              |
| 1:C:219:GLU:HA   | 1:C:219:GLU:OE1  | 2.17                     | 0.44              |
| 1:H:425:LEU:HA   | 1:H:425:LEU:HD23 | 1.60                     | 0.44              |
| 1:E:143:ASN:O    | 1:E:145:SER:N    | 2.51                     | 0.44              |
| 1:F:56:LEU:CB    | 1:F:57:PRO:HD3   | 2.47                     | 0.44              |
| 1:D:219:GLU:HG3  | 1:D:220:LEU:N    | 2.32                     | 0.44              |
| 1:F:143:ASN:HB3  | 1:F:148:ARG:HH21 | 1.79                     | 0.44              |
| 1:B:756:GLN:HG2  | 1:B:757:ILE:CD1  | 2.40                     | 0.44              |
| 1:C:232:LYS:O    | 1:C:235:GLU:HB2  | 2.17                     | 0.44              |
| 1:G:32:LEU:CD1   | 1:G:32:LEU:O     | 2.65                     | 0.44              |
| 1:E:590:LEU:HB2  | 1:E:671:PRO:HG3  | 1.99                     | 0.44              |
| 1:C:221:LYS:HE3  | 1:C:223:GLU:HB2  | 1.99                     | 0.44              |
| 1:H:65:GLU:C     | 1:H:67:GLY:N     | 2.70                     | 0.44              |
| 1:F:79:ALA:CB    | 1:F:88:LEU:HD23  | 2.48                     | 0.44              |
| 1:D:407:LYS:HB2  | 1:D:408:PRO:HD2  | 1.99                     | 0.44              |
| 1:C:178:LEU:N    | 1:C:179:PRO:HD2  | 2.33                     | 0.44              |
| 1:F:245:ASN:O    | 1:F:249:VAL:HG23 | 2.18                     | 0.44              |
| 1:F:259:LEU:HD21 | 1:F:267:THR:HG22 | 1.99                     | 0.44              |
| 1:D:780:ARG:HD2  | 1:D:780:ARG:HA   | 1.70                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:278:VAL:CG2  | 1:H:766:THR:HG21 | 2.47                     | 0.44              |
| 1:B:93:ARG:H     | 1:B:96:VAL:CG2   | 2.30                     | 0.44              |
| 1:D:434:CYS:SG   | 1:D:479:ILE:HG13 | 2.58                     | 0.44              |
| 1:H:483:PHE:CE1  | 1:H:487:ALA:HB3  | 2.53                     | 0.44              |
| 1:G:400:LEU:HD12 | 1:G:400:LEU:C    | 2.38                     | 0.44              |
| 1:B:587:LEU:HD13 | 1:B:608:VAL:CG1  | 2.47                     | 0.44              |
| 1:C:527:GLY:O    | 1:C:755:TRP:NE1  | 2.51                     | 0.44              |
| 1:F:370:ARG:CB   | 1:F:375:ILE:HA   | 2.48                     | 0.44              |
| 1:D:695:CYS:SG   | 1:D:696:LYS:HD3  | 2.57                     | 0.44              |
| 1:B:484:GLN:HG2  | 1:B:488:GLY:HA2  | 2.00                     | 0.44              |
| 1:D:315:LEU:HA   | 1:D:315:LEU:HD12 | 1.77                     | 0.44              |
| 1:F:225:LEU:HD12 | 1:F:225:LEU:N    | 2.32                     | 0.44              |
| 1:A:583:ARG:HH11 | 1:A:583:ARG:HG2  | 1.81                     | 0.44              |
| 1:E:315:LEU:HD23 | 1:E:319:MSE:CE   | 2.48                     | 0.44              |
| 1:F:43:ILE:CG1   | 1:F:82:LEU:HA    | 2.46                     | 0.44              |
| 1:B:80:ILE:HG12  | 1:B:87:ALA:O     | 2.18                     | 0.44              |
| 1:A:195:MSE:CE   | 1:A:242:TRP:CD2  | 2.88                     | 0.44              |
| 1:C:390:GLU:OE1  | 1:C:796:ARG:HD2  | 2.17                     | 0.44              |
| 1:F:65:GLU:HG3   | 1:F:70:PHE:HB3   | 2.00                     | 0.44              |
| 1:F:140:GLU:N    | 1:F:141:PRO:CD   | 2.76                     | 0.44              |
| 1:B:135:LEU:HD21 | 1:C:789:MSE:HE2  | 2.00                     | 0.44              |
| 1:F:284:LEU:HD22 | 1:F:284:LEU:N    | 2.33                     | 0.44              |
| 1:C:534:PHE:O    | 1:C:687:CYS:HA   | 2.18                     | 0.44              |
| 1:A:419:ASN:OD1  | 1:A:435:THR:HB   | 2.18                     | 0.44              |
| 1:C:327:GLY:O    | 1:C:328:LEU:HD23 | 2.17                     | 0.44              |
| 1:F:526:PRO:HG2  | 1:F:677:PHE:CE1  | 2.53                     | 0.44              |
| 1:H:514:ILE:HG13 | 1:H:515:ASP:N    | 2.33                     | 0.44              |
| 1:B:594:TYR:CE1  | 1:B:601:ARG:HG2  | 2.53                     | 0.44              |
| 1:H:304:GLN:HB3  | 3:H:902:FRU:O1   | 2.17                     | 0.44              |
| 1:D:59:GLN:O     | 1:D:63:LYS:HD2   | 2.17                     | 0.44              |
| 1:A:63:LYS:O     | 1:A:64:LEU:C     | 2.55                     | 0.44              |
| 1:G:169:LYS:HG2  | 1:G:176:SER:OG   | 2.18                     | 0.44              |
| 1:G:131:GLY:CA   | 1:G:134:THR:CG2  | 2.93                     | 0.44              |
| 1:F:67:GLY:HA3   | 1:F:68:PRO:HD2   | 1.53                     | 0.44              |
| 1:B:142:PHE:O    | 1:B:780:ARG:NH1  | 2.51                     | 0.44              |
| 1:E:66:GLY:HA2   | 1:E:71:ASP:OD1   | 2.18                     | 0.44              |
| 1:F:159:VAL:HG13 | 1:F:160:ASP:N    | 2.33                     | 0.44              |
| 1:G:136:GLU:HG2  | 1:G:509:ARG:HD2  | 1.99                     | 0.44              |
| 1:B:416:SER:CB   | 1:B:464:GLN:HE21 | 2.30                     | 0.44              |
| 1:C:484:GLN:HA   | 1:C:488:GLY:HA2  | 1.98                     | 0.44              |
| 1:C:441:GLU:OE1  | 1:C:441:GLU:HA   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:65:GLU:HG3   | 1:G:70:PHE:HB2   | 1.98                     | 0.44              |
| 1:G:70:PHE:CZ    | 1:G:71:ASP:OD1   | 2.71                     | 0.44              |
| 1:E:789:MSE:CE   | 1:H:789:MSE:C    | 2.87                     | 0.44              |
| 1:F:789:MSE:CE   | 1:G:789:MSE:CG   | 2.91                     | 0.44              |
| 1:D:43:ILE:O     | 1:D:44:LEU:CB    | 2.64                     | 0.44              |
| 1:E:245:ASN:O    | 1:E:249:VAL:HG23 | 2.17                     | 0.44              |
| 1:G:692:PHE:CD1  | 1:G:692:PHE:N    | 2.86                     | 0.44              |
| 1:H:65:GLU:OE2   | 1:H:65:GLU:HA    | 2.17                     | 0.44              |
| 1:F:137:LEU:HD11 | 1:F:790:PHE:CZ   | 2.53                     | 0.44              |
| 1:E:730:LYS:HE3  | 5:E:921:MLA:HC22 | 1.99                     | 0.44              |
| 1:E:415:TYR:HA   | 1:E:437:ALA:O    | 2.18                     | 0.44              |
| 1:D:73:LEU:N     | 1:D:73:LEU:HD12  | 2.33                     | 0.44              |
| 1:H:444:LYS:HE3  | 1:H:584:VAL:HG11 | 1.99                     | 0.44              |
| 1:H:679:LEU:O    | 1:H:683:GLU:HG3  | 2.18                     | 0.44              |
| 1:H:50:ILE:O     | 1:H:54:GLU:HB3   | 2.18                     | 0.44              |
| 1:A:221:LYS:HE2  | 1:A:221:LYS:HB3  | 1.67                     | 0.44              |
| 1:E:277:MSE:HB3  | 1:E:277:MSE:HE3  | 1.83                     | 0.44              |
| 1:A:789:MSE:HE1  | 1:D:786:TYR:O    | 2.18                     | 0.43              |
| 1:E:789:MSE:SE   | 1:H:789:MSE:CE   | 3.14                     | 0.43              |
| 1:A:315:LEU:C    | 1:A:319:MSE:CE   | 2.86                     | 0.43              |
| 1:B:89:ALA:HA    | 1:B:99:TYR:HA    | 1.99                     | 0.43              |
| 1:E:35:ARG:CD    | 1:E:104:LEU:HA   | 2.46                     | 0.43              |
| 1:H:99:TYR:HE2   | 1:H:114:PRO:HB3  | 1.83                     | 0.43              |
| 1:C:71:ASP:HA    | 1:C:74:LYS:CB    | 2.48                     | 0.43              |
| 1:C:597:ASN:C    | 1:C:597:ASN:OD1  | 2.57                     | 0.43              |
| 1:E:112:LEU:N    | 1:E:112:LEU:HD23 | 2.32                     | 0.43              |
| 1:F:580:ARG:NH1  | 2:F:901:UDP:O1B  | 2.51                     | 0.43              |
| 1:A:217:LEU:HD23 | 1:A:217:LEU:HA   | 1.80                     | 0.43              |
| 1:D:376:VAL:HG21 | 1:D:388:TYR:CE2  | 2.53                     | 0.43              |
| 1:G:435:THR:HG23 | 1:G:475:THR:CB   | 2.48                     | 0.43              |
| 1:E:693:ALA:HB3  | 1:E:703:ILE:HD12 | 2.00                     | 0.43              |
| 1:C:279:PHE:HB2  | 1:C:409:ASP:OD2  | 2.17                     | 0.43              |
| 1:G:219:GLU:OE1  | 1:G:219:GLU:HA   | 2.18                     | 0.43              |
| 1:G:223:GLU:CD   | 1:G:223:GLU:H    | 2.22                     | 0.43              |
| 1:D:452:TRP:CG   | 1:D:453:LYS:N    | 2.86                     | 0.43              |
| 1:H:284:LEU:HD22 | 1:H:284:LEU:N    | 2.33                     | 0.43              |
| 1:G:70:PHE:HD2   | 1:G:70:PHE:O     | 2.02                     | 0.43              |
| 1:C:685:MSE:HE1  | 1:C:703:ILE:HG13 | 2.00                     | 0.43              |
| 1:F:83:PRO:HB2   | 1:F:84:PRO:CD    | 2.48                     | 0.43              |
| 1:H:315:LEU:CB   | 1:H:319:MSE:HE3  | 2.44                     | 0.43              |
| 1:D:102:VAL:CG2  | 1:D:109:VAL:HG22 | 2.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:281:VAL:HB   | 1:B:334:ILE:HG23 | 2.00                     | 0.43              |
| 1:G:524:VAL:HG12 | 1:G:758:TYR:CD2  | 2.53                     | 0.43              |
| 1:G:63:LYS:O     | 1:G:65:GLU:N     | 2.51                     | 0.43              |
| 1:E:135:LEU:HD22 | 1:H:793:LEU:HD11 | 1.99                     | 0.43              |
| 1:E:60:THR:OG1   | 1:E:61:ARG:N     | 2.52                     | 0.43              |
| 1:F:187:HIS:NE2  | 1:F:276:PRO:O    | 2.49                     | 0.43              |
| 1:H:545:LYS:HB2  | 1:H:545:LYS:NZ   | 2.33                     | 0.43              |
| 1:G:295:VAL:HG23 | 7:G:892:HOH:O    | 2.18                     | 0.43              |
| 1:B:586:ASN:HB3  | 1:B:671:PRO:O    | 2.18                     | 0.43              |
| 1:H:86:VAL:O     | 1:H:101:ARG:HA   | 2.18                     | 0.43              |
| 1:F:442:LYS:HB2  | 7:F:872:HOH:O    | 2.17                     | 0.43              |
| 1:C:306:VAL:HG21 | 2:C:901:UDP:H4'  | 2.00                     | 0.43              |
| 1:A:528:ALA:HA   | 7:A:827:HOH:O    | 2.17                     | 0.43              |
| 1:C:91:ARG:HD2   | 1:C:97:TRP:CZ2   | 2.52                     | 0.43              |
| 1:C:86:VAL:HG12  | 1:C:102:VAL:HB   | 2.00                     | 0.43              |
| 1:A:70:PHE:CD2   | 1:A:71:ASP:HA    | 2.53                     | 0.43              |
| 1:E:340:LEU:HB2  | 1:E:366:ARG:HB3  | 1.99                     | 0.43              |
| 1:H:131:GLY:C    | 1:H:134:THR:HG23 | 2.39                     | 0.43              |
| 1:H:757:ILE:HG22 | 1:H:761:ARG:CG   | 2.46                     | 0.43              |
| 1:G:156:GLY:HA3  | 1:G:523:ILE:HG13 | 2.00                     | 0.43              |
| 1:H:56:LEU:HG    | 1:H:70:PHE:CE1   | 2.53                     | 0.43              |
| 1:E:415:TYR:CG   | 1:E:416:SER:N    | 2.87                     | 0.43              |
| 1:G:524:VAL:HA   | 7:G:820:HOH:O    | 2.18                     | 0.43              |
| 1:A:599:ARG:O    | 1:A:603:LEU:HD12 | 2.17                     | 0.43              |
| 1:F:734:ASP:HA   | 1:F:735:PRO:HD2  | 1.89                     | 0.43              |
| 1:H:102:VAL:HA   | 1:H:109:VAL:HA   | 2.01                     | 0.43              |
| 1:D:156:GLY:HA3  | 1:D:523:ILE:HG13 | 2.01                     | 0.43              |
| 1:G:68:PRO:O     | 1:G:70:PHE:N     | 2.52                     | 0.43              |
| 1:D:61:ARG:HB3   | 1:G:405:ASN:OD1  | 2.19                     | 0.43              |
| 1:A:39:LYS:HZ1   | 1:A:105:HIS:HD2  | 1.65                     | 0.43              |
| 1:H:217:LEU:HD11 | 1:H:233:PHE:HZ   | 1.84                     | 0.43              |
| 1:A:43:ILE:C     | 1:A:44:LEU:HG    | 2.37                     | 0.43              |
| 1:G:131:GLY:C    | 1:G:134:THR:HG23 | 2.39                     | 0.43              |
| 1:B:419:ASN:HB3  | 1:B:471:ALA:HB1  | 1.99                     | 0.43              |
| 1:G:552:GLU:O    | 1:G:556:SER:HB3  | 2.19                     | 0.43              |
| 1:B:22:LEU:HD13  | 1:B:25:GLU:OE2   | 2.19                     | 0.43              |
| 1:D:373:LYS:HE3  | 1:D:373:LYS:HB2  | 1.90                     | 0.43              |
| 1:B:49:ILE:O     | 1:B:53:PHE:CB    | 2.66                     | 0.43              |
| 1:F:794:LYS:C    | 1:F:797:PRO:HD2  | 2.39                     | 0.43              |
| 1:A:673:LEU:HA   | 1:A:673:LEU:HD23 | 1.74                     | 0.43              |
| 1:A:565:CYS:HB3  | 1:A:566:VAL:H    | 1.66                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:317:ILE:HG22 | 1:C:318:GLU:N    | 2.32                     | 0.43              |
| 1:A:278:VAL:HG22 | 1:A:766:THR:HG21 | 1.99                     | 0.43              |
| 1:H:71:ASP:O     | 1:H:75:SER:HB3   | 2.18                     | 0.43              |
| 1:E:216:TYR:HD1  | 1:E:216:TYR:O    | 2.01                     | 0.43              |
| 1:A:56:LEU:HD13  | 1:A:63:LYS:HD2   | 2.01                     | 0.43              |
| 1:F:143:ASN:HB3  | 1:F:148:ARG:HH22 | 1.77                     | 0.43              |
| 1:F:178:LEU:CB   | 1:F:179:PRO:HD3  | 2.48                     | 0.43              |
| 1:H:315:LEU:HD12 | 1:H:315:LEU:HA   | 1.51                     | 0.43              |
| 1:B:178:LEU:N    | 1:B:179:PRO:CD   | 2.81                     | 0.43              |
| 1:B:293:ASP:O    | 1:B:294:ASN:HB2  | 2.19                     | 0.43              |
| 1:A:209:THR:HG23 | 1:A:236:ILE:HB   | 2.01                     | 0.43              |
| 1:F:419:ASN:HB3  | 1:F:471:ALA:CB   | 2.49                     | 0.43              |
| 1:F:156:GLY:HA3  | 1:F:523:ILE:HG13 | 1.99                     | 0.43              |
| 1:C:183:PHE:HD1  | 1:C:774:HIS:ND1  | 2.16                     | 0.43              |
| 1:H:348:THR:O    | 1:H:351:GLU:HG2  | 2.19                     | 0.43              |
| 1:E:433:GLN:O    | 1:E:476:ASP:HB2  | 2.18                     | 0.43              |
| 1:F:713:ASP:OD1  | 1:F:713:ASP:C    | 2.57                     | 0.43              |
| 1:F:479:ILE:HD11 | 1:F:762:LEU:CD1  | 2.49                     | 0.43              |
| 1:B:583:ARG:HG2  | 1:B:583:ARG:HH11 | 1.84                     | 0.43              |
| 1:B:45:GLN:HA    | 1:B:80:ILE:HA    | 2.01                     | 0.43              |
| 1:E:340:LEU:O    | 1:E:342:PRO:HD3  | 2.19                     | 0.43              |
| 1:G:131:GLY:O    | 1:G:134:THR:HG23 | 2.18                     | 0.43              |
| 1:B:63:LYS:CG    | 1:B:64:LEU:N     | 2.81                     | 0.43              |
| 1:A:564:LEU:HD22 | 1:A:613:ARG:CZ   | 2.49                     | 0.43              |
| 1:G:435:THR:HG23 | 1:G:475:THR:HB   | 2.00                     | 0.43              |
| 1:H:518:ASP:OD1  | 1:H:520:LYS:HG2  | 2.19                     | 0.43              |
| 1:G:781:LEU:HD12 | 1:G:781:LEU:HA   | 1.68                     | 0.43              |
| 1:D:170:LEU:HD12 | 1:D:170:LEU:HA   | 1.78                     | 0.43              |
| 1:A:41:LYS:O     | 1:A:44:LEU:HD12  | 2.18                     | 0.43              |
| 1:B:48:GLN:O     | 1:B:52:GLU:N     | 2.51                     | 0.43              |
| 1:F:146:ILE:CG2  | 1:F:147:PRO:N    | 2.82                     | 0.43              |
| 1:F:131:GLY:O    | 1:F:134:THR:CG2  | 2.64                     | 0.43              |
| 1:H:143:ASN:CB   | 1:H:148:ARG:HH22 | 2.31                     | 0.43              |
| 1:E:125:VAL:HG22 | 1:E:126:ASP:N    | 2.33                     | 0.43              |
| 1:B:534:PHE:HB2  | 1:B:535:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:230:GLU:O    | 1:C:234:GLU:HG3  | 2.18                     | 0.43              |
| 1:D:462:SER:O    | 1:D:798:LEU:HD13 | 2.19                     | 0.43              |
| 1:C:139:PHE:CE1  | 1:C:787:LEU:HD21 | 2.54                     | 0.43              |
| 1:B:352:ARG:NH2  | 1:B:403:GLU:OE2  | 2.43                     | 0.43              |
| 1:H:236:ILE:HD11 | 1:H:238:LEU:HD12 | 2.01                     | 0.43              |
| 1:F:193:ASN:ND2  | 1:F:197:SER:HA   | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:571:LYS:HD2  | 1:E:571:LYS:H    | 1.82                     | 0.43              |
| 1:E:44:LEU:CD1   | 1:E:45:GLN:H     | 2.32                     | 0.43              |
| 1:A:39:LYS:HZ3   | 1:A:105:HIS:HD2  | 1.65                     | 0.43              |
| 1:F:83:PRO:CB    | 1:F:85:TRP:H     | 2.25                     | 0.43              |
| 1:A:65:GLU:C     | 1:A:67:GLY:N     | 2.71                     | 0.43              |
| 1:F:80:ILE:CD1   | 1:F:117:PHE:CE2  | 3.02                     | 0.43              |
| 1:G:43:ILE:O     | 1:G:44:LEU:HG    | 2.18                     | 0.43              |
| 1:D:586:ASN:HB3  | 1:D:671:PRO:O    | 2.19                     | 0.43              |
| 1:E:680:THR:CG2  | 2:E:901:UDP:H3'  | 2.48                     | 0.43              |
| 1:H:163:ASN:HD21 | 1:H:269:GLU:HB2  | 1.84                     | 0.43              |
| 1:E:629:MSE:HG2  | 1:E:644:TRP:CH2  | 2.54                     | 0.43              |
| 1:A:564:LEU:HA   | 1:A:564:LEU:HD12 | 1.47                     | 0.43              |
| 1:F:459:TYR:O    | 1:F:460:HIS:HB2  | 2.19                     | 0.43              |
| 1:E:292:GLN:OE1  | 1:E:356:VAL:HA   | 2.19                     | 0.43              |
| 1:A:581:LEU:HD11 | 1:A:625:GLU:HG3  | 2.01                     | 0.43              |
| 1:C:514:ILE:HG13 | 1:C:515:ASP:N    | 2.34                     | 0.43              |
| 1:D:142:PHE:HB3  | 1:D:783:ALA:HB2  | 2.01                     | 0.43              |
| 1:B:339:ARG:HD2  | 1:B:369:PHE:CE2  | 2.53                     | 0.43              |
| 1:D:638:LEU:HD23 | 1:D:638:LEU:HA   | 1.78                     | 0.43              |
| 1:D:30:LEU:O     | 1:D:33:LEU:N     | 2.52                     | 0.42              |
| 1:B:131:GLY:CA   | 1:B:134:THR:HG23 | 2.43                     | 0.42              |
| 1:D:125:VAL:CG1  | 1:D:505:PRO:HG2  | 2.44                     | 0.42              |
| 1:B:29:VAL:HG11  | 1:E:405:ASN:OD1  | 2.18                     | 0.42              |
| 1:A:173:ASP:HB3  | 1:A:176:SER:HB3  | 2.00                     | 0.42              |
| 1:F:685:MSE:HE2  | 1:F:745:GLY:HA2  | 2.00                     | 0.42              |
| 1:F:493:VAL:HG23 | 1:F:497:GLU:HG2  | 2.00                     | 0.42              |
| 1:E:321:GLN:OE1  | 1:E:321:GLN:HA   | 2.19                     | 0.42              |
| 1:D:449:ASP:HB2  | 1:D:504:LEU:CD2  | 2.49                     | 0.42              |
| 1:A:583:ARG:HG2  | 1:A:583:ARG:NH1  | 2.34                     | 0.42              |
| 1:G:339:ARG:HH12 | 1:G:380:ILE:HG13 | 1.83                     | 0.42              |
| 1:H:88:LEU:N     | 1:H:100:LEU:O    | 2.46                     | 0.42              |
| 1:A:582:ASP:HB2  | 1:A:621:GLU:OE1  | 2.18                     | 0.42              |
| 1:F:320:LEU:HA   | 1:F:320:LEU:HD23 | 1.68                     | 0.42              |
| 1:G:780:ARG:HA   | 1:G:780:ARG:HD2  | 1.81                     | 0.42              |
| 1:A:39:LYS:NZ    | 1:A:105:HIS:CD2  | 2.84                     | 0.42              |
| 1:G:146:ILE:HG22 | 1:G:147:PRO:N    | 2.34                     | 0.42              |
| 1:F:497:GLU:HB2  | 1:F:516:VAL:CG2  | 2.49                     | 0.42              |
| 1:H:415:TYR:O    | 1:H:419:ASN:ND2  | 2.52                     | 0.42              |
| 1:H:435:THR:HG23 | 1:H:475:THR:HB   | 2.01                     | 0.42              |
| 1:F:630:TYR:O    | 1:F:633:ILE:HB   | 2.20                     | 0.42              |
| 1:B:63:LYS:HG3   | 1:B:64:LEU:N     | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:298:TYR:CE1  | 1:C:649:MSE:CE   | 3.02                     | 0.42              |
| 1:H:553:LEU:HD23 | 1:H:645:ILE:HD13 | 2.01                     | 0.42              |
| 1:C:226:TYR:O    | 1:C:230:GLU:HB2  | 2.19                     | 0.42              |
| 1:E:730:LYS:NZ   | 5:E:921:MLA:HC22 | 2.33                     | 0.42              |
| 1:E:556:SER:HB3  | 1:E:643:ARG:NH2  | 2.35                     | 0.42              |
| 1:E:301:THR:HG23 | 1:E:305:VAL:HG21 | 2.01                     | 0.42              |
| 1:D:542:ARG:HD2  | 1:D:659:ARG:HD2  | 2.00                     | 0.42              |
| 1:D:333:ARG:NH2  | 1:D:363:ASP:OD1  | 2.51                     | 0.42              |
| 1:B:82:LEU:C     | 1:B:83:PRO:O     | 2.58                     | 0.42              |
| 1:D:61:ARG:HA    | 1:D:63:LYS:CD    | 2.38                     | 0.42              |
| 1:C:46:GLN:HB2   | 1:C:50:ILE:CG2   | 2.50                     | 0.42              |
| 1:B:113:GLN:HA   | 1:B:114:PRO:HD3  | 1.92                     | 0.42              |
| 1:D:441:GLU:HG2  | 1:D:464:GLN:NE2  | 2.34                     | 0.42              |
| 1:C:60:THR:O     | 1:C:62:LYS:N     | 2.53                     | 0.42              |
| 1:B:230:GLU:OE1  | 1:B:240:ARG:NH1  | 2.52                     | 0.42              |
| 1:F:145:SER:CB   | 1:F:779:ASP:OD2  | 2.65                     | 0.42              |
| 1:G:125:VAL:HG12 | 1:G:126:ASP:N    | 2.34                     | 0.42              |
| 1:C:284:LEU:HD22 | 1:C:284:LEU:N    | 2.34                     | 0.42              |
| 1:G:371:THR:HG21 | 1:G:804:LEU:HD13 | 2.00                     | 0.42              |
| 1:C:470:PHE:CE1  | 1:C:791:TYR:HB2  | 2.54                     | 0.42              |
| 1:H:565:CYS:HB2  | 1:H:642:PHE:O    | 2.19                     | 0.42              |
| 1:D:278:VAL:CG2  | 1:D:766:THR:HG21 | 2.48                     | 0.42              |
| 1:E:45:GLN:CB    | 1:E:79:ALA:O     | 2.68                     | 0.42              |
| 1:B:20:GLU:OE1   | 1:B:71:ASP:CB    | 2.67                     | 0.42              |
| 1:E:794:LYS:HE2  | 1:E:794:LYS:HA   | 2.01                     | 0.42              |
| 1:G:148:ARG:HD2  | 1:G:515:ASP:OD2  | 2.20                     | 0.42              |
| 1:A:41:LYS:HE3   | 1:A:54:GLU:OE1   | 2.18                     | 0.42              |
| 1:H:89:ALA:HA    | 1:H:99:TYR:HA    | 2.01                     | 0.42              |
| 1:F:400:LEU:CD1  | 1:F:400:LEU:C    | 2.85                     | 0.42              |
| 1:G:86:VAL:O     | 1:G:101:ARG:HA   | 2.20                     | 0.42              |
| 1:C:71:ASP:O     | 1:C:75:SER:HB2   | 2.20                     | 0.42              |
| 1:D:386:TRP:N    | 1:D:387:PRO:HD2  | 2.34                     | 0.42              |
| 1:A:216:TYR:CE2  | 1:A:232:LYS:HG2  | 2.53                     | 0.42              |
| 1:D:580:ARG:HD3  | 2:D:901:UDP:O2B  | 2.19                     | 0.42              |
| 1:A:693:ALA:HB3  | 1:A:703:ILE:HD12 | 2.00                     | 0.42              |
| 1:F:752:LYS:HB2  | 1:F:753:TYR:CE2  | 2.55                     | 0.42              |
| 1:B:730:LYS:HE3  | 5:B:921:MLA:O1A  | 2.20                     | 0.42              |
| 1:A:752:LYS:HB2  | 1:A:753:TYR:CE2  | 2.54                     | 0.42              |
| 1:A:688:GLY:O    | 1:A:690:PRO:HD3  | 2.20                     | 0.42              |
| 1:H:322:ARG:HD2  | 1:H:763:LEU:CD1  | 2.50                     | 0.42              |
| 1:E:491:GLU:H    | 1:E:491:GLU:CD   | 2.22                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:82:LEU:CD1   | 1:G:83:PRO:HD3   | 2.49                     | 0.42              |
| 1:G:65:GLU:OE2   | 1:G:65:GLU:HA    | 2.19                     | 0.42              |
| 1:H:72:LEU:HA    | 1:H:75:SER:CB    | 2.37                     | 0.42              |
| 1:E:60:THR:O     | 1:E:63:LYS:CD    | 2.68                     | 0.42              |
| 1:B:30:LEU:O     | 1:B:33:LEU:HB2   | 2.19                     | 0.42              |
| 1:F:216:TYR:CD2  | 1:F:232:LYS:HG2  | 2.55                     | 0.42              |
| 1:F:794:LYS:O    | 1:F:797:PRO:HD2  | 2.19                     | 0.42              |
| 1:E:119:HIS:HE1  | 1:E:509:ARG:NH2  | 2.18                     | 0.42              |
| 1:H:609:VAL:HG22 | 1:H:645:ILE:HB   | 2.00                     | 0.42              |
| 1:F:645:ILE:HG22 | 1:F:646:SER:O    | 2.19                     | 0.42              |
| 1:D:566:VAL:O    | 1:D:640:GLY:CA   | 2.68                     | 0.42              |
| 1:C:547:HIS:HD2  | 1:C:660:TYR:CE2  | 2.37                     | 0.42              |
| 3:F:902:FRU:H61  | 7:F:888:HOH:O    | 2.19                     | 0.42              |
| 1:H:528:ALA:HA   | 7:H:834:HOH:O    | 2.18                     | 0.42              |
| 1:G:65:GLU:CG    | 1:G:70:PHE:CB    | 2.97                     | 0.42              |
| 1:A:52:GLU:O     | 1:A:53:PHE:C     | 2.56                     | 0.42              |
| 1:B:56:LEU:HD22  | 1:B:56:LEU:HA    | 1.93                     | 0.42              |
| 1:B:420:LEU:HD13 | 1:B:420:LEU:O    | 2.19                     | 0.42              |
| 1:B:321:GLN:O    | 1:B:325:GLN:HG3  | 2.20                     | 0.42              |
| 1:E:155:ILE:HB   | 1:E:483:PHE:HE2  | 1.85                     | 0.42              |
| 1:B:629:MSE:HE1  | 1:B:642:PHE:HZ   | 1.85                     | 0.42              |
| 1:H:339:ARG:NH2  | 1:H:378:LYS:O    | 2.52                     | 0.42              |
| 1:D:60:THR:O     | 1:D:63:LYS:CD    | 2.68                     | 0.42              |
| 1:F:468:ASP:O    | 1:F:472:MSE:HB2  | 2.18                     | 0.42              |
| 1:E:216:TYR:HD1  | 1:E:216:TYR:C    | 2.23                     | 0.42              |
| 1:H:76:THR:O     | 1:H:77:GLN:HB2   | 2.20                     | 0.42              |
| 1:F:794:LYS:HA   | 1:F:794:LYS:HD2  | 1.66                     | 0.42              |
| 1:A:773:LYS:HB2  | 1:A:773:LYS:HE3  | 1.81                     | 0.42              |
| 1:F:135:LEU:HD22 | 1:G:793:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:322:ARG:O    | 1:A:326:GLN:HG2  | 2.20                     | 0.42              |
| 1:F:507:LEU:HA   | 1:F:507:LEU:HD12 | 1.75                     | 0.42              |
| 1:D:183:PHE:HZ   | 1:D:277:MSE:SE   | 2.52                     | 0.42              |
| 1:E:315:LEU:CD2  | 1:E:319:MSE:CE   | 2.98                     | 0.42              |
| 1:D:63:LYS:O     | 1:D:64:LEU:C     | 2.58                     | 0.42              |
| 1:B:56:LEU:HD21  | 1:B:65:GLU:CD    | 2.40                     | 0.42              |
| 1:D:43:ILE:HG23  | 1:D:124:LEU:CD1  | 2.49                     | 0.42              |
| 1:E:796:ARG:HB2  | 1:E:797:PRO:CD   | 2.46                     | 0.42              |
| 1:F:63:LYS:HG3   | 1:F:63:LYS:H     | 1.59                     | 0.42              |
| 1:E:226:TYR:CE2  | 1:E:240:ARG:CG   | 3.02                     | 0.42              |
| 1:A:203:LEU:O    | 1:A:207:GLN:HB3  | 2.20                     | 0.42              |
| 1:H:596:LYS:CE   | 1:H:636:TYR:OH   | 2.68                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:287:HIS:HB3  | 1:A:417:ASP:OD2  | 2.20                     | 0.42              |
| 1:F:441:GLU:OE1  | 1:F:441:GLU:HA   | 2.19                     | 0.42              |
| 1:H:796:ARG:HB2  | 1:H:797:PRO:HD3  | 2.00                     | 0.42              |
| 1:C:301:THR:HG23 | 1:C:305:VAL:HG21 | 2.02                     | 0.42              |
| 1:B:435:THR:HG23 | 1:B:475:THR:HB   | 2.02                     | 0.42              |
| 1:H:617:SER:HB3  | 1:H:623:LYS:HG3  | 2.01                     | 0.42              |
| 1:A:99:TYR:CD2   | 1:A:99:TYR:N     | 2.88                     | 0.42              |
| 1:E:99:TYR:N     | 1:E:99:TYR:CD2   | 2.88                     | 0.42              |
| 1:G:50:ILE:O     | 1:G:52:GLU:N     | 2.53                     | 0.42              |
| 1:E:789:MSE:HE2  | 1:H:789:MSE:CB   | 2.40                     | 0.42              |
| 1:C:50:ILE:O     | 1:C:52:GLU:N     | 2.52                     | 0.42              |
| 1:F:43:ILE:CG2   | 1:F:44:LEU:N     | 2.63                     | 0.42              |
| 1:B:99:TYR:OH    | 1:B:114:PRO:HG3  | 2.20                     | 0.42              |
| 1:D:629:MSE:CE   | 1:D:629:MSE:CA   | 2.95                     | 0.42              |
| 1:B:33:LEU:O     | 1:B:36:VAL:N     | 2.43                     | 0.42              |
| 1:A:146:ILE:HD11 | 1:A:162:LEU:CD1  | 2.50                     | 0.42              |
| 1:C:119:HIS:CE1  | 1:C:509:ARG:CZ   | 3.02                     | 0.42              |
| 1:H:140:GLU:N    | 1:H:141:PRO:CD   | 2.82                     | 0.42              |
| 1:C:339:ARG:HH12 | 1:C:380:ILE:N    | 2.18                     | 0.42              |
| 1:C:540:LYS:HE3  | 1:C:540:LYS:HB2  | 1.91                     | 0.42              |
| 1:C:572:LYS:HE3  | 1:C:605:ASN:CG   | 2.40                     | 0.42              |
| 1:G:417:ASP:O    | 1:G:421:VAL:HG23 | 2.19                     | 0.42              |
| 1:E:462:SER:HB2  | 1:E:507:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:348:THR:O    | 1:A:351:GLU:HG2  | 2.20                     | 0.42              |
| 1:C:81:VAL:HB    | 1:C:86:VAL:HG23  | 2.02                     | 0.42              |
| 1:F:434:CYS:HG   | 1:F:479:ILE:HG13 | 1.85                     | 0.42              |
| 1:F:46:GLN:HG2   | 1:F:50:ILE:HG22  | 2.02                     | 0.42              |
| 1:B:91:ARG:HA    | 1:B:92:PRO:HD2   | 1.86                     | 0.42              |
| 1:A:252:MSE:SE   | 1:A:274:ARG:HD2  | 2.70                     | 0.42              |
| 1:B:162:LEU:HD11 | 1:B:772:TRP:CE3  | 2.55                     | 0.42              |
| 1:C:136:GLU:OE2  | 1:C:509:ARG:NH1  | 2.53                     | 0.42              |
| 1:A:141:PRO:HB2  | 1:D:782:GLU:HG3  | 2.01                     | 0.42              |
| 1:D:206:LEU:O    | 1:D:210:LEU:HG   | 2.19                     | 0.42              |
| 1:B:465:PHE:HD2  | 1:B:504:LEU:HD11 | 1.84                     | 0.42              |
| 1:E:435:THR:HG23 | 1:E:475:THR:HB   | 2.00                     | 0.42              |
| 1:A:290:PHE:HD2  | 7:A:882:HOH:O    | 2.03                     | 0.42              |
| 1:F:716:HIS:HB3  | 4:F:913:SO4:S    | 2.59                     | 0.42              |
| 1:A:437:ALA:O    | 1:A:438:HIS:HB2  | 2.20                     | 0.42              |
| 1:E:743:LYS:HA   | 1:E:746:LEU:HD12 | 2.02                     | 0.42              |
| 1:G:446:PRO:O    | 1:G:447:ASP:HB2  | 2.20                     | 0.42              |
| 1:F:371:THR:OG1  | 1:F:373:LYS:HE3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:238:LEU:HA   | 1:C:238:LEU:HD23 | 1.81                     | 0.42              |
| 1:A:545:LYS:H    | 1:A:545:LYS:CD   | 2.32                     | 0.42              |
| 1:C:83:PRO:CG    | 1:C:84:PRO:CD    | 2.88                     | 0.41              |
| 1:A:789:MSE:CE   | 1:D:789:MSE:C    | 2.89                     | 0.41              |
| 1:H:46:GLN:HB3   | 1:H:51:ALA:CB    | 2.29                     | 0.41              |
| 1:E:63:LYS:O     | 1:E:64:LEU:C     | 2.59                     | 0.41              |
| 1:C:752:LYS:HB2  | 1:C:753:TYR:CE2  | 2.55                     | 0.41              |
| 1:H:73:LEU:O     | 1:H:76:THR:HG23  | 2.19                     | 0.41              |
| 1:B:62:LYS:HE3   | 1:B:62:LYS:HB2   | 1.83                     | 0.41              |
| 1:G:55:ALA:O     | 1:G:59:GLN:HB2   | 2.20                     | 0.41              |
| 1:C:216:TYR:CE2  | 1:C:232:LYS:HE2  | 2.55                     | 0.41              |
| 1:H:308:ILE:HG22 | 1:H:336:ILE:HD13 | 2.01                     | 0.41              |
| 1:D:433:GLN:HG2  | 1:D:475:THR:OG1  | 2.20                     | 0.41              |
| 1:A:339:ARG:HD2  | 1:A:369:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:582:ASP:C    | 1:A:582:ASP:OD1  | 2.58                     | 0.41              |
| 1:H:659:ARG:O    | 1:H:662:CYS:HB2  | 2.20                     | 0.41              |
| 1:A:726:ASP:O    | 1:A:730:LYS:HG3  | 2.20                     | 0.41              |
| 1:B:276:PRO:HG3  | 1:B:326:GLN:HB3  | 2.02                     | 0.41              |
| 1:F:749:ILE:HD13 | 1:F:749:ILE:HA   | 1.86                     | 0.41              |
| 1:H:375:ILE:HG13 | 1:H:375:ILE:O    | 2.16                     | 0.41              |
| 1:C:180:LEU:HD12 | 1:C:180:LEU:O    | 2.20                     | 0.41              |
| 1:G:82:LEU:CD1   | 1:G:83:PRO:CD    | 2.88                     | 0.41              |
| 1:D:173:ASP:CB   | 1:D:176:SER:HB2  | 2.46                     | 0.41              |
| 1:E:65:GLU:HG2   | 1:E:70:PHE:HB2   | 2.02                     | 0.41              |
| 1:F:81:VAL:CG1   | 1:F:86:VAL:CB    | 2.98                     | 0.41              |
| 1:H:113:GLN:HB3  | 1:H:114:PRO:HD2  | 2.02                     | 0.41              |
| 1:F:65:GLU:O     | 1:F:66:GLY:C     | 2.57                     | 0.41              |
| 1:C:217:LEU:HD22 | 1:C:246:ALA:HB1  | 2.03                     | 0.41              |
| 1:B:22:LEU:HA    | 1:B:22:LEU:HD23  | 1.91                     | 0.41              |
| 1:H:672:ALA:HB3  | 1:H:694:THR:HG21 | 2.03                     | 0.41              |
| 1:C:468:ASP:O    | 1:C:472:MSE:HB2  | 2.20                     | 0.41              |
| 1:F:743:LYS:O    | 1:F:747:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:606:LEU:HD23 | 1:A:642:PHE:CD1  | 2.55                     | 0.41              |
| 1:G:778:LEU:N    | 1:G:778:LEU:HD12 | 2.35                     | 0.41              |
| 1:G:641:GLN:N    | 1:G:641:GLN:CD   | 2.73                     | 0.41              |
| 1:F:404:LEU:HA   | 1:F:404:LEU:HD23 | 1.86                     | 0.41              |
| 1:E:44:LEU:O     | 1:E:81:VAL:CG1   | 2.68                     | 0.41              |
| 1:F:789:MSE:HE3  | 1:G:789:MSE:C    | 2.40                     | 0.41              |
| 1:C:67:GLY:O     | 1:C:70:PHE:HB3   | 2.20                     | 0.41              |
| 1:F:275:VAL:O    | 1:F:277:MSE:HG3  | 2.20                     | 0.41              |
| 1:B:438:HIS:O    | 1:B:439:ALA:HB2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:287:HIS:HB3  | 1:C:417:ASP:OD2  | 2.20                     | 0.41              |
| 1:E:664:THR:O    | 1:E:665:LYS:HB2  | 2.19                     | 0.41              |
| 1:C:328:LEU:HD23 | 1:C:328:LEU:HA   | 1.76                     | 0.41              |
| 1:F:291:ALA:HB3  | 1:F:295:VAL:HG11 | 2.02                     | 0.41              |
| 1:F:327:GLY:O    | 1:F:328:LEU:HD23 | 2.20                     | 0.41              |
| 1:C:433:GLN:O    | 1:C:476:ASP:HB2  | 2.20                     | 0.41              |
| 1:D:633:ILE:HD11 | 1:D:642:PHE:HE2  | 1.85                     | 0.41              |
| 1:G:502:PHE:N    | 1:G:502:PHE:CD2  | 2.88                     | 0.41              |
| 1:G:798:LEU:HD23 | 1:G:798:LEU:HA   | 1.88                     | 0.41              |
| 1:H:21:THR:O     | 1:H:21:THR:HG23  | 2.19                     | 0.41              |
| 1:C:52:GLU:O     | 1:C:57:PRO:HD2   | 2.19                     | 0.41              |
| 1:C:146:ILE:CD1  | 1:C:162:LEU:HD13 | 2.51                     | 0.41              |
| 1:A:146:ILE:CD1  | 1:A:162:LEU:HD13 | 2.50                     | 0.41              |
| 1:E:177:LEU:HD23 | 1:E:177:LEU:HA   | 1.92                     | 0.41              |
| 1:A:149:PRO:HB3  | 1:A:161:PHE:CD1  | 2.55                     | 0.41              |
| 1:B:283:ILE:HD12 | 1:B:312:VAL:CG1  | 2.50                     | 0.41              |
| 1:E:298:TYR:CE1  | 1:E:649:MSE:HE1  | 2.56                     | 0.41              |
| 1:E:452:TRP:CG   | 1:E:453:LYS:N    | 2.88                     | 0.41              |
| 1:H:599:ARG:NH2  | 1:H:726:ASP:OD1  | 2.53                     | 0.41              |
| 1:C:118:LEU:HA   | 1:C:118:LEU:HD23 | 1.83                     | 0.41              |
| 1:F:315:LEU:CD1  | 1:F:762:LEU:HD23 | 2.50                     | 0.41              |
| 1:A:39:LYS:H     | 1:A:39:LYS:HG3   | 1.61                     | 0.41              |
| 1:E:564:LEU:HD22 | 1:E:613:ARG:CZ   | 2.49                     | 0.41              |
| 1:D:536:TYR:CD1  | 1:D:537:THR:HG23 | 2.55                     | 0.41              |
| 1:G:621:GLU:O    | 1:G:625:GLU:HB2  | 2.21                     | 0.41              |
| 1:G:415:TYR:HA   | 1:G:437:ALA:O    | 2.21                     | 0.41              |
| 1:D:449:ASP:HA   | 1:D:504:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:479:ILE:CD1  | 1:A:762:LEU:HD13 | 2.51                     | 0.41              |
| 1:D:660:TYR:O    | 1:D:663:ASP:HB2  | 2.19                     | 0.41              |
| 1:H:615:LYS:HG3  | 7:H:865:HOH:O    | 2.20                     | 0.41              |
| 1:B:399:GLU:O    | 1:B:402:LYS:HB2  | 2.20                     | 0.41              |
| 1:E:44:LEU:C     | 1:E:124:LEU:HD21 | 2.41                     | 0.41              |
| 1:D:27:ASN:HB2   | 1:D:30:LEU:HD23  | 2.03                     | 0.41              |
| 1:D:102:VAL:HG13 | 1:D:102:VAL:O    | 2.20                     | 0.41              |
| 1:B:449:ASP:OD1  | 1:B:450:ILE:N    | 2.48                     | 0.41              |
| 1:B:158:GLY:HA3  | 1:B:519:PRO:O    | 2.19                     | 0.41              |
| 1:C:518:ASP:OD1  | 1:C:519:PRO:HD2  | 2.20                     | 0.41              |
| 1:C:802:VAL:HA   | 1:C:803:PRO:HD3  | 1.93                     | 0.41              |
| 1:E:438:HIS:O    | 1:E:439:ALA:HB2  | 2.20                     | 0.41              |
| 1:H:503:THR:O    | 1:H:504:LEU:HD23 | 2.20                     | 0.41              |
| 1:D:438:HIS:O    | 1:D:439:ALA:HB2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:207:GLN:HG3  | 1:B:211:ARG:NH2  | 2.35                     | 0.41              |
| 1:E:284:LEU:HD21 | 1:E:425:LEU:HD12 | 2.02                     | 0.41              |
| 1:B:378:LYS:HD3  | 1:B:805:ALA:HB1  | 2.03                     | 0.41              |
| 1:F:329:ASN:O    | 1:F:331:LYS:NZ   | 2.45                     | 0.41              |
| 1:B:536:TYR:CE1  | 1:B:537:THR:HG23 | 2.55                     | 0.41              |
| 1:D:272:LEU:HD23 | 1:D:272:LEU:HA   | 1.80                     | 0.41              |
| 1:E:583:ARG:HH11 | 1:E:583:ARG:HG2  | 1.85                     | 0.41              |
| 1:E:223:GLU:CD   | 1:E:223:GLU:N    | 2.74                     | 0.41              |
| 1:B:93:ARG:H     | 1:B:96:VAL:HG23  | 1.86                     | 0.41              |
| 1:B:111:GLU:O    | 1:B:112:LEU:HD23 | 2.21                     | 0.41              |
| 1:B:146:ILE:HG22 | 1:B:147:PRO:N    | 2.34                     | 0.41              |
| 1:G:284:LEU:HD22 | 1:G:284:LEU:N    | 2.36                     | 0.41              |
| 1:A:73:LEU:HD22  | 1:A:90:VAL:HG11  | 2.03                     | 0.41              |
| 1:C:233:PHE:HE1  | 1:C:249:VAL:HG11 | 1.85                     | 0.41              |
| 1:B:23:VAL:O     | 1:B:23:VAL:HG13  | 2.19                     | 0.41              |
| 1:A:276:PRO:HG3  | 1:A:326:GLN:CB   | 2.51                     | 0.41              |
| 1:A:497:GLU:HB2  | 1:A:516:VAL:CG2  | 2.51                     | 0.41              |
| 1:H:44:LEU:O     | 1:H:80:ILE:HA    | 2.21                     | 0.41              |
| 1:D:581:LEU:CD2  | 1:D:626:MSE:HG3  | 2.51                     | 0.41              |
| 1:G:795:TYR:CD2  | 1:G:795:TYR:C    | 2.94                     | 0.41              |
| 1:E:272:LEU:HD23 | 1:E:272:LEU:HA   | 1.75                     | 0.41              |
| 1:C:212:LYS:HB3  | 1:C:212:LYS:HE2  | 1.97                     | 0.41              |
| 1:F:86:VAL:HG12  | 1:F:102:VAL:O    | 2.21                     | 0.41              |
| 1:F:284:LEU:HD13 | 1:F:337:LEU:HB2  | 2.03                     | 0.41              |
| 1:D:532:ILE:CD1  | 1:D:652:VAL:HG22 | 2.49                     | 0.41              |
| 1:G:259:LEU:CD2  | 1:G:267:THR:HG22 | 2.50                     | 0.41              |
| 1:A:670:GLN:OE1  | 1:A:672:ALA:HB2  | 2.20                     | 0.41              |
| 1:C:194:LEU:CD2  | 1:C:328:LEU:HD11 | 2.51                     | 0.41              |
| 1:E:295:VAL:HB   | 1:E:301:THR:HG21 | 2.03                     | 0.41              |
| 1:A:590:LEU:HD21 | 1:A:606:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:411:ILE:HG13 | 1:A:431:VAL:HG11 | 2.03                     | 0.41              |
| 1:G:630:TYR:CE1  | 1:G:644:TRP:HZ3  | 2.39                     | 0.41              |
| 1:H:532:ILE:HG13 | 1:H:651:ARG:NH1  | 2.36                     | 0.41              |
| 1:E:469:ILE:HA   | 1:E:469:ILE:HD13 | 1.93                     | 0.41              |
| 1:A:137:LEU:HD11 | 1:A:790:PHE:CZ   | 2.56                     | 0.41              |
| 1:B:177:LEU:HA   | 1:B:177:LEU:HD23 | 1.81                     | 0.41              |
| 1:E:102:VAL:O    | 1:E:102:VAL:HG12 | 2.19                     | 0.41              |
| 1:A:82:LEU:C     | 1:A:83:PRO:O     | 2.59                     | 0.41              |
| 1:D:178:LEU:N    | 1:D:179:PRO:HD2  | 2.35                     | 0.41              |
| 1:C:629:MSE:O    | 1:C:633:ILE:HG13 | 2.21                     | 0.41              |
| 1:H:89:ALA:HB2   | 1:H:99:TYR:HD1   | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:578:MSE:HA   | 1:B:609:VAL:O    | 2.20                     | 0.41              |
| 1:G:208:HIS:CE1  | 1:G:211:ARG:HH22 | 2.38                     | 0.41              |
| 1:G:73:LEU:C     | 1:G:75:SER:N     | 2.75                     | 0.41              |
| 1:D:534:PHE:HB2  | 1:D:535:PRO:CD   | 2.50                     | 0.41              |
| 1:F:497:GLU:HB2  | 1:F:516:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:149:PRO:HD3  | 1:A:161:PHE:CE2  | 2.56                     | 0.41              |
| 1:A:420:LEU:CD1  | 1:A:420:LEU:C    | 2.88                     | 0.41              |
| 1:A:682:VAL:HG13 | 1:A:749:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:793:LEU:HB3  | 1:D:793:LEU:CB   | 2.51                     | 0.41              |
| 1:H:91:ARG:HA    | 1:H:92:PRO:HD2   | 1.93                     | 0.41              |
| 1:C:195:MSE:HE1  | 1:C:241:GLY:CA   | 2.50                     | 0.41              |
| 1:F:518:ASP:OD1  | 1:F:520:LYS:HG2  | 2.21                     | 0.41              |
| 1:D:155:ILE:HG21 | 1:D:487:ALA:HB2  | 2.03                     | 0.41              |
| 1:E:386:TRP:HH2  | 1:E:416:SER:HB3  | 1.86                     | 0.41              |
| 1:G:438:HIS:O    | 1:G:439:ALA:HB2  | 2.21                     | 0.41              |
| 1:D:284:LEU:CD2  | 1:D:284:LEU:N    | 2.84                     | 0.41              |
| 1:B:436:ILE:HG12 | 1:B:479:ILE:HB   | 2.03                     | 0.41              |
| 1:H:452:TRP:CG   | 1:H:453:LYS:N    | 2.89                     | 0.41              |
| 1:H:472:MSE:HG3  | 1:H:514:ILE:HD13 | 2.02                     | 0.41              |
| 1:A:437:ALA:C    | 1:A:439:ALA:H    | 2.23                     | 0.41              |
| 1:D:597:ASN:O    | 1:D:601:ARG:HG3  | 2.20                     | 0.41              |
| 1:C:330:ILE:HG22 | 1:C:331:LYS:N    | 2.36                     | 0.41              |
| 1:G:174:LYS:N    | 1:G:174:LYS:HD2  | 2.36                     | 0.41              |
| 1:D:623:LYS:HE3  | 1:D:623:LYS:HB2  | 1.80                     | 0.41              |
| 1:C:502:PHE:CZ   | 1:C:510:VAL:HG21 | 2.55                     | 0.41              |
| 1:F:565:CYS:HB2  | 1:F:642:PHE:O    | 2.21                     | 0.41              |
| 1:D:692:PHE:CD2  | 1:D:710:PHE:HB2  | 2.55                     | 0.41              |
| 1:F:151:LEU:HA   | 1:F:151:LEU:HD23 | 1.77                     | 0.41              |
| 1:B:469:ILE:HA   | 1:B:469:ILE:HD13 | 1.96                     | 0.41              |
| 1:A:315:LEU:CG   | 1:A:319:MSE:HE2  | 2.48                     | 0.41              |
| 1:A:30:LEU:CD1   | 1:A:62:LYS:O     | 2.68                     | 0.41              |
| 1:G:304:GLN:HB3  | 3:G:902:FRU:C1   | 2.37                     | 0.41              |
| 1:F:117:PHE:O    | 1:F:120:PHE:HB2  | 2.21                     | 0.41              |
| 1:E:206:LEU:HD11 | 1:E:210:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:298:TYR:CE1  | 1:A:649:MSE:CE   | 3.01                     | 0.41              |
| 1:H:315:LEU:HG   | 1:H:319:MSE:HE2  | 2.02                     | 0.41              |
| 1:H:588:SER:HB3  | 1:H:625:GLU:OE2  | 2.21                     | 0.41              |
| 1:E:431:VAL:CG1  | 1:E:432:THR:N    | 2.83                     | 0.41              |
| 1:D:547:HIS:O    | 1:D:551:GLU:HG3  | 2.21                     | 0.41              |
| 1:B:445:TYR:O    | 1:B:448:SER:HB3  | 2.21                     | 0.41              |
| 1:F:746:LEU:HA   | 1:F:746:LEU:HD23 | 1.94                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:148:ARG:HD3  | 1:D:148:ARG:HA   | 1.87                     | 0.41              |
| 1:G:564:LEU:HA   | 1:G:564:LEU:HD12 | 1.74                     | 0.41              |
| 1:H:287:HIS:C    | 1:H:287:HIS:CD2  | 2.94                     | 0.41              |
| 1:D:34:SER:HA    | 1:D:59:GLN:HE22  | 1.86                     | 0.40              |
| 1:A:512:HIS:NE2  | 1:A:515:ASP:HB2  | 2.36                     | 0.40              |
| 1:D:564:LEU:HD23 | 1:D:564:LEU:HA   | 1.81                     | 0.40              |
| 1:E:48:GLN:HG3   | 1:E:76:THR:O     | 2.21                     | 0.40              |
| 1:B:380:ILE:HD11 | 1:B:805:ALA:CB   | 2.51                     | 0.40              |
| 1:E:448:SER:HB2  | 1:E:461:PHE:CD2  | 2.56                     | 0.40              |
| 1:H:414:ASN:O    | 1:H:418:GLY:HA3  | 2.21                     | 0.40              |
| 1:A:183:PHE:HD1  | 1:A:774:HIS:ND1  | 2.19                     | 0.40              |
| 1:H:69:PHE:CG    | 1:H:69:PHE:O     | 2.74                     | 0.40              |
| 1:A:88:LEU:HD23  | 1:A:88:LEU:O     | 2.20                     | 0.40              |
| 1:A:88:LEU:N     | 1:A:88:LEU:CD2   | 2.84                     | 0.40              |
| 1:H:692:PHE:CD1  | 1:H:692:PHE:N    | 2.89                     | 0.40              |
| 1:A:567:LEU:HA   | 1:A:567:LEU:HD23 | 1.87                     | 0.40              |
| 1:E:514:ILE:HG13 | 1:E:515:ASP:N    | 2.36                     | 0.40              |
| 1:G:172:HIS:CE1  | 1:G:261:GLU:O    | 2.75                     | 0.40              |
| 1:F:86:VAL:CG1   | 1:F:102:VAL:HB   | 2.51                     | 0.40              |
| 1:H:131:GLY:O    | 1:H:134:THR:CG2  | 2.65                     | 0.40              |
| 1:B:390:GLU:OE1  | 1:B:796:ARG:HD2  | 2.21                     | 0.40              |
| 1:A:135:LEU:HD12 | 1:A:136:GLU:H    | 1.86                     | 0.40              |
| 1:H:155:ILE:HB   | 1:H:483:PHE:CE2  | 2.56                     | 0.40              |
| 1:C:645:ILE:CG2  | 1:C:648:GLN:NE2  | 2.84                     | 0.40              |
| 1:F:370:ARG:HB3  | 1:F:375:ILE:HA   | 2.04                     | 0.40              |
| 1:F:449:ASP:HA   | 1:F:504:LEU:CD2  | 2.52                     | 0.40              |
| 1:F:281:VAL:HG22 | 1:F:410:LEU:HB3  | 2.02                     | 0.40              |
| 1:E:322:ARG:HD2  | 1:E:763:LEU:HD13 | 2.02                     | 0.40              |
| 1:G:719:GLN:HG3  | 4:G:913:SO4:O3   | 2.21                     | 0.40              |
| 1:E:316:GLU:OE1  | 1:E:361:TYR:N    | 2.42                     | 0.40              |
| 1:D:50:ILE:H     | 1:D:50:ILE:HG13  | 1.60                     | 0.40              |
| 1:H:705:HIS:C    | 1:H:705:HIS:CD2  | 2.95                     | 0.40              |
| 1:G:318:GLU:HG3  | 1:G:763:LEU:HD12 | 2.03                     | 0.40              |
| 1:D:61:ARG:C     | 1:D:63:LYS:N     | 2.73                     | 0.40              |
| 1:A:70:PHE:HD2   | 1:A:71:ASP:HA    | 1.87                     | 0.40              |
| 1:F:578:MSE:HG3  | 1:F:609:VAL:HB   | 2.03                     | 0.40              |
| 1:D:462:SER:HB2  | 1:D:507:LEU:CD2  | 2.51                     | 0.40              |
| 1:E:252:MSE:SE   | 1:E:274:ARG:HB3  | 2.72                     | 0.40              |
| 1:D:493:VAL:HG22 | 1:D:494:GLY:N    | 2.35                     | 0.40              |
| 1:C:282:VAL:HG21 | 1:C:400:LEU:HD22 | 2.03                     | 0.40              |
| 1:A:534:PHE:O    | 1:A:687:CYS:HA   | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:252:MSE:SE   | 1:C:274:ARG:HG2  | 2.71                     | 0.40              |
| 1:F:625:GLU:HG2  | 7:F:827:HOH:O    | 2.21                     | 0.40              |
| 1:B:279:PHE:HB2  | 1:B:409:ASP:OD2  | 2.21                     | 0.40              |
| 1:A:376:VAL:HG21 | 1:A:388:TYR:CE2  | 2.57                     | 0.40              |
| 1:H:566:VAL:O    | 1:H:640:GLY:HA2  | 2.21                     | 0.40              |
| 1:E:545:LYS:HB2  | 1:E:545:LYS:HE3  | 1.95                     | 0.40              |
| 1:A:137:LEU:HD11 | 1:A:790:PHE:CE1  | 2.56                     | 0.40              |
| 1:F:316:GLU:N    | 1:F:319:MSE:CE   | 2.85                     | 0.40              |
| 1:D:146:ILE:HG13 | 1:D:772:TRP:CZ2  | 2.57                     | 0.40              |
| 1:A:70:PHE:HD2   | 1:A:71:ASP:N     | 2.20                     | 0.40              |
| 1:B:49:ILE:HG13  | 1:B:49:ILE:H     | 1.39                     | 0.40              |
| 1:D:338:THR:HG23 | 1:D:366:ARG:HG2  | 2.02                     | 0.40              |
| 1:B:163:ASN:HD21 | 1:B:269:GLU:CG   | 2.33                     | 0.40              |
| 1:B:716:HIS:CB   | 4:B:913:SO4:O4   | 2.66                     | 0.40              |
| 1:E:386:TRP:N    | 1:E:387:PRO:HD2  | 2.36                     | 0.40              |
| 1:A:339:ARG:HH12 | 1:A:380:ILE:HG13 | 1.85                     | 0.40              |
| 1:E:591:VAL:HG13 | 1:E:638:LEU:CD1  | 2.51                     | 0.40              |
| 1:E:591:VAL:CG1  | 1:E:638:LEU:HD11 | 2.51                     | 0.40              |
| 1:H:181:LEU:HD13 | 1:H:206:LEU:HD22 | 2.02                     | 0.40              |
| 1:F:698:GLY:N    | 1:F:699:PRO:CD   | 2.84                     | 0.40              |
| 1:C:469:ILE:HA   | 1:C:469:ILE:HD13 | 1.92                     | 0.40              |
| 1:B:746:LEU:HD23 | 1:B:746:LEU:HA   | 1.93                     | 0.40              |
| 1:E:148:ARG:HA   | 1:E:149:PRO:HD2  | 1.89                     | 0.40              |
| 1:C:34:SER:OG    | 1:C:55:ALA:HB1   | 2.21                     | 0.40              |
| 1:A:315:LEU:C    | 1:A:319:MSE:HE2  | 2.41                     | 0.40              |
| 1:B:92:PRO:HG2   | 1:B:96:VAL:HG21  | 1.93                     | 0.40              |
| 1:A:146:ILE:HD11 | 1:A:772:TRP:CZ2  | 2.57                     | 0.40              |
| 1:A:670:GLN:NE2  | 7:A:849:HOH:O    | 2.53                     | 0.40              |
| 1:F:441:GLU:OE1  | 1:F:444:LYS:HE3  | 2.21                     | 0.40              |
| 1:B:479:ILE:HD11 | 1:B:762:LEU:CD1  | 2.52                     | 0.40              |
| 1:C:154:TYR:OH   | 1:D:262:ALA:HB3  | 2.22                     | 0.40              |
| 1:B:118:LEU:HD22 | 1:B:503:THR:HG22 | 2.02                     | 0.40              |
| 1:E:444:LYS:HE2  | 1:E:444:LYS:HB3  | 1.97                     | 0.40              |
| 1:C:679:LEU:HA   | 1:C:679:LEU:HD23 | 1.89                     | 0.40              |
| 1:B:649:MSE:H    | 1:B:649:MSE:HG2  | 1.59                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 779/816 (96%)   | 730 (94%)  | 45 (6%)  | 4 (0%)   | 34          | 70 |
| 1   | B     | 791/816 (97%)   | 734 (93%)  | 56 (7%)  | 1 (0%)   | 56          | 86 |
| 1   | C     | 779/816 (96%)   | 734 (94%)  | 42 (5%)  | 3 (0%)   | 39          | 74 |
| 1   | D     | 779/816 (96%)   | 736 (94%)  | 38 (5%)  | 5 (1%)   | 30          | 66 |
| 1   | E     | 779/816 (96%)   | 737 (95%)  | 38 (5%)  | 4 (0%)   | 34          | 70 |
| 1   | F     | 779/816 (96%)   | 734 (94%)  | 39 (5%)  | 6 (1%)   | 24          | 58 |
| 1   | G     | 779/816 (96%)   | 736 (94%)  | 39 (5%)  | 4 (0%)   | 34          | 70 |
| 1   | H     | 795/816 (97%)   | 750 (94%)  | 42 (5%)  | 3 (0%)   | 39          | 74 |
| All | All   | 6260/6528 (96%) | 5891 (94%) | 339 (5%) | 30 (0%)  | 34          | 70 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 48  | GLN  |
| 1   | D     | 106 | ALA  |
| 1   | E     | 83  | PRO  |
| 1   | A     | 52  | GLU  |
| 1   | A     | 83  | PRO  |
| 1   | F     | 58  | GLU  |
| 1   | G     | 68  | PRO  |
| 1   | G     | 69  | PHE  |
| 1   | H     | 108 | VAL  |
| 1   | B     | 83  | PRO  |
| 1   | E     | 63  | LYS  |
| 1   | F     | 57  | PRO  |
| 1   | F     | 63  | LYS  |
| 1   | F     | 68  | PRO  |
| 1   | F     | 69  | PHE  |
| 1   | A     | 51  | ALA  |
| 1   | A     | 63  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 63  | LYS  |
| 1   | C     | 565 | CYS  |
| 1   | D     | 63  | LYS  |
| 1   | D     | 56  | LEU  |
| 1   | G     | 63  | LYS  |
| 1   | G     | 70  | PHE  |
| 1   | H     | 63  | LYS  |
| 1   | D     | 57  | PRO  |
| 1   | E     | 84  | PRO  |
| 1   | H     | 145 | SER  |
| 1   | F     | 43  | ILE  |
| 1   | D     | 49  | ILE  |
| 1   | E     | 82  | LEU  |

### 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     | 667/704 (95%)   | 626 (94%)  | 41 (6%)  | 23          | 55 |
| 1   | B     | 663/704 (94%)   | 626 (94%)  | 37 (6%)  | 26          | 59 |
| 1   | C     | 666/704 (95%)   | 622 (93%)  | 44 (7%)  | 21          | 50 |
| 1   | D     | 659/704 (94%)   | 624 (95%)  | 35 (5%)  | 28          | 62 |
| 1   | E     | 662/704 (94%)   | 620 (94%)  | 42 (6%)  | 22          | 53 |
| 1   | F     | 668/704 (95%)   | 635 (95%)  | 33 (5%)  | 31          | 66 |
| 1   | G     | 668/704 (95%)   | 626 (94%)  | 42 (6%)  | 22          | 53 |
| 1   | H     | 663/704 (94%)   | 623 (94%)  | 40 (6%)  | 24          | 56 |
| All | All   | 5316/5632 (94%) | 5002 (94%) | 314 (6%) | 24          | 57 |

All (314) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | LYS  |
| 1   | A     | 45  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | GLN  |
| 1   | A     | 52  | GLU  |
| 1   | A     | 54  | GLU  |
| 1   | A     | 56  | LEU  |
| 1   | A     | 59  | GLN  |
| 1   | A     | 70  | PHE  |
| 1   | A     | 73  | LEU  |
| 1   | A     | 86  | VAL  |
| 1   | A     | 88  | LEU  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 105 | HIS  |
| 1   | A     | 111 | GLU  |
| 1   | A     | 140 | GLU  |
| 1   | A     | 148 | ARG  |
| 1   | A     | 164 | ARG  |
| 1   | A     | 195 | MSE  |
| 1   | A     | 248 | ARG  |
| 1   | A     | 255 | LEU  |
| 1   | A     | 258 | ASP  |
| 1   | A     | 285 | SER  |
| 1   | A     | 293 | ASP  |
| 1   | A     | 307 | TYR  |
| 1   | A     | 321 | GLN  |
| 1   | A     | 322 | ARG  |
| 1   | A     | 340 | LEU  |
| 1   | A     | 434 | CYS  |
| 1   | A     | 484 | GLN  |
| 1   | A     | 493 | VAL  |
| 1   | A     | 530 | MSE  |
| 1   | A     | 545 | LYS  |
| 1   | A     | 556 | SER  |
| 1   | A     | 602 | GLU  |
| 1   | A     | 616 | GLU  |
| 1   | A     | 618 | LYS  |
| 1   | A     | 670 | GLN  |
| 1   | A     | 736 | SER  |
| 1   | A     | 750 | GLU  |
| 1   | A     | 757 | ILE  |
| 1   | A     | 781 | LEU  |
| 1   | B     | 22  | LEU  |
| 1   | B     | 23  | VAL  |
| 1   | B     | 24  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 30  | LEU  |
| 1   | B     | 43  | ILE  |
| 1   | B     | 49  | ILE  |
| 1   | B     | 50  | ILE  |
| 1   | B     | 56  | LEU  |
| 1   | B     | 60  | THR  |
| 1   | B     | 70  | PHE  |
| 1   | B     | 72  | LEU  |
| 1   | B     | 99  | TYR  |
| 1   | B     | 105 | HIS  |
| 1   | B     | 111 | GLU  |
| 1   | B     | 128 | VAL  |
| 1   | B     | 132 | ASN  |
| 1   | B     | 151 | LEU  |
| 1   | B     | 216 | TYR  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 248 | ARG  |
| 1   | B     | 258 | ASP  |
| 1   | B     | 293 | ASP  |
| 1   | B     | 321 | GLN  |
| 1   | B     | 345 | VAL  |
| 1   | B     | 358 | ASP  |
| 1   | B     | 493 | VAL  |
| 1   | B     | 503 | THR  |
| 1   | B     | 531 | SER  |
| 1   | B     | 545 | LYS  |
| 1   | B     | 630 | TYR  |
| 1   | B     | 646 | SER  |
| 1   | B     | 649 | MSE  |
| 1   | B     | 670 | GLN  |
| 1   | B     | 722 | ASP  |
| 1   | B     | 756 | GLN  |
| 1   | B     | 757 | ILE  |
| 1   | B     | 779 | ASP  |
| 1   | C     | 29  | VAL  |
| 1   | C     | 30  | LEU  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 37  | GLU  |
| 1   | C     | 44  | LEU  |
| 1   | C     | 45  | GLN  |
| 1   | C     | 46  | GLN  |
| 1   | C     | 52  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 54  | GLU  |
| 1   | C     | 56  | LEU  |
| 1   | C     | 59  | GLN  |
| 1   | C     | 63  | LYS  |
| 1   | C     | 65  | GLU  |
| 1   | C     | 69  | PHE  |
| 1   | C     | 86  | VAL  |
| 1   | C     | 105 | HIS  |
| 1   | C     | 109 | VAL  |
| 1   | C     | 119 | HIS  |
| 1   | C     | 120 | PHE  |
| 1   | C     | 148 | ARG  |
| 1   | C     | 167 | SER  |
| 1   | C     | 174 | LYS  |
| 1   | C     | 216 | TYR  |
| 1   | C     | 240 | ARG  |
| 1   | C     | 248 | ARG  |
| 1   | C     | 258 | ASP  |
| 1   | C     | 284 | LEU  |
| 1   | C     | 358 | ASP  |
| 1   | C     | 373 | LYS  |
| 1   | C     | 405 | ASN  |
| 1   | C     | 420 | LEU  |
| 1   | C     | 508 | TYR  |
| 1   | C     | 545 | LYS  |
| 1   | C     | 556 | SER  |
| 1   | C     | 580 | ARG  |
| 1   | C     | 616 | GLU  |
| 1   | C     | 646 | SER  |
| 1   | C     | 665 | LYS  |
| 1   | C     | 670 | GLN  |
| 1   | C     | 708 | SER  |
| 1   | C     | 757 | ILE  |
| 1   | C     | 760 | GLN  |
| 1   | C     | 777 | ASN  |
| 1   | C     | 806 | GLN  |
| 1   | D     | 27  | ASN  |
| 1   | D     | 29  | VAL  |
| 1   | D     | 44  | LEU  |
| 1   | D     | 52  | GLU  |
| 1   | D     | 54  | GLU  |
| 1   | D     | 56  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 76  | THR  |
| 1   | D     | 108 | VAL  |
| 1   | D     | 119 | HIS  |
| 1   | D     | 120 | PHE  |
| 1   | D     | 125 | VAL  |
| 1   | D     | 132 | ASN  |
| 1   | D     | 164 | ARG  |
| 1   | D     | 170 | LEU  |
| 1   | D     | 197 | SER  |
| 1   | D     | 216 | TYR  |
| 1   | D     | 219 | GLU  |
| 1   | D     | 251 | ASP  |
| 1   | D     | 258 | ASP  |
| 1   | D     | 269 | GLU  |
| 1   | D     | 286 | PRO  |
| 1   | D     | 321 | GLN  |
| 1   | D     | 360 | GLU  |
| 1   | D     | 454 | LYS  |
| 1   | D     | 491 | GLU  |
| 1   | D     | 556 | SER  |
| 1   | D     | 563 | HIS  |
| 1   | D     | 570 | LYS  |
| 1   | D     | 629 | MSE  |
| 1   | D     | 708 | SER  |
| 1   | D     | 750 | GLU  |
| 1   | D     | 757 | ILE  |
| 1   | D     | 779 | ASP  |
| 1   | D     | 794 | LYS  |
| 1   | D     | 806 | GLN  |
| 1   | E     | 30  | LEU  |
| 1   | E     | 32  | LEU  |
| 1   | E     | 35  | ARG  |
| 1   | E     | 44  | LEU  |
| 1   | E     | 45  | GLN  |
| 1   | E     | 54  | GLU  |
| 1   | E     | 56  | LEU  |
| 1   | E     | 59  | GLN  |
| 1   | E     | 61  | ARG  |
| 1   | E     | 70  | PHE  |
| 1   | E     | 73  | LEU  |
| 1   | E     | 85  | TRP  |
| 1   | E     | 102 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 105 | HIS  |
| 1   | E     | 112 | LEU  |
| 1   | E     | 125 | VAL  |
| 1   | E     | 148 | ARG  |
| 1   | E     | 153 | LYS  |
| 1   | E     | 167 | SER  |
| 1   | E     | 193 | ASN  |
| 1   | E     | 216 | TYR  |
| 1   | E     | 235 | GLU  |
| 1   | E     | 240 | ARG  |
| 1   | E     | 293 | ASP  |
| 1   | E     | 340 | LEU  |
| 1   | E     | 358 | ASP  |
| 1   | E     | 375 | ILE  |
| 1   | E     | 401 | SER  |
| 1   | E     | 457 | ASP  |
| 1   | E     | 463 | CYS  |
| 1   | E     | 491 | GLU  |
| 1   | E     | 492 | THR  |
| 1   | E     | 493 | VAL  |
| 1   | E     | 516 | VAL  |
| 1   | E     | 530 | MSE  |
| 1   | E     | 572 | LYS  |
| 1   | E     | 653 | ARG  |
| 1   | E     | 670 | GLN  |
| 1   | E     | 750 | GLU  |
| 1   | E     | 759 | SER  |
| 1   | E     | 777 | ASN  |
| 1   | E     | 781 | LEU  |
| 1   | F     | 32  | LEU  |
| 1   | F     | 44  | LEU  |
| 1   | F     | 45  | GLN  |
| 1   | F     | 54  | GLU  |
| 1   | F     | 56  | LEU  |
| 1   | F     | 59  | GLN  |
| 1   | F     | 60  | THR  |
| 1   | F     | 65  | GLU  |
| 1   | F     | 69  | PHE  |
| 1   | F     | 82  | LEU  |
| 1   | F     | 100 | LEU  |
| 1   | F     | 123 | GLU  |
| 1   | F     | 140 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 153 | LYS  |
| 1   | F     | 178 | LEU  |
| 1   | F     | 205 | THR  |
| 1   | F     | 216 | TYR  |
| 1   | F     | 240 | ARG  |
| 1   | F     | 285 | SER  |
| 1   | F     | 311 | GLN  |
| 1   | F     | 315 | LEU  |
| 1   | F     | 412 | ILE  |
| 1   | F     | 420 | LEU  |
| 1   | F     | 516 | VAL  |
| 1   | F     | 545 | LYS  |
| 1   | F     | 628 | LYS  |
| 1   | F     | 629 | MSE  |
| 1   | F     | 647 | SER  |
| 1   | F     | 649 | MSE  |
| 1   | F     | 670 | GLN  |
| 1   | F     | 696 | LYS  |
| 1   | F     | 773 | LYS  |
| 1   | F     | 778 | LEU  |
| 1   | G     | 30  | LEU  |
| 1   | G     | 32  | LEU  |
| 1   | G     | 41  | LYS  |
| 1   | G     | 48  | GLN  |
| 1   | G     | 50  | ILE  |
| 1   | G     | 54  | GLU  |
| 1   | G     | 56  | LEU  |
| 1   | G     | 61  | ARG  |
| 1   | G     | 65  | GLU  |
| 1   | G     | 70  | PHE  |
| 1   | G     | 73  | LEU  |
| 1   | G     | 82  | LEU  |
| 1   | G     | 100 | LEU  |
| 1   | G     | 119 | HIS  |
| 1   | G     | 124 | LEU  |
| 1   | G     | 125 | VAL  |
| 1   | G     | 140 | GLU  |
| 1   | G     | 148 | ARG  |
| 1   | G     | 153 | LYS  |
| 1   | G     | 170 | LEU  |
| 1   | G     | 202 | ASN  |
| 1   | G     | 205 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 222 | SER  |
| 1   | G     | 258 | ASP  |
| 1   | G     | 315 | LEU  |
| 1   | G     | 425 | LEU  |
| 1   | G     | 491 | GLU  |
| 1   | G     | 493 | VAL  |
| 1   | G     | 516 | VAL  |
| 1   | G     | 545 | LYS  |
| 1   | G     | 556 | SER  |
| 1   | G     | 561 | LYS  |
| 1   | G     | 571 | LYS  |
| 1   | G     | 602 | GLU  |
| 1   | G     | 664 | THR  |
| 1   | G     | 670 | GLN  |
| 1   | G     | 736 | SER  |
| 1   | G     | 756 | GLN  |
| 1   | G     | 757 | ILE  |
| 1   | G     | 759 | SER  |
| 1   | G     | 781 | LEU  |
| 1   | G     | 784 | ARG  |
| 1   | H     | 11  | VAL  |
| 1   | H     | 18  | LEU  |
| 1   | H     | 21  | THR  |
| 1   | H     | 22  | LEU  |
| 1   | H     | 32  | LEU  |
| 1   | H     | 33  | LEU  |
| 1   | H     | 43  | ILE  |
| 1   | H     | 46  | GLN  |
| 1   | H     | 48  | GLN  |
| 1   | H     | 49  | ILE  |
| 1   | H     | 50  | ILE  |
| 1   | H     | 60  | THR  |
| 1   | H     | 61  | ARG  |
| 1   | H     | 69  | PHE  |
| 1   | H     | 72  | LEU  |
| 1   | H     | 82  | LEU  |
| 1   | H     | 146 | ILE  |
| 1   | H     | 148 | ARG  |
| 1   | H     | 176 | SER  |
| 1   | H     | 178 | LEU  |
| 1   | H     | 207 | GLN  |
| 1   | H     | 240 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 251 | ASP  |
| 1   | H     | 315 | LEU  |
| 1   | H     | 345 | VAL  |
| 1   | H     | 353 | LEU  |
| 1   | H     | 417 | ASP  |
| 1   | H     | 450 | ILE  |
| 1   | H     | 481 | SER  |
| 1   | H     | 493 | VAL  |
| 1   | H     | 516 | VAL  |
| 1   | H     | 540 | LYS  |
| 1   | H     | 545 | LYS  |
| 1   | H     | 556 | SER  |
| 1   | H     | 563 | HIS  |
| 1   | H     | 564 | LEU  |
| 1   | H     | 572 | LYS  |
| 1   | H     | 750 | GLU  |
| 1   | H     | 759 | SER  |
| 1   | H     | 779 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 45  | GLN  |
| 1   | A     | 59  | GLN  |
| 1   | A     | 105 | HIS  |
| 1   | A     | 172 | HIS  |
| 1   | A     | 189 | HIS  |
| 1   | A     | 207 | GLN  |
| 1   | A     | 287 | HIS  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 414 | ASN  |
| 1   | A     | 711 | HIS  |
| 1   | B     | 48  | GLN  |
| 1   | B     | 119 | HIS  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 311 | GLN  |
| 1   | C     | 59  | GLN  |
| 1   | C     | 119 | HIS  |
| 1   | C     | 172 | HIS  |
| 1   | C     | 207 | GLN  |
| 1   | C     | 287 | HIS  |
| 1   | C     | 311 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 414 | ASN  |
| 1   | C     | 512 | HIS  |
| 1   | D     | 48  | GLN  |
| 1   | D     | 59  | GLN  |
| 1   | D     | 163 | ASN  |
| 1   | D     | 207 | GLN  |
| 1   | D     | 208 | HIS  |
| 1   | D     | 719 | GLN  |
| 1   | D     | 806 | GLN  |
| 1   | E     | 119 | HIS  |
| 1   | E     | 193 | ASN  |
| 1   | E     | 207 | GLN  |
| 1   | E     | 325 | GLN  |
| 1   | E     | 737 | HIS  |
| 1   | E     | 774 | HIS  |
| 1   | F     | 59  | GLN  |
| 1   | F     | 172 | HIS  |
| 1   | F     | 207 | GLN  |
| 1   | F     | 414 | ASN  |
| 1   | F     | 747 | GLN  |
| 1   | G     | 27  | ASN  |
| 1   | G     | 45  | GLN  |
| 1   | G     | 46  | GLN  |
| 1   | G     | 48  | GLN  |
| 1   | G     | 172 | HIS  |
| 1   | G     | 190 | GLN  |
| 1   | G     | 202 | ASN  |
| 1   | G     | 204 | ASN  |
| 1   | G     | 207 | GLN  |
| 1   | G     | 321 | GLN  |
| 1   | G     | 414 | ASN  |
| 1   | H     | 12  | HIS  |
| 1   | H     | 45  | GLN  |
| 1   | H     | 130 | ASN  |
| 1   | H     | 189 | HIS  |
| 1   | H     | 204 | ASN  |
| 1   | H     | 207 | GLN  |
| 1   | H     | 321 | GLN  |
| 1   | H     | 325 | GLN  |
| 1   | H     | 705 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 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 | $\# Z  > 2$ |
| 2   | UDP  | A     | 901 | -    | 18,26,26     | 1.00 | 0           | 23,40,40    | 1.02 | 1 (4%)      |
| 3   | FRU  | A     | 902 | -    | 11,12,12     | 0.77 | 0           | 10,18,18    | 0.80 | 0           |
| 4   | SO4  | A     | 911 | -    | 4,4,4        | 0.19 | 0           | 6,6,6       | 0.26 | 0           |
| 4   | SO4  | A     | 912 | -    | 4,4,4        | 0.09 | 0           | 6,6,6       | 0.17 | 0           |
| 4   | SO4  | A     | 913 | -    | 4,4,4        | 0.09 | 0           | 6,6,6       | 0.33 | 0           |
| 5   | MLA  | A     | 921 | -    | 0,6,6        | 0.00 | -           | 0,7,7       | 0.00 | -           |
| 2   | UDP  | B     | 901 | -    | 18,26,26     | 0.90 | 0           | 23,40,40    | 1.09 | 1 (4%)      |
| 3   | FRU  | B     | 902 | -    | 11,12,12     | 0.78 | 1 (9%)      | 10,18,18    | 0.83 | 0           |
| 4   | SO4  | B     | 911 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.17 | 0           |
| 4   | SO4  | B     | 912 | -    | 4,4,4        | 0.09 | 0           | 6,6,6       | 0.32 | 0           |
| 4   | SO4  | B     | 913 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.24 | 0           |
| 5   | MLA  | B     | 921 | -    | 0,6,6        | 0.00 | -           | 0,7,7       | 0.00 | -           |
| 2   | UDP  | C     | 901 | -    | 18,26,26     | 0.94 | 0           | 23,40,40    | 0.99 | 1 (4%)      |
| 3   | FRU  | C     | 902 | -    | 11,12,12     | 0.67 | 0           | 10,18,18    | 0.84 | 0           |
| 4   | SO4  | C     | 911 | -    | 4,4,4        | 0.10 | 0           | 6,6,6       | 0.25 | 0           |
| 4   | SO4  | C     | 912 | -    | 4,4,4        | 0.04 | 0           | 6,6,6       | 0.16 | 0           |
| 4   | SO4  | C     | 913 | -    | 4,4,4        | 0.09 | 0           | 6,6,6       | 0.11 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | MLA  | C     | 921 | -    | 0,6,6        | 0.00 | -        | 0,7,7       | 0.00 | -        |
| 2   | UDP  | D     | 901 | -    | 18,26,26     | 1.06 | 0        | 23,40,40    | 1.08 | 1 (4%)   |
| 3   | FRU  | D     | 902 | -    | 11,12,12     | 1.02 | 1 (9%)   | 10,18,18    | 1.23 | 2 (20%)  |
| 4   | SO4  | D     | 911 | -    | 4,4,4        | 0.17 | 0        | 6,6,6       | 0.26 | 0        |
| 4   | SO4  | D     | 912 | -    | 4,4,4        | 0.03 | 0        | 6,6,6       | 0.10 | 0        |
| 4   | SO4  | D     | 913 | -    | 4,4,4        | 0.11 | 0        | 6,6,6       | 0.17 | 0        |
| 5   | MLA  | D     | 921 | -    | 0,6,6        | 0.00 | -        | 0,7,7       | 0.00 | -        |
| 2   | UDP  | E     | 901 | -    | 18,26,26     | 0.98 | 0        | 23,40,40    | 1.09 | 1 (4%)   |
| 3   | FRU  | E     | 902 | -    | 11,12,12     | 0.70 | 0        | 10,18,18    | 0.82 | 0        |
| 4   | SO4  | E     | 911 | -    | 4,4,4        | 0.17 | 0        | 6,6,6       | 0.32 | 0        |
| 4   | SO4  | E     | 912 | -    | 4,4,4        | 0.12 | 0        | 6,6,6       | 0.12 | 0        |
| 4   | SO4  | E     | 913 | -    | 4,4,4        | 0.15 | 0        | 6,6,6       | 0.23 | 0        |
| 5   | MLA  | E     | 921 | -    | 0,6,6        | 0.00 | -        | 0,7,7       | 0.00 | -        |
| 2   | UDP  | F     | 901 | -    | 18,26,26     | 0.91 | 0        | 23,40,40    | 0.98 | 1 (4%)   |
| 3   | FRU  | F     | 902 | -    | 11,12,12     | 0.71 | 0        | 10,18,18    | 0.71 | 0        |
| 4   | SO4  | F     | 911 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.38 | 0        |
| 4   | SO4  | F     | 912 | -    | 4,4,4        | 0.09 | 0        | 6,6,6       | 0.20 | 0        |
| 4   | SO4  | F     | 913 | -    | 4,4,4        | 0.13 | 0        | 6,6,6       | 0.20 | 0        |
| 5   | MLA  | F     | 921 | -    | 0,6,6        | 0.00 | -        | 0,7,7       | 0.00 | -        |
| 2   | UDP  | G     | 901 | -    | 18,26,26     | 0.99 | 0        | 23,40,40    | 0.97 | 1 (4%)   |
| 3   | FRU  | G     | 902 | -    | 11,12,12     | 0.72 | 0        | 10,18,18    | 0.76 | 0        |
| 4   | SO4  | G     | 911 | -    | 4,4,4        | 0.19 | 0        | 6,6,6       | 0.13 | 0        |
| 4   | SO4  | G     | 912 | -    | 4,4,4        | 0.06 | 0        | 6,6,6       | 0.07 | 0        |
| 4   | SO4  | G     | 913 | -    | 4,4,4        | 0.04 | 0        | 6,6,6       | 0.09 | 0        |
| 5   | MLA  | G     | 921 | -    | 0,6,6        | 0.00 | -        | 0,7,7       | 0.00 | -        |
| 2   | UDP  | H     | 901 | -    | 18,26,26     | 1.02 | 0        | 23,40,40    | 1.02 | 1 (4%)   |
| 3   | FRU  | H     | 902 | -    | 11,12,12     | 0.89 | 1 (9%)   | 10,18,18    | 1.06 | 0        |
| 4   | SO4  | H     | 911 | -    | 4,4,4        | 0.20 | 0        | 6,6,6       | 0.23 | 0        |
| 4   | SO4  | H     | 912 | -    | 4,4,4        | 0.05 | 0        | 6,6,6       | 0.13 | 0        |
| 4   | SO4  | H     | 913 | -    | 4,4,4        | 0.13 | 0        | 6,6,6       | 0.18 | 0        |
| 5   | MLA  | H     | 921 | -    | 0,6,6        | 0.00 | -        | 0,7,7       | 0.00 | -        |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | UDP  | A     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | A     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | A     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | SO4  | A     | 912 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | A     | 913 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 5   | MLA  | A     | 921 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | UDP  | B     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | B     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | B     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | B     | 912 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | B     | 913 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 5   | MLA  | B     | 921 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | UDP  | C     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | C     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | C     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | C     | 912 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | C     | 913 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 5   | MLA  | C     | 921 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | UDP  | D     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | D     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | D     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | D     | 912 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | D     | 913 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 5   | MLA  | D     | 921 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | UDP  | E     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | E     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | E     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | E     | 912 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | E     | 913 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 5   | MLA  | E     | 921 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | UDP  | F     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | F     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | F     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | F     | 912 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | F     | 913 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 5   | MLA  | F     | 921 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | UDP  | G     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | G     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | G     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | G     | 912 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SO4  | G     | 913 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 5   | MLA  | G     | 921 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | UDP  | H     | 901 | -    | -       | 0/12/32/32 | 0/2/2/2 |
| 3   | FRU  | H     | 902 | -    | -       | 0/5/24/24  | 0/1/1/1 |
| 4   | SO4  | H     | 911 | -    | -       | 0/0/0/0    | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 4   | SO4  | H     | 912 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 4   | SO4  | H     | 913 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | MLA  | H     | 921 | -    | -       | 0/0/4/4  | 0/0/0/0 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | H     | 902 | FRU  | O2-C2 | 2.19 | 1.44        | 1.41     |
| 3   | B     | 902 | FRU  | O2-C2 | 2.30 | 1.44        | 1.41     |
| 3   | D     | 902 | FRU  | C1-C2 | 2.35 | 1.56        | 1.52     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | E     | 901 | UDP  | PA-O3A-PB | -3.84 | 119.78      | 132.67   |
| 2   | B     | 901 | UDP  | PA-O3A-PB | -3.69 | 120.30      | 132.67   |
| 2   | A     | 901 | UDP  | PA-O3A-PB | -3.55 | 120.76      | 132.67   |
| 2   | D     | 901 | UDP  | PA-O3A-PB | -3.48 | 121.02      | 132.67   |
| 2   | G     | 901 | UDP  | PA-O3A-PB | -2.89 | 122.99      | 132.67   |
| 2   | F     | 901 | UDP  | PA-O3A-PB | -2.72 | 123.53      | 132.67   |
| 2   | C     | 901 | UDP  | PA-O3A-PB | -2.72 | 123.55      | 132.67   |
| 2   | H     | 901 | UDP  | PA-O3A-PB | -2.72 | 123.55      | 132.67   |
| 3   | D     | 902 | FRU  | O2-C2-O5  | -2.07 | 105.11      | 109.37   |
| 3   | D     | 902 | FRU  | O1-C1-C2  | 2.47  | 116.18      | 111.39   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 33 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 902 | FRU  | 1       | 0            |
| 4   | A     | 913 | SO4  | 1       | 0            |
| 4   | B     | 912 | SO4  | 1       | 0            |
| 4   | B     | 913 | SO4  | 2       | 0            |
| 5   | B     | 921 | MLA  | 1       | 0            |
| 2   | C     | 901 | UDP  | 1       | 0            |
| 3   | C     | 902 | FRU  | 1       | 0            |
| 2   | D     | 901 | UDP  | 2       | 0            |
| 2   | E     | 901 | UDP  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | E     | 902 | FRU  | 1       | 0            |
| 4   | E     | 912 | SO4  | 1       | 0            |
| 5   | E     | 921 | MLA  | 5       | 0            |
| 2   | F     | 901 | UDP  | 1       | 0            |
| 3   | F     | 902 | FRU  | 1       | 0            |
| 4   | F     | 913 | SO4  | 2       | 0            |
| 2   | G     | 901 | UDP  | 1       | 0            |
| 3   | G     | 902 | FRU  | 4       | 0            |
| 4   | G     | 913 | SO4  | 1       | 0            |
| 3   | H     | 902 | FRU  | 1       | 0            |
| 4   | H     | 913 | SO4  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 769/816 (94%)   | -0.23  | 29 (3%) 44 38  | 13, 27, 90, 116       | 0     |
| 1   | B     | 781/816 (95%)   | 0.09   | 57 (7%) 18 12  | 16, 33, 98, 131       | 0     |
| 1   | C     | 769/816 (94%)   | -0.11  | 28 (3%) 46 39  | 20, 38, 83, 122       | 0     |
| 1   | D     | 769/816 (94%)   | -0.23  | 26 (3%) 49 42  | 14, 28, 80, 111       | 0     |
| 1   | E     | 769/816 (94%)   | -0.15  | 35 (4%) 36 31  | 14, 30, 95, 118       | 0     |
| 1   | F     | 769/816 (94%)   | -0.24  | 24 (3%) 52 46  | 10, 26, 73, 111       | 0     |
| 1   | G     | 769/816 (94%)   | -0.27  | 18 (2%) 64 59  | 14, 30, 70, 108       | 0     |
| 1   | H     | 785/816 (96%)   | 0.04   | 61 (7%) 16 11  | 17, 35, 92, 117       | 0     |
| All | All   | 6180/6528 (94%) | -0.14  | 278 (4%) 37 31 | 10, 31, 87, 131       | 0     |

All (278) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 86  | VAL  | 8.3  |
| 1   | B     | 105 | HIS  | 7.9  |
| 1   | H     | 83  | PRO  | 7.8  |
| 1   | B     | 102 | VAL  | 7.6  |
| 1   | H     | 18  | LEU  | 7.1  |
| 1   | B     | 84  | PRO  | 7.0  |
| 1   | H     | 86  | VAL  | 6.9  |
| 1   | H     | 21  | THR  | 6.9  |
| 1   | B     | 21  | THR  | 6.8  |
| 1   | B     | 109 | VAL  | 6.8  |
| 1   | B     | 69  | PHE  | 6.6  |
| 1   | H     | 69  | PHE  | 6.5  |
| 1   | G     | 70  | PHE  | 6.4  |
| 1   | H     | 130 | ASN  | 6.4  |
| 1   | B     | 23  | VAL  | 6.3  |
| 1   | H     | 70  | PHE  | 6.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 42  | GLY  | 6.2  |
| 1   | H     | 107 | LEU  | 6.2  |
| 1   | F     | 68  | PRO  | 6.1  |
| 1   | E     | 44  | LEU  | 5.9  |
| 1   | B     | 22  | LEU  | 5.9  |
| 1   | H     | 23  | VAL  | 5.9  |
| 1   | G     | 69  | PHE  | 5.8  |
| 1   | E     | 32  | LEU  | 5.8  |
| 1   | H     | 12  | HIS  | 5.4  |
| 1   | H     | 102 | VAL  | 5.4  |
| 1   | D     | 32  | LEU  | 5.4  |
| 1   | B     | 19  | ASN  | 5.4  |
| 1   | B     | 43  | ILE  | 5.3  |
| 1   | H     | 57  | PRO  | 5.3  |
| 1   | B     | 70  | PHE  | 5.2  |
| 1   | C     | 68  | PRO  | 5.2  |
| 1   | E     | 71  | ASP  | 5.1  |
| 1   | D     | 59  | GLN  | 5.1  |
| 1   | H     | 106 | ALA  | 5.0  |
| 1   | D     | 71  | ASP  | 5.0  |
| 1   | D     | 31  | ALA  | 5.0  |
| 1   | A     | 107 | LEU  | 4.9  |
| 1   | H     | 42  | GLY  | 4.9  |
| 1   | E     | 70  | PHE  | 4.8  |
| 1   | A     | 27  | ASN  | 4.8  |
| 1   | E     | 35  | ARG  | 4.7  |
| 1   | E     | 56  | LEU  | 4.7  |
| 1   | H     | 22  | LEU  | 4.7  |
| 1   | H     | 19  | ASN  | 4.7  |
| 1   | B     | 45  | GLN  | 4.7  |
| 1   | B     | 18  | LEU  | 4.7  |
| 1   | B     | 38  | ALA  | 4.7  |
| 1   | B     | 106 | ALA  | 4.6  |
| 1   | H     | 43  | ILE  | 4.6  |
| 1   | G     | 42  | GLY  | 4.6  |
| 1   | H     | 103 | ASN  | 4.6  |
| 1   | H     | 13  | SER  | 4.4  |
| 1   | E     | 106 | ALA  | 4.4  |
| 1   | C     | 106 | ALA  | 4.4  |
| 1   | H     | 54  | GLU  | 4.4  |
| 1   | B     | 126 | ASP  | 4.4  |
| 1   | D     | 107 | LEU  | 4.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 31  | ALA  | 4.4  |
| 1   | H     | 59  | GLN  | 4.3  |
| 1   | H     | 11  | VAL  | 4.3  |
| 1   | D     | 108 | VAL  | 4.2  |
| 1   | B     | 57  | PRO  | 4.2  |
| 1   | F     | 105 | HIS  | 4.2  |
| 1   | A     | 70  | PHE  | 4.1  |
| 1   | H     | 26  | ARG  | 4.1  |
| 1   | E     | 28  | GLU  | 4.1  |
| 1   | H     | 105 | HIS  | 4.0  |
| 1   | C     | 60  | THR  | 4.0  |
| 1   | H     | 82  | LEU  | 4.0  |
| 1   | B     | 103 | ASN  | 3.9  |
| 1   | A     | 57  | PRO  | 3.9  |
| 1   | H     | 38  | ALA  | 3.9  |
| 1   | E     | 46  | GLN  | 3.9  |
| 1   | H     | 109 | VAL  | 3.8  |
| 1   | D     | 42  | GLY  | 3.8  |
| 1   | H     | 28  | GLU  | 3.8  |
| 1   | E     | 59  | GLN  | 3.8  |
| 1   | B     | 53  | PHE  | 3.8  |
| 1   | A     | 67  | GLY  | 3.8  |
| 1   | B     | 58  | GLU  | 3.8  |
| 1   | E     | 64  | LEU  | 3.7  |
| 1   | C     | 69  | PHE  | 3.7  |
| 1   | G     | 71  | ASP  | 3.7  |
| 1   | C     | 59  | GLN  | 3.7  |
| 1   | B     | 83  | PRO  | 3.7  |
| 1   | A     | 31  | ALA  | 3.7  |
| 1   | F     | 71  | ASP  | 3.7  |
| 1   | C     | 105 | HIS  | 3.7  |
| 1   | H     | 60  | THR  | 3.7  |
| 1   | B     | 28  | GLU  | 3.6  |
| 1   | A     | 30  | LEU  | 3.6  |
| 1   | E     | 57  | PRO  | 3.6  |
| 1   | B     | 60  | THR  | 3.6  |
| 1   | G     | 59  | GLN  | 3.6  |
| 1   | A     | 105 | HIS  | 3.6  |
| 1   | D     | 72  | LEU  | 3.6  |
| 1   | E     | 67  | GLY  | 3.6  |
| 1   | A     | 104 | LEU  | 3.6  |
| 1   | B     | 47  | ASN  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 128 | VAL  | 3.5  |
| 1   | A     | 69  | PHE  | 3.5  |
| 1   | A     | 44  | LEU  | 3.5  |
| 1   | B     | 101 | ARG  | 3.5  |
| 1   | H     | 84  | PRO  | 3.4  |
| 1   | H     | 56  | LEU  | 3.4  |
| 1   | D     | 28  | GLU  | 3.4  |
| 1   | B     | 29  | VAL  | 3.4  |
| 1   | B     | 17  | ARG  | 3.4  |
| 1   | E     | 51  | ALA  | 3.4  |
| 1   | H     | 129 | LYS  | 3.4  |
| 1   | C     | 104 | LEU  | 3.4  |
| 1   | E     | 68  | PRO  | 3.3  |
| 1   | E     | 55  | ALA  | 3.3  |
| 1   | C     | 51  | ALA  | 3.3  |
| 1   | D     | 41  | LYS  | 3.3  |
| 1   | D     | 46  | GLN  | 3.3  |
| 1   | B     | 65  | GLU  | 3.3  |
| 1   | C     | 43  | ILE  | 3.3  |
| 1   | C     | 29  | VAL  | 3.2  |
| 1   | F     | 58  | GLU  | 3.2  |
| 1   | E     | 45  | GLN  | 3.2  |
| 1   | D     | 67  | GLY  | 3.2  |
| 1   | A     | 66  | GLY  | 3.1  |
| 1   | B     | 108 | VAL  | 3.1  |
| 1   | E     | 52  | GLU  | 3.1  |
| 1   | H     | 17  | ARG  | 3.1  |
| 1   | F     | 46  | GLN  | 3.1  |
| 1   | C     | 52  | GLU  | 3.1  |
| 1   | C     | 46  | GLN  | 3.1  |
| 1   | F     | 82  | LEU  | 3.1  |
| 1   | B     | 59  | GLN  | 3.1  |
| 1   | B     | 37  | GLU  | 3.1  |
| 1   | A     | 42  | GLY  | 3.1  |
| 1   | D     | 55  | ALA  | 3.0  |
| 1   | D     | 54  | GLU  | 3.0  |
| 1   | F     | 59  | GLN  | 3.0  |
| 1   | E     | 105 | HIS  | 3.0  |
| 1   | B     | 55  | ALA  | 3.0  |
| 1   | G     | 46  | GLN  | 3.0  |
| 1   | H     | 104 | LEU  | 3.0  |
| 1   | H     | 73  | LEU  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 129 | LYS  | 3.0  |
| 1   | E     | 33  | LEU  | 3.0  |
| 1   | B     | 54  | GLU  | 2.9  |
| 1   | H     | 44  | LEU  | 2.9  |
| 1   | C     | 130 | ASN  | 2.9  |
| 1   | E     | 27  | ASN  | 2.9  |
| 1   | G     | 51  | ALA  | 2.9  |
| 1   | C     | 57  | PRO  | 2.9  |
| 1   | F     | 70  | PHE  | 2.9  |
| 1   | F     | 128 | VAL  | 2.9  |
| 1   | G     | 104 | LEU  | 2.9  |
| 1   | B     | 130 | ASN  | 2.9  |
| 1   | C     | 83  | PRO  | 2.8  |
| 1   | A     | 46  | GLN  | 2.8  |
| 1   | C     | 31  | ALA  | 2.8  |
| 1   | A     | 59  | GLN  | 2.8  |
| 1   | E     | 39  | LYS  | 2.8  |
| 1   | C     | 44  | LEU  | 2.8  |
| 1   | E     | 38  | ALA  | 2.7  |
| 1   | H     | 108 | VAL  | 2.7  |
| 1   | H     | 58  | GLU  | 2.7  |
| 1   | H     | 219 | GLU  | 2.7  |
| 1   | B     | 62  | LYS  | 2.7  |
| 1   | B     | 81  | VAL  | 2.7  |
| 1   | E     | 43  | ILE  | 2.7  |
| 1   | B     | 630 | TYR  | 2.7  |
| 1   | A     | 72  | LEU  | 2.7  |
| 1   | H     | 55  | ALA  | 2.7  |
| 1   | F     | 69  | PHE  | 2.7  |
| 1   | H     | 228 | GLU  | 2.7  |
| 1   | B     | 26  | ARG  | 2.7  |
| 1   | E     | 29  | VAL  | 2.7  |
| 1   | D     | 69  | PHE  | 2.7  |
| 1   | E     | 72  | LEU  | 2.7  |
| 1   | E     | 235 | GLU  | 2.7  |
| 1   | F     | 65  | GLU  | 2.6  |
| 1   | F     | 44  | LEU  | 2.6  |
| 1   | G     | 44  | LEU  | 2.6  |
| 1   | A     | 128 | VAL  | 2.6  |
| 1   | B     | 88  | LEU  | 2.6  |
| 1   | H     | 71  | ASP  | 2.6  |
| 1   | C     | 38  | ALA  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 29  | VAL  | 2.6  |
| 1   | A     | 71  | ASP  | 2.6  |
| 1   | G     | 82  | LEU  | 2.6  |
| 1   | E     | 30  | LEU  | 2.5  |
| 1   | B     | 46  | GLN  | 2.5  |
| 1   | A     | 68  | PRO  | 2.5  |
| 1   | B     | 221 | LYS  | 2.5  |
| 1   | C     | 32  | LEU  | 2.5  |
| 1   | A     | 82  | LEU  | 2.5  |
| 1   | D     | 104 | LEU  | 2.5  |
| 1   | E     | 104 | LEU  | 2.5  |
| 1   | H     | 33  | LEU  | 2.5  |
| 1   | D     | 57  | PRO  | 2.5  |
| 1   | B     | 24  | SER  | 2.5  |
| 1   | B     | 16  | GLU  | 2.5  |
| 1   | H     | 111 | GLU  | 2.4  |
| 1   | C     | 55  | ALA  | 2.4  |
| 1   | G     | 130 | ASN  | 2.4  |
| 1   | D     | 109 | VAL  | 2.4  |
| 1   | G     | 105 | HIS  | 2.4  |
| 1   | B     | 52  | GLU  | 2.4  |
| 1   | A     | 43  | ILE  | 2.4  |
| 1   | D     | 540 | LYS  | 2.4  |
| 1   | F     | 42  | GLY  | 2.4  |
| 1   | B     | 85  | TRP  | 2.4  |
| 1   | D     | 43  | ILE  | 2.4  |
| 1   | H     | 630 | TYR  | 2.4  |
| 1   | F     | 172 | HIS  | 2.4  |
| 1   | B     | 73  | LEU  | 2.3  |
| 1   | B     | 31  | ALA  | 2.3  |
| 1   | F     | 54  | GLU  | 2.3  |
| 1   | H     | 232 | LYS  | 2.3  |
| 1   | H     | 75  | SER  | 2.3  |
| 1   | H     | 110 | GLU  | 2.3  |
| 1   | D     | 52  | GLU  | 2.3  |
| 1   | G     | 60  | THR  | 2.3  |
| 1   | H     | 40  | GLY  | 2.3  |
| 1   | F     | 33  | LEU  | 2.3  |
| 1   | E     | 40  | GLY  | 2.3  |
| 1   | E     | 50  | ILE  | 2.3  |
| 1   | H     | 36  | VAL  | 2.3  |
| 1   | H     | 52  | GLU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 56  | LEU  | 2.3  |
| 1   | C     | 39  | LYS  | 2.3  |
| 1   | F     | 176 | SER  | 2.3  |
| 1   | H     | 37  | GLU  | 2.3  |
| 1   | H     | 65  | GLU  | 2.3  |
| 1   | A     | 85  | TRP  | 2.3  |
| 1   | B     | 74  | LYS  | 2.3  |
| 1   | G     | 68  | PRO  | 2.3  |
| 1   | A     | 52  | GLU  | 2.2  |
| 1   | A     | 34  | SER  | 2.2  |
| 1   | G     | 28  | GLU  | 2.2  |
| 1   | H     | 16  | GLU  | 2.2  |
| 1   | F     | 220 | LEU  | 2.2  |
| 1   | C     | 129 | LYS  | 2.2  |
| 1   | C     | 127 | GLY  | 2.2  |
| 1   | F     | 28  | GLU  | 2.2  |
| 1   | E     | 54  | GLU  | 2.2  |
| 1   | B     | 127 | GLY  | 2.1  |
| 1   | F     | 66  | GLY  | 2.1  |
| 1   | A     | 61  | ARG  | 2.1  |
| 1   | D     | 51  | ALA  | 2.1  |
| 1   | H     | 29  | VAL  | 2.1  |
| 1   | H     | 231 | ALA  | 2.1  |
| 1   | A     | 103 | ASN  | 2.1  |
| 1   | H     | 74  | LYS  | 2.1  |
| 1   | C     | 128 | VAL  | 2.1  |
| 1   | D     | 220 | LEU  | 2.1  |
| 1   | D     | 105 | HIS  | 2.1  |
| 1   | F     | 126 | ASP  | 2.1  |
| 1   | C     | 41  | LYS  | 2.1  |
| 1   | B     | 100 | LEU  | 2.1  |
| 1   | B     | 180 | LEU  | 2.1  |
| 1   | C     | 58  | GLU  | 2.1  |
| 1   | C     | 126 | ASP  | 2.1  |
| 1   | G     | 223 | GLU  | 2.1  |
| 1   | A     | 178 | LEU  | 2.1  |
| 1   | F     | 72  | LEU  | 2.1  |
| 1   | H     | 127 | GLY  | 2.0  |
| 1   | G     | 43  | ILE  | 2.0  |
| 1   | H     | 733 | GLU  | 2.0  |
| 1   | A     | 108 | VAL  | 2.0  |
| 1   | E     | 83  | PRO  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 201 | GLN  | 2.0  |
| 1   | B     | 107 | LEU  | 2.0  |
| 1   | E     | 244 | ASP  | 2.0  |
| 1   | H     | 216 | TYR  | 2.0  |
| 1   | B     | 206 | LEU  | 2.0  |
| 1   | F     | 40  | GLY  | 2.0  |
| 1   | D     | 83  | PRO  | 2.0  |
| 1   | H     | 236 | ILE  | 2.0  |
| 1   | G     | 129 | LYS  | 2.0  |
| 1   | A     | 54  | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | SO4  | H     | 913 | 5/5   | 0.89 | 0.42 | 15.97 | 64,70,86,101               | 0     |
| 5   | MLA  | D     | 921 | 7/7   | 0.94 | 0.33 | 6.76  | 33,40,44,47                | 0     |
| 5   | MLA  | H     | 921 | 7/7   | 0.89 | 0.41 | 6.27  | 53,58,69,69                | 0     |
| 5   | MLA  | E     | 921 | 7/7   | 0.95 | 0.37 | 5.04  | 34,38,43,43                | 0     |
| 4   | SO4  | B     | 913 | 5/5   | 0.91 | 0.28 | 4.78  | 53,54,65,78                | 0     |
| 5   | MLA  | C     | 921 | 7/7   | 0.89 | 0.41 | 4.14  | 56,60,68,77                | 0     |
| 4   | SO4  | A     | 911 | 5/5   | 0.97 | 0.22 | 4.01  | 31,35,46,58                | 0     |
| 4   | SO4  | G     | 911 | 5/5   | 0.96 | 0.24 | 3.52  | 32,40,56,64                | 0     |
| 4   | SO4  | E     | 913 | 5/5   | 0.95 | 0.21 | 3.22  | 44,47,62,71                | 0     |
| 5   | MLA  | F     | 921 | 7/7   | 0.93 | 0.23 | 2.60  | 30,35,36,36                | 0     |
| 5   | MLA  | B     | 921 | 7/7   | 0.94 | 0.26 | 2.54  | 38,45,50,53                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | SO4  | D     | 911 | 5/5   | 0.95 | 0.20 | 2.42  | 38,41,56,67                | 0     |
| 5   | MLA  | G     | 921 | 7/7   | 0.92 | 0.27 | 2.21  | 46,49,59,59                | 0     |
| 4   | SO4  | F     | 911 | 5/5   | 0.95 | 0.20 | 2.09  | 32,36,45,64                | 0     |
| 4   | SO4  | E     | 911 | 5/5   | 0.94 | 0.17 | 1.41  | 31,35,59,60                | 0     |
| 5   | MLA  | A     | 921 | 7/7   | 0.93 | 0.19 | 1.21  | 27,31,34,36                | 0     |
| 2   | UDP  | F     | 901 | 25/25 | 0.99 | 0.18 | 1.04  | 14,18,23,25                | 0     |
| 3   | FRU  | C     | 902 | 12/12 | 0.93 | 0.21 | 1.00  | 30,36,44,50                | 0     |
| 4   | SO4  | D     | 913 | 5/5   | 0.96 | 0.16 | 0.90  | 44,46,53,63                | 0     |
| 6   | K    | C     | 931 | 1/1   | 0.95 | 0.25 | 0.79  | 69,69,69,69                | 0     |
| 2   | UDP  | B     | 901 | 25/25 | 0.98 | 0.18 | 0.61  | 19,25,30,34                | 0     |
| 4   | SO4  | C     | 911 | 5/5   | 0.96 | 0.16 | 0.53  | 44,46,57,63                | 0     |
| 3   | FRU  | B     | 902 | 12/12 | 0.96 | 0.17 | 0.48  | 25,30,35,35                | 0     |
| 4   | SO4  | H     | 911 | 5/5   | 0.95 | 0.15 | 0.37  | 37,38,69,70                | 0     |
| 4   | SO4  | F     | 913 | 5/5   | 0.97 | 0.15 | 0.25  | 40,44,61,64                | 0     |
| 2   | UDP  | H     | 901 | 25/25 | 0.98 | 0.17 | 0.18  | 22,28,36,38                | 0     |
| 2   | UDP  | G     | 901 | 25/25 | 0.99 | 0.17 | 0.15  | 14,21,25,35                | 0     |
| 3   | FRU  | H     | 902 | 12/12 | 0.94 | 0.17 | 0.09  | 22,29,34,37                | 0     |
| 4   | SO4  | G     | 913 | 5/5   | 0.95 | 0.17 | 0.08  | 52,58,68,74                | 0     |
| 4   | SO4  | B     | 911 | 5/5   | 0.95 | 0.14 | -0.07 | 37,42,50,70                | 0     |
| 3   | FRU  | E     | 902 | 12/12 | 0.97 | 0.17 | -0.14 | 18,25,30,32                | 0     |
| 6   | K    | F     | 931 | 1/1   | 0.82 | 0.21 | -0.24 | 69,69,69,69                | 0     |
| 2   | UDP  | E     | 901 | 25/25 | 0.99 | 0.17 | -0.28 | 17,21,27,29                | 0     |
| 6   | K    | B     | 931 | 1/1   | 0.91 | 0.22 | -0.29 | 74,74,74,74                | 0     |
| 3   | FRU  | D     | 902 | 12/12 | 0.96 | 0.15 | -0.39 | 18,25,31,32                | 0     |
| 2   | UDP  | D     | 901 | 25/25 | 0.99 | 0.15 | -0.43 | 17,21,25,30                | 0     |
| 6   | K    | D     | 931 | 1/1   | 0.93 | 0.17 | -0.44 | 61,61,61,61                | 0     |
| 2   | UDP  | A     | 901 | 25/25 | 0.99 | 0.16 | -0.44 | 14,17,21,24                | 0     |
| 3   | FRU  | F     | 902 | 12/12 | 0.97 | 0.15 | -0.46 | 17,22,28,35                | 0     |
| 3   | FRU  | G     | 902 | 12/12 | 0.96 | 0.15 | -0.46 | 18,25,34,34                | 0     |
| 2   | UDP  | C     | 901 | 25/25 | 0.98 | 0.15 | -0.52 | 21,31,40,42                | 0     |
| 6   | K    | H     | 931 | 1/1   | 0.96 | 0.17 | -0.62 | 61,61,61,61                | 0     |
| 6   | K    | E     | 931 | 1/1   | 0.90 | 0.16 | -1.02 | 64,64,64,64                | 0     |
| 3   | FRU  | A     | 902 | 12/12 | 0.97 | 0.13 | -1.62 | 16,22,27,28                | 0     |
| 6   | K    | A     | 931 | 1/1   | 0.94 | 0.09 | -1.91 | 61,61,61,61                | 0     |
| 6   | K    | G     | 931 | 1/1   | 0.93 | 0.10 | -2.49 | 57,57,57,57                | 0     |
| 4   | SO4  | F     | 912 | 5/5   | 0.93 | 0.19 | -     | 46,50,62,76                | 0     |
| 4   | SO4  | E     | 912 | 5/5   | 0.91 | 0.32 | -     | 47,55,63,84                | 0     |
| 4   | SO4  | D     | 912 | 5/5   | 0.92 | 0.28 | -     | 54,74,96,98                | 0     |
| 4   | SO4  | H     | 912 | 5/5   | 0.93 | 0.30 | -     | 63,66,76,94                | 0     |
| 4   | SO4  | B     | 912 | 5/5   | 0.94 | 0.24 | -     | 49,67,79,88                | 0     |
| 4   | SO4  | A     | 912 | 5/5   | 0.93 | 0.21 | -     | 47,55,59,81                | 0     |
| 4   | SO4  | C     | 913 | 5/5   | 0.92 | 0.36 | -     | 63,74,75,89                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 4   | SO4  | A     | 913 | 5/5   | 0.96 | 0.19 | -    | 42,44,52,59                 | 0     |
| 4   | SO4  | C     | 912 | 5/5   | 0.90 | 0.38 | -    | 71,74,96,104                | 0     |
| 4   | SO4  | G     | 912 | 5/5   | 0.95 | 0.30 | -    | 48,67,72,86                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.