



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:13 AM UTC

PDB ID : 4WL1 / pdb\_00004wl1  
Title : Structure of WzzE Polysaccharide Co-polymerase  
Authors : Kalynych, S.; Cherney, M.; Cygler, M.  
Deposited on : 2014-10-05  
Resolution : 5.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

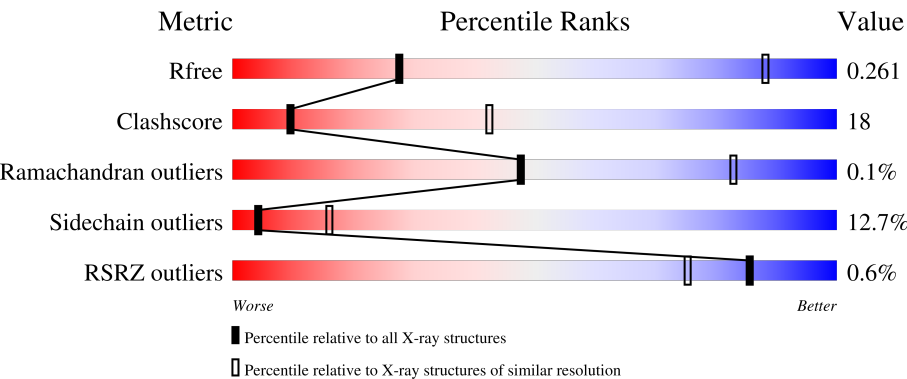
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 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 5.99 Å.

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



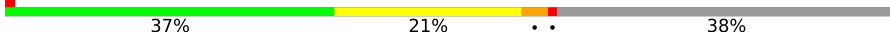
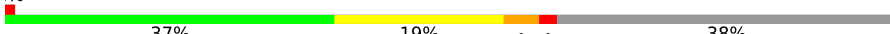
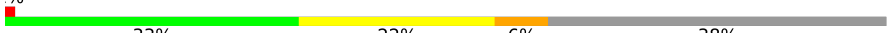
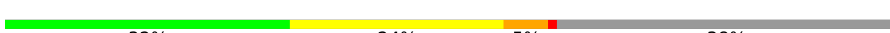
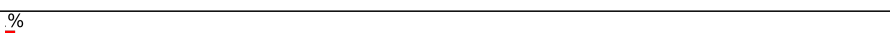
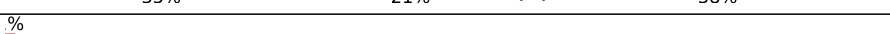
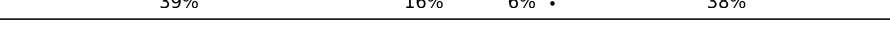
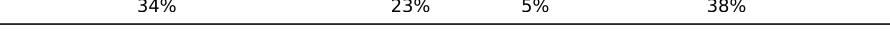
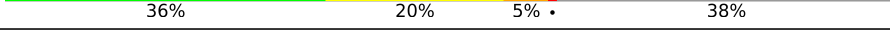
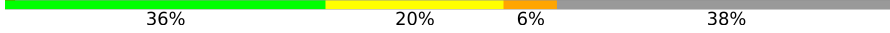
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1138 (7.94-4.00)                                      |
| Clashscore            | 190562                      | 1204 (7.94-4.00)                                      |
| Ramachandran outliers | 187476                      | 1029 (7.94-4.00)                                      |
| Sidechain outliers    | 187428                      | 1019 (7.94-3.98)                                      |
| RSRZ outliers         | 180081                      | 1131 (7.94-4.00)                                      |

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

| Mol | Chain | Length | Quality of chain                              |
|-----|-------|--------|-----------------------------------------------|
| 1   | A     | 356    | <div><div></div><div>36%19%6%•38%</div></div> |
| 1   | B     | 356    | <div><div></div><div>32%25%••38%</div></div>  |
| 1   | C     | 356    | <div><div></div><div>39%19%••38%</div></div>  |
| 1   | D     | 356    | <div><div></div><div>31%24%6%•38%</div></div> |
| 1   | E     | 356    | <div><div>%</div><div>38%19%••38%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | F     | 356    |    |
| 1   | G     | 356    |    |
| 1   | H     | 356    |    |
| 1   | I     | 356    |    |
| 1   | J     | 356    |    |
| 1   | K     | 356    |    |
| 1   | L     | 356    |    |
| 1   | M     | 356    |    |
| 1   | N     | 356    |    |
| 1   | O     | 356    |    |
| 1   | P     | 356    |    |
| 1   | Q     | 356    |    |
| 1   | R     | 356    |  |
| 1   | S     | 356    |  |
| 1   | T     | 356    |  |
| 1   | U     | 356    |  |
| 1   | V     | 356    |  |
| 1   | W     | 356    |  |
| 1   | X     | 356    |  |
| 1   | Y     | 356    |  |
| 1   | Z     | 356    |  |
| 1   | a     | 356    |  |
| 1   | b     | 356    |  |
| 1   | c     | 356    |  |
| 1   | d     | 356    |  |

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| Mol | Chain | Length | Quality of chain                              |
|-----|-------|--------|-----------------------------------------------|
| 1   | e     | 356    | <div><div></div><div>36%19%5%•38%</div></div> |
| 1   | f     | 356    | <div><div></div><div>32%22%7%•38%</div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 57504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lipopolysaccharide biosynthesis protein WzzE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | B     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | C     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | D     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | E     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | F     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | G     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | H     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | I     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | J     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | K     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | L     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | M     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | N     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | O     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | P     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Q     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | R     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | S     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | T     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | U     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | V     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | W     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | X     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | Y     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | Z     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | a     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | b     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | c     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | d     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | e     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |
| 1   | f     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1797  | 1124 | 321 | 344 | 8 |         |         |       |

There are 288 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| A     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| A     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| A     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| A     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| A     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| A     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| A     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| B     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| B     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| B     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| B     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| B     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| B     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| B     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| B     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| B     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| C     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| C     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| C     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| C     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| C     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| C     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| C     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| C     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| C     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| D     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| D     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| D     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| D     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| D     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| D     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| D     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| D     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| D     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| E     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| E     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| E     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| E     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| E     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| E     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| E     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| E     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| E     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| F     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| F     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| F     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| F     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| F     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| F     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| F     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| F     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| F     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| G     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| G     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| G     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| G     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| G     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| G     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| G     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| G     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| G     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| H     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| H     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| H     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| H     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| H     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| H     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| H     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| H     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| H     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| I     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| I     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| I     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| I     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| I     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| I     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| I     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| I     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| I     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| J     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| J     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| J     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| J     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| J     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| J     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| J     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| J     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| J     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| K     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| K     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| K     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| K     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| K     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| K     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| K     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| K     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| K     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| L     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| L     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| L     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| L     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| L     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| L     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| L     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| L     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| L     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| M     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| M     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| M     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| M     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| M     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| M     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| M     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| M     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| M     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| N     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| N     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| N     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| N     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| N     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| N     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| N     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| N     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| N     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| O     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| O     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| O     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| O     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| O     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| O     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| O     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| O     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| O     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| P     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| P     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| P     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| P     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| P     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| P     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| P     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| P     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| P     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| Q     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| Q     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| Q     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| Q     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| Q     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| Q     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| Q     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| Q     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| Q     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| R     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| R     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| R     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| R     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| R     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| R     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| R     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| R     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| R     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| S     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| S     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| S     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| S     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| S     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| S     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| S     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| S     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| S     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| T     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| T     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| T     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| T     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| T     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| T     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| T     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| T     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| T     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| U     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| U     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| U     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| U     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| U     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| U     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| U     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| U     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| U     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| V     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| V     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| V     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| V     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| V     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| V     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| V     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| V     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| V     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| W     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| W     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| W     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| W     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| W     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| W     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| W     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| W     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| W     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| X     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| X     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| X     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| X     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| X     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| X     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| X     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| X     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| X     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| Y     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| Y     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| Y     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| Y     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| Y     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| Y     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| Y     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| Y     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| Y     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| Z     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| Z     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| Z     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| Z     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| Z     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| Z     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| Z     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| Z     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| Z     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| a     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| a     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| a     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| a     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| a     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| a     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| a     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| a     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| a     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| b     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| b     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| b     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| b     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| b     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| b     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| b     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| b     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| b     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| c     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| c     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| c     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| c     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| c     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| c     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| c     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| c     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| c     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| d     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| d     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| d     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| d     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| d     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| d     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| d     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| d     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| d     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| e     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| e     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| e     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| e     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| e     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| e     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| e     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| e     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| e     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |
| f     | -6      | MET      | -      | initiating methionine | UNP P0AG01 |
| f     | -5      | GLY      | -      | expression tag        | UNP P0AG01 |
| f     | -4      | SER      | -      | expression tag        | UNP P0AG01 |
| f     | -3      | HIS      | -      | expression tag        | UNP P0AG01 |
| f     | -2      | HIS      | -      | expression tag        | UNP P0AG01 |
| f     | -1      | HIS      | -      | expression tag        | UNP P0AG01 |
| f     | 0       | HIS      | -      | expression tag        | UNP P0AG01 |
| f     | 1       | HIS      | -      | expression tag        | UNP P0AG01 |
| f     | 2       | HIS      | -      | expression tag        | UNP P0AG01 |



Chain C: 39% 19% 38%

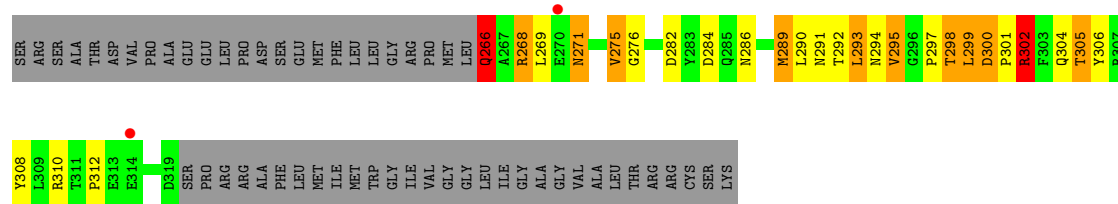
|     |      |      |      |     |
|-----|------|------|------|-----|
| ALA | VAL  | K134 | GLN  | MET |
| PHE | PRO  | A135 | E55  | GLY |
| LEU | ALA  |      | W56  | SER |
| MET | GLU  | I143 |      | HIS |
| ILE | GLU  | M144 | A60  | HIS |
| MET | LEU  |      | T61  | HIS |
| TRP | PRO  | I150 | T62  | HIS |
| GLY | ASP  | P151 |      | HIS |
| ILE | SER  | G152 | T66  | THR |
| VAL | GLU  |      | V67  | THR |
| GLY | MET  | T155 | N68  | GLN |
| GLY | PHE  |      | N69  | PRO |
| LEU | LEU  | D160 | L70  | MET |
| ILE | LEU  |      |      | PRO |
| GLY | GLY  | K163 | Y73  | GLY |
| ALA | ARG  |      | Y74  | LYS |
| GLY | PRO  | T168 | S75  | PRO |
| VAL | MET  | A169 | Q76  | ALA |
| ALA | LEU  | P170 | Q77  | GLU |
| LEU |      | D171 | Q78  | ASP |
| THR | Q266 |      |      | ALA |
| ARG | L272 | A187 | L83  | ALA |
| ARG | Q273 |      | D84  | ASN |
| CYS |      | L191 | V85  | GLU |
| SER | D282 | N192 | ARG  | LEU |
| LYS | Y283 | E193 | SER  | ASP |
|     |      | D194 | ASN  | ILE |
|     |      | L195 | MET  | ARG |
|     | N286 | K196 | ALA  | GLY |
|     | R287 |      | ALA  | LEU |
|     | A288 |      | SER  | PHE |
|     | R289 | W199 | ALA  | ARG |
|     | L290 | M206 | GLN  | THR |
|     | N291 |      | P95  | LEU |
|     | T292 | V210 | S96  | TRP |
|     | L293 |      | N97  | ALA |
|     | N294 | Q213 | N98  | GLY |
|     | V295 |      |      | LYS |
|     | G296 |      | A101 | LEU |
|     | P297 | V216 | Y102 | TRP |
|     | T298 |      | K103 | TRP |
|     | L299 | M225 | E104 | ILE |
|     | D300 |      | F105 | GLY |
|     |      | E229 | V106 | MET |
|     | F303 | Q230 | M107 | GLY |
|     | Q304 | ALA  |      | LEU |
|     | T305 | LEU  |      | ALA |
|     | V306 | LYS  |      | ALA |
|     | R307 | ILE  | T114 | PHE |
|     |      | ALA  |      | ALA |
|     | T311 | GLU  | Q121 | LEU |
|     | P312 | GLN  | T122 | ILE |
|     |      | HIS  | D123 | ALA |
|     |      | ILE  | Y124 | LEU |
|     | V316 | ASN  | Y125 | LEU |
|     | R317 | ILE  | K126 | ALA |
|     | R318 | SER  | Q127 | THR |
|     | D319 | ARG  | R128 | THR |
|     | SER  | SER  | M129 | PHE |
| PRO | PRO  | ALA  |      | PHE |
| ARG | ARG  | THR  | N132 | ALA |
|     |      | ASP  | S133 | ASP |

Chain D:

31% 24% 6% 38%

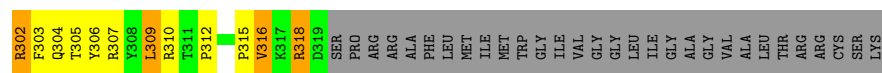
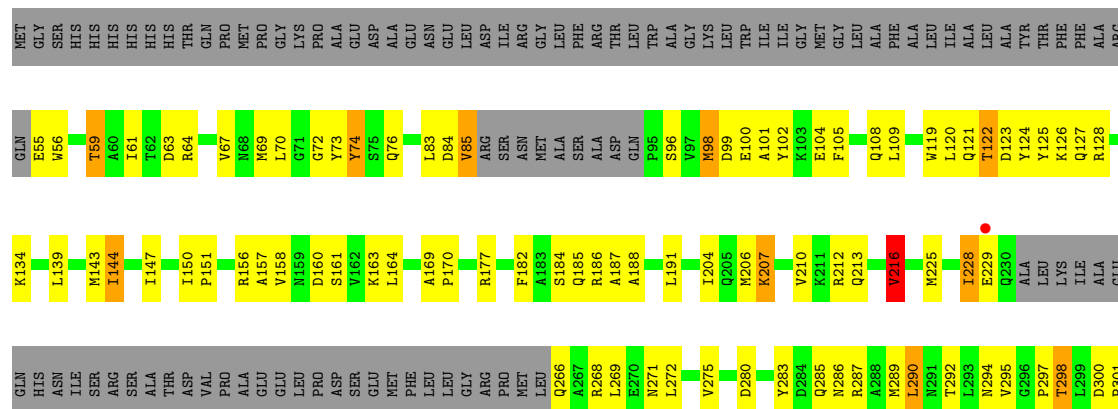
| Amino Acid | Category |
|------------|----------|
| Met        | Grey     |
| Gly        | Grey     |
| His        | Green    |
| His        | Green    |
| His        | Green    |
| His        | Green    |
| His        | Green    |
| Thr        | Green    |
| Gln        | Green    |
| Pro        | Green    |
| Pro        | Green    |
| Gly        | Green    |
| Lys        | Green    |
| Pro        | Green    |
| Ala        | Green    |
| Ala        | Green    |
| Asp        | Green    |
| Ala        | Green    |
| Glu        | Green    |
| Asn        | Green    |
| Glu        | Green    |
| Leu        | Green    |
| Asp        | Green    |
| Ile        | Green    |
| Arg        | Green    |
| Gly        | Green    |
| Leu        | Green    |
| Phe        | Green    |
| Asn        | Green    |
| Met        | Green    |
| Thr        | Green    |
| Leu        | Green    |
| Trp        | Green    |
| Ala        | Green    |
| Gly        | Green    |
| Lys        | Green    |
| Leu        | Green    |
| Trp        | Green    |
| Ile        | Green    |
| Ile        | Green    |
| Met        | Grey     |
| Gly        | Grey     |
| Leu        | Grey     |
| Ala        | Grey     |
| Phe        | Grey     |
| Ala        | Grey     |
| Leu        | Grey     |
| Ile        | Grey     |
| Leu        | Grey     |
| Ala        | Grey     |
| Leu        | Grey     |
| Ala        | Grey     |
| Ala        | Grey     |
| Thr        | Grey     |
| Trp        | Grey     |
| Phe        | Grey     |
| Phe        | Grey     |
| Ala        | Grey     |

[illegible]



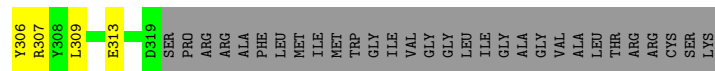
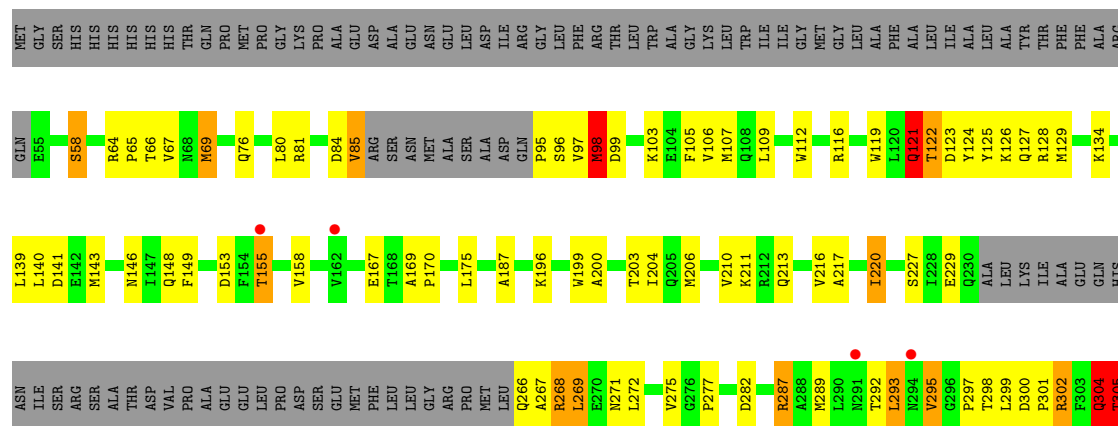
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain F: 33% 24% • 38%



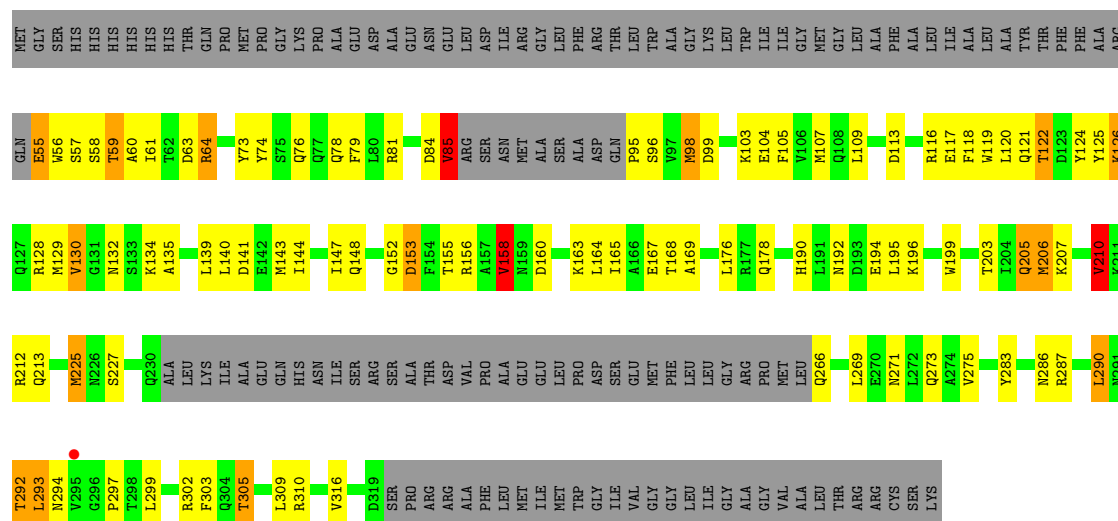
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain G: 37% 21% • • 38%



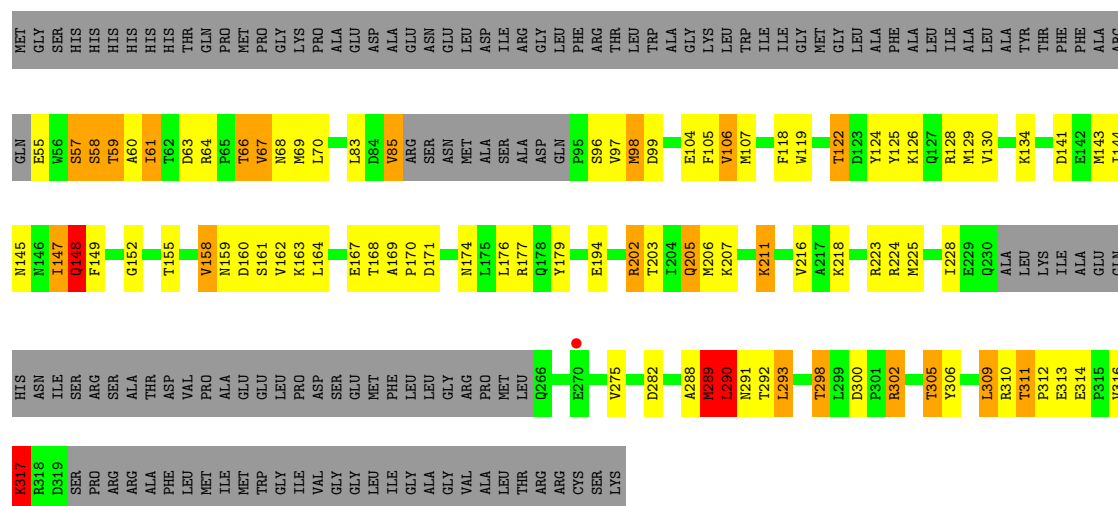
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain H: 34% 23% • • 38%



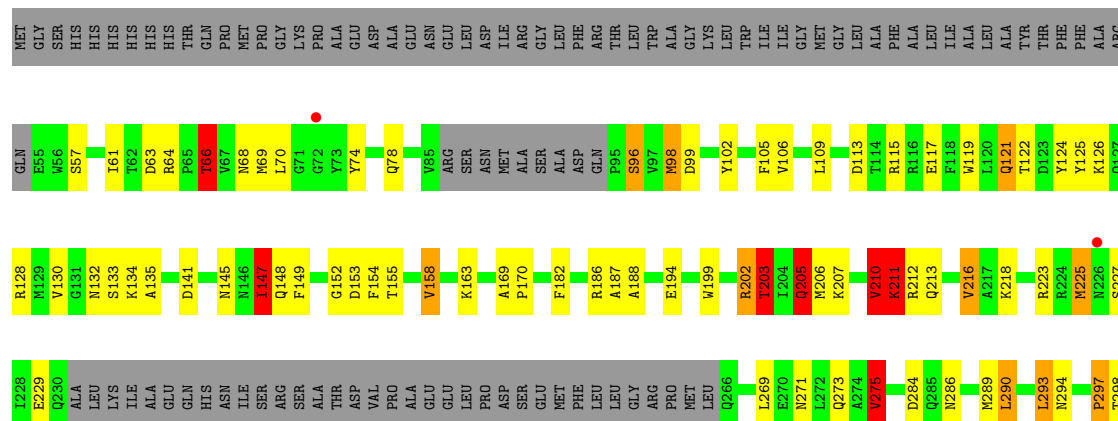
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

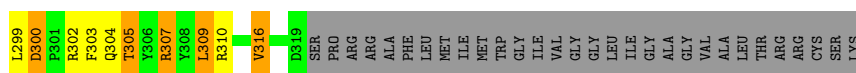
Chain I: 36% 19% 6% • 38%



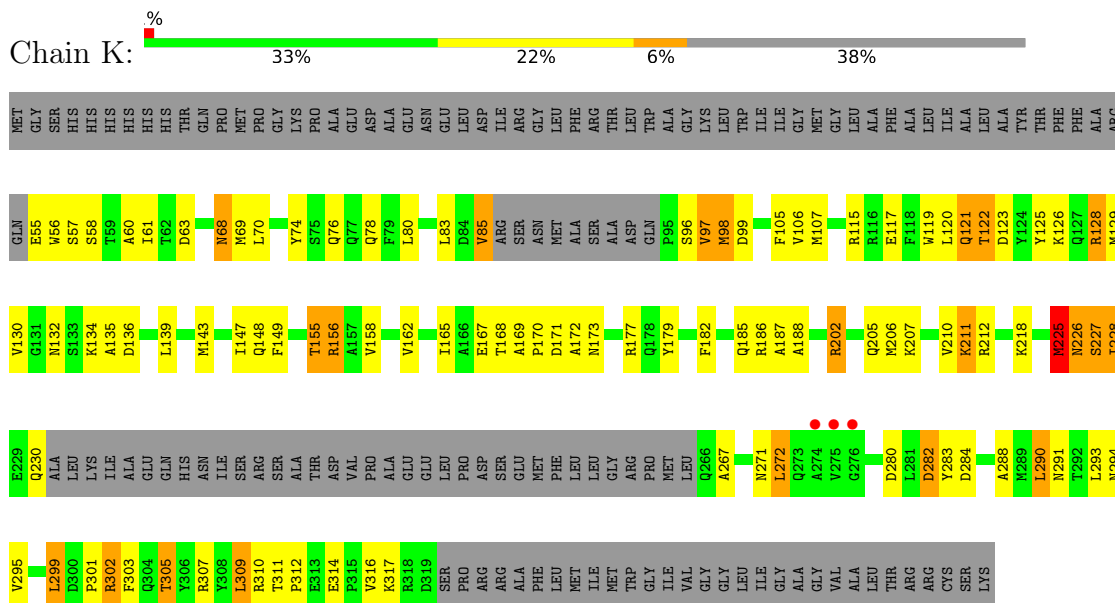
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain J: 37% 19% • • 38%

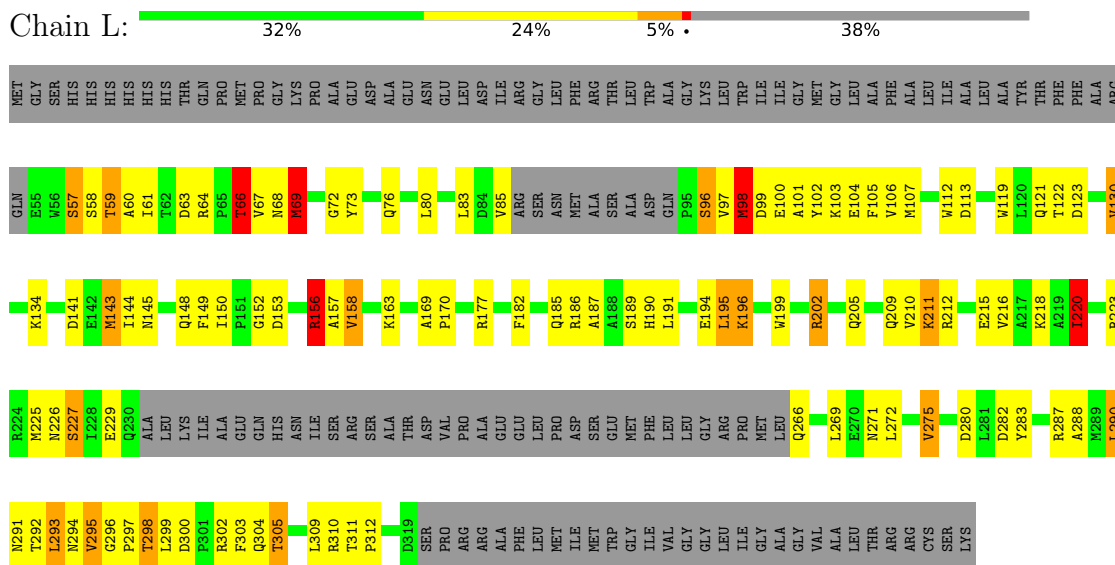




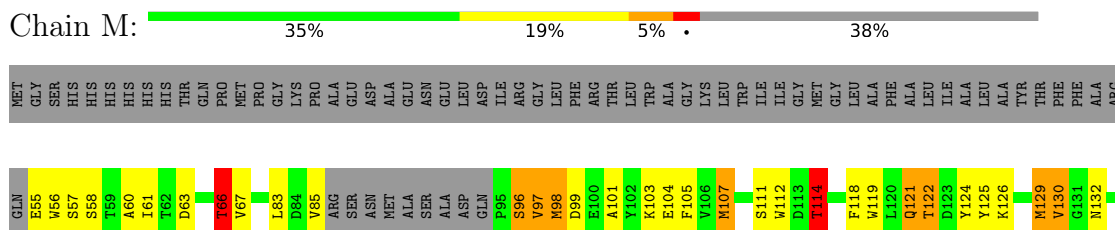
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

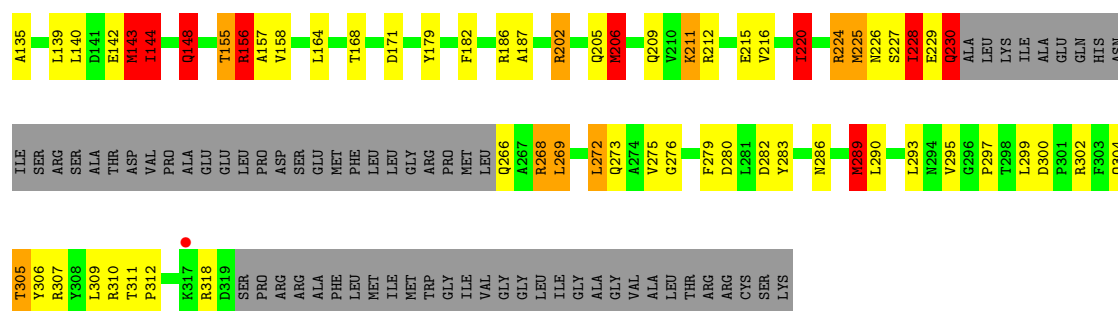


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

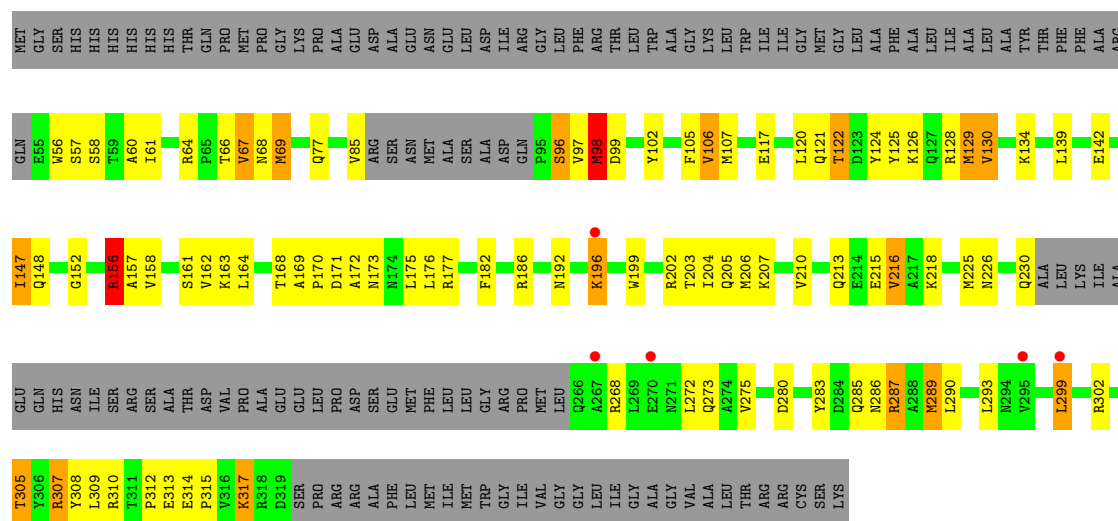
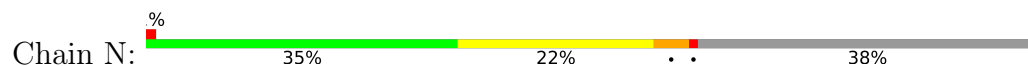


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

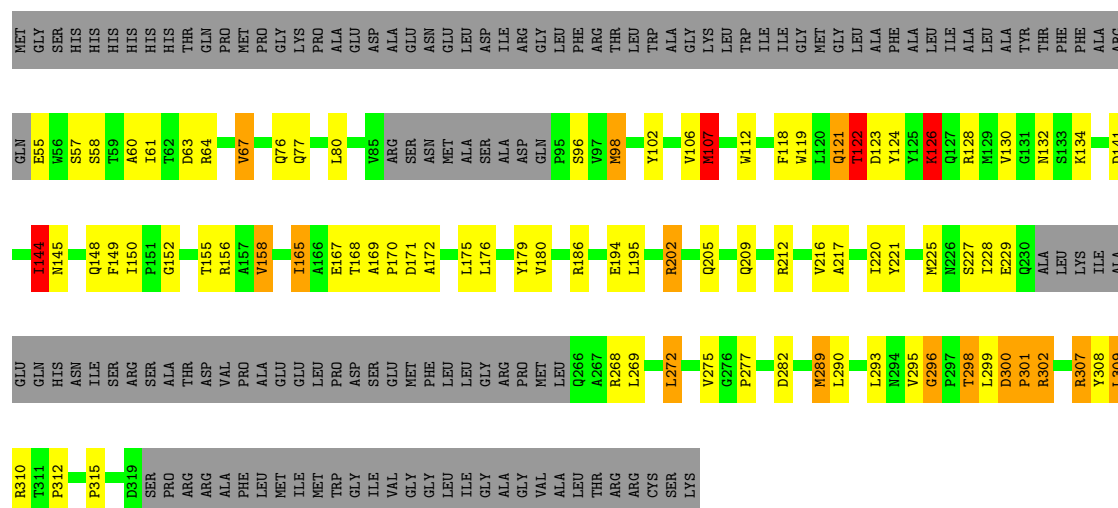




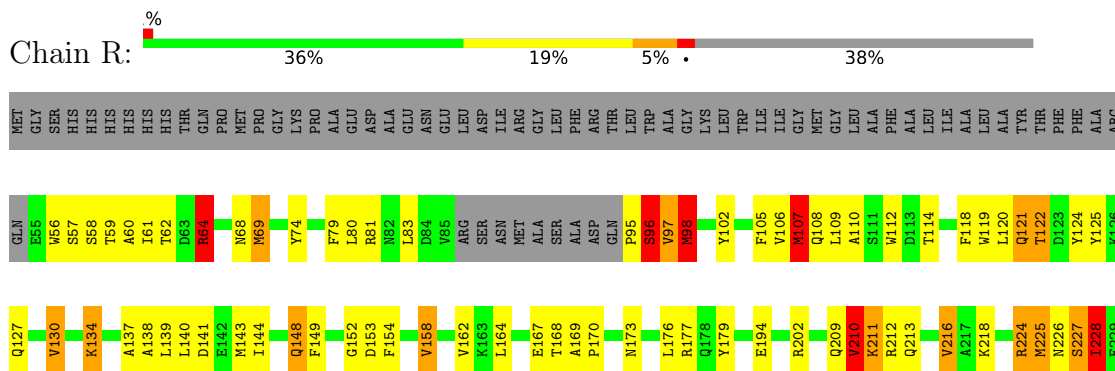
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

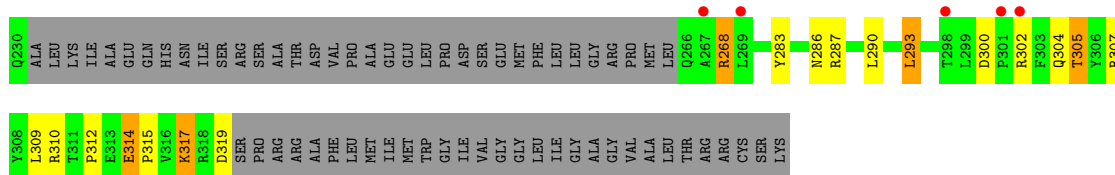


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

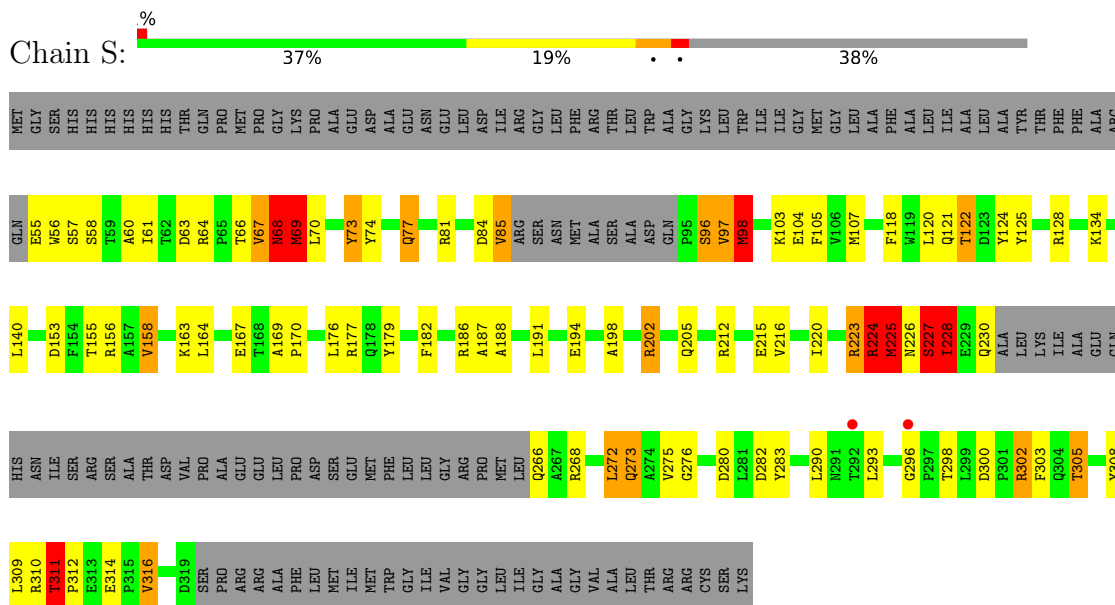


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

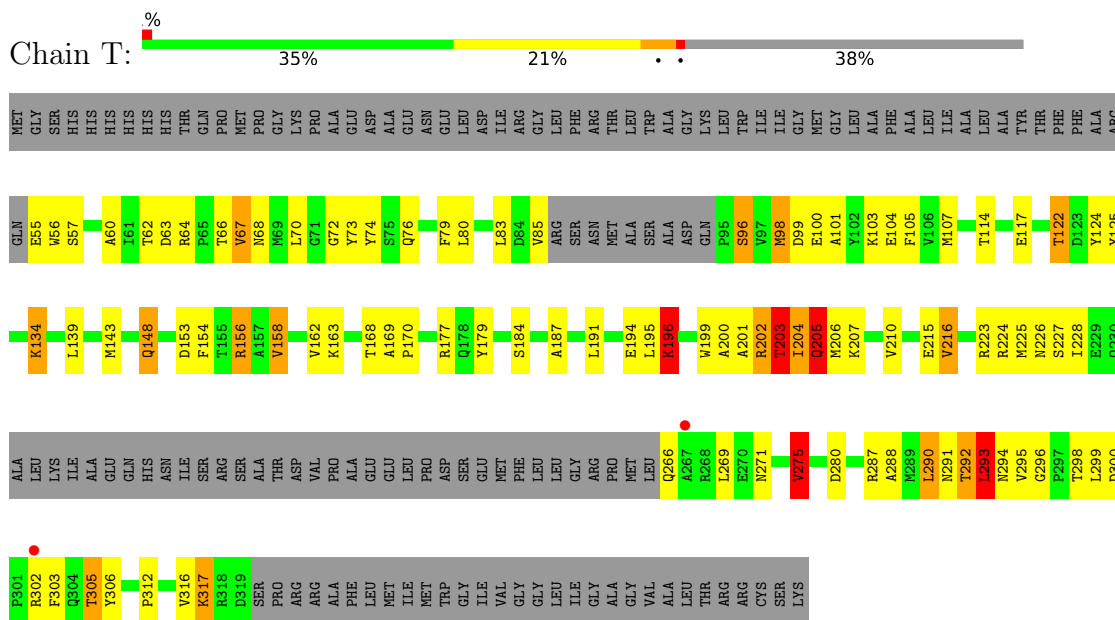




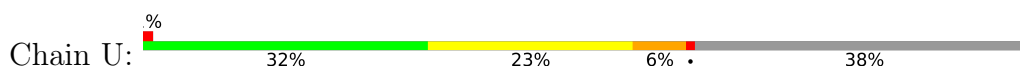
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

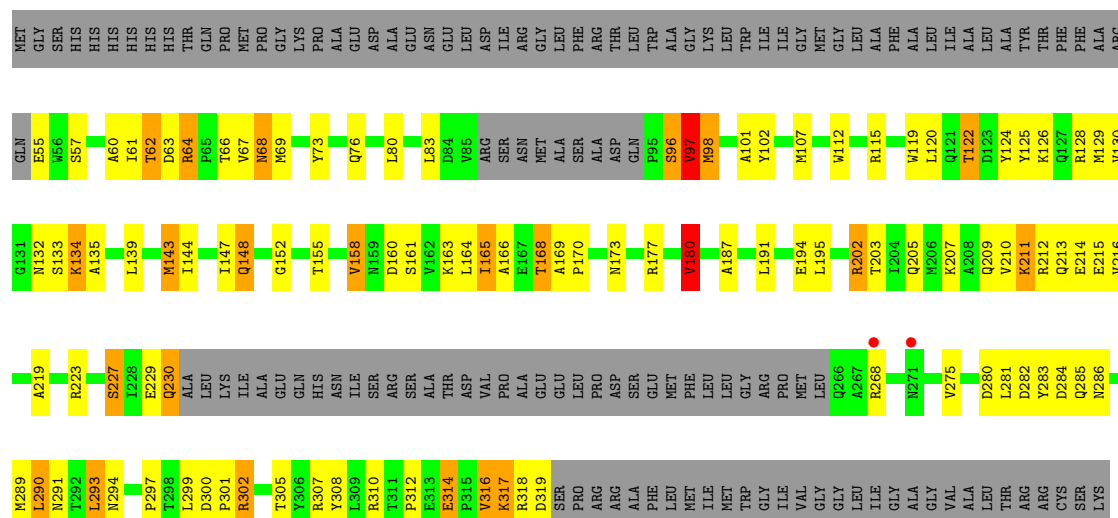


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

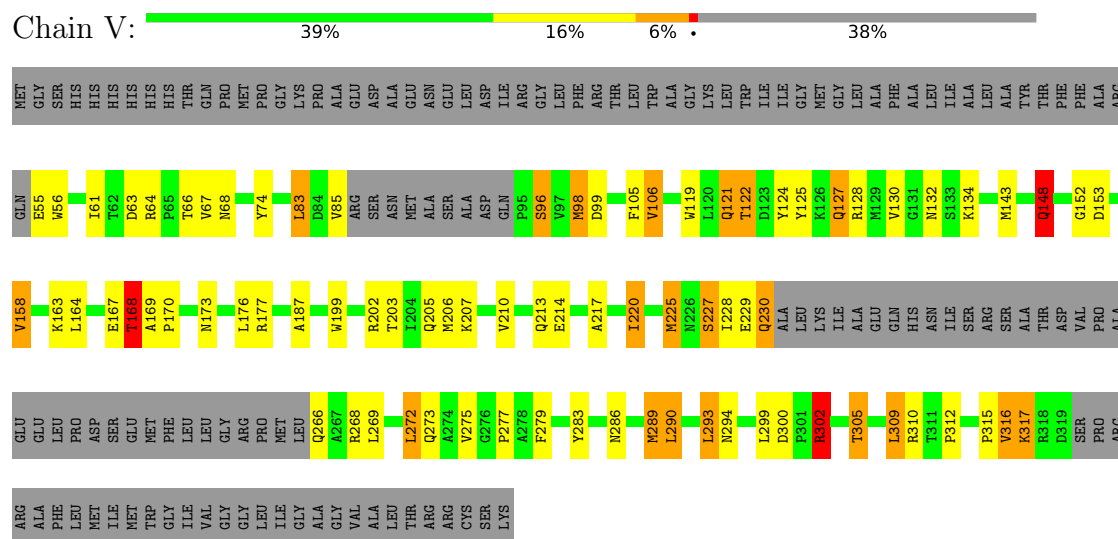


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

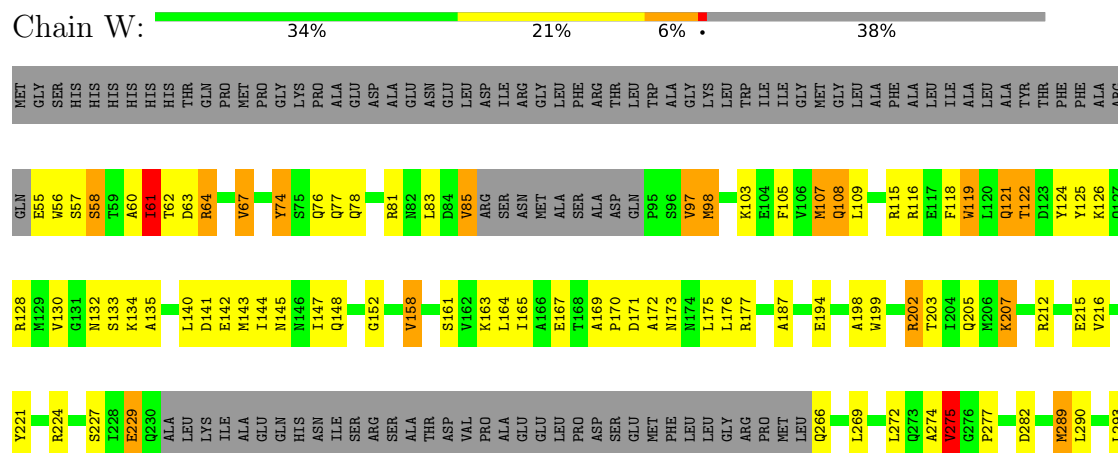


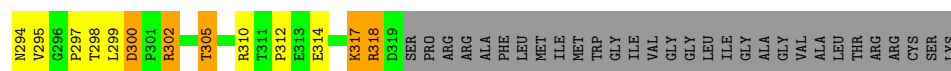


• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

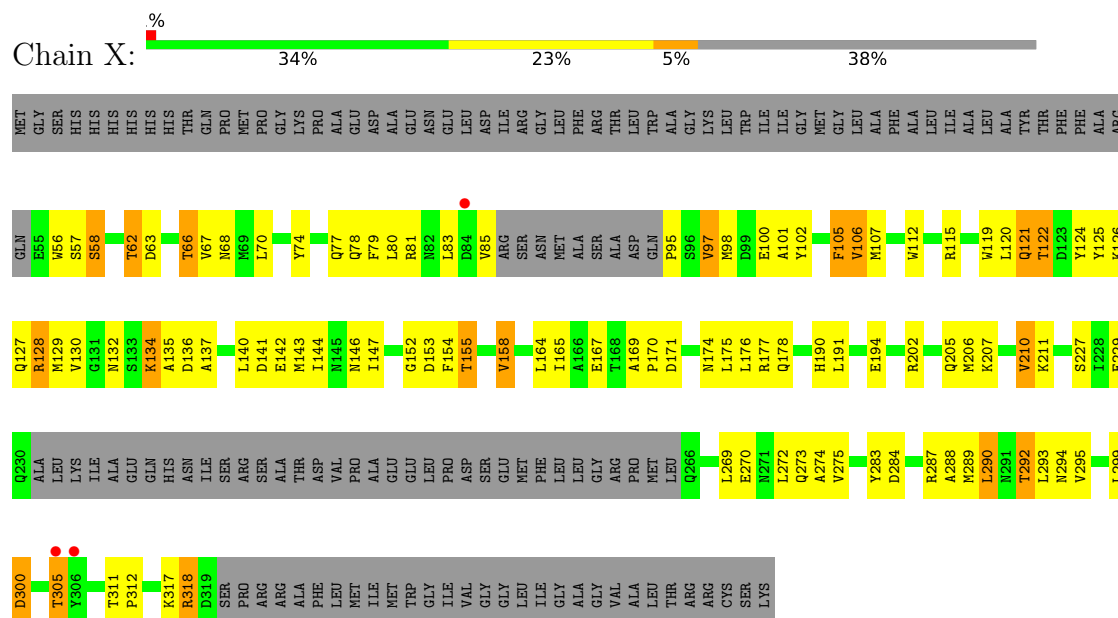


• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

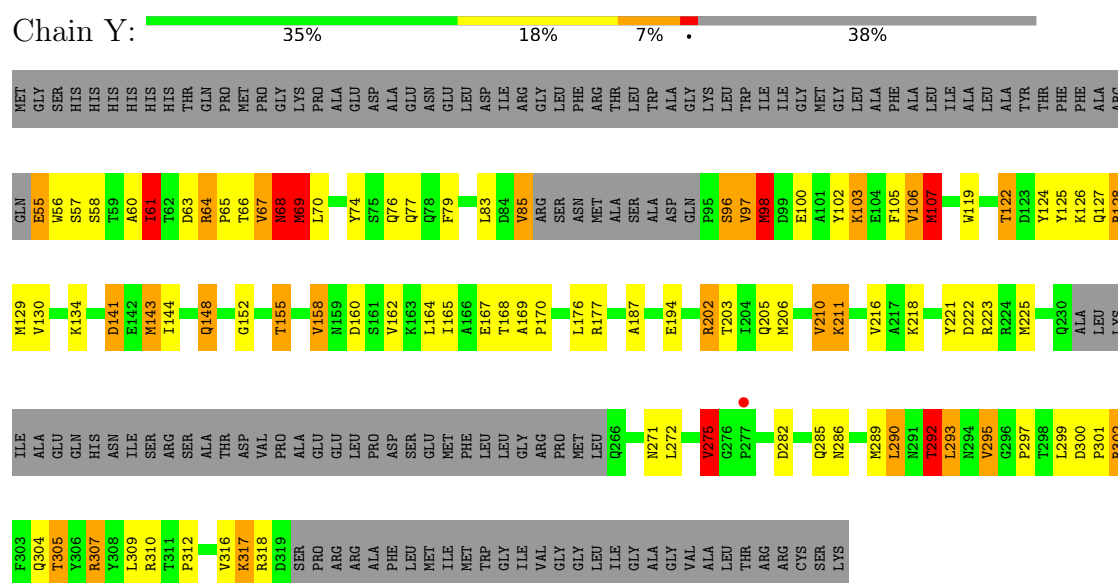




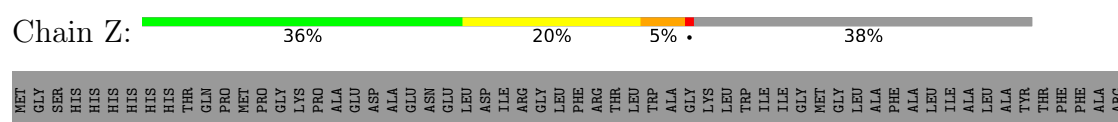
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

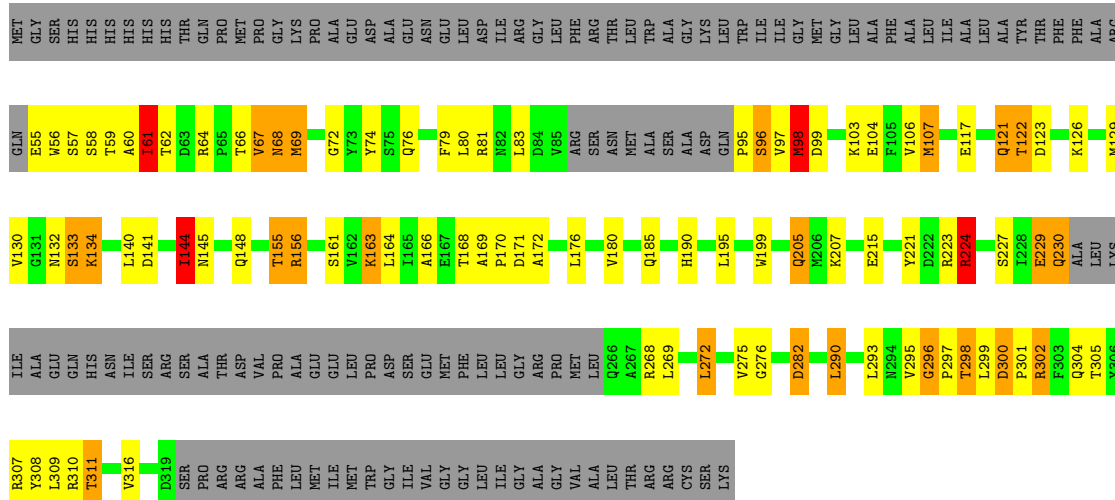


• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

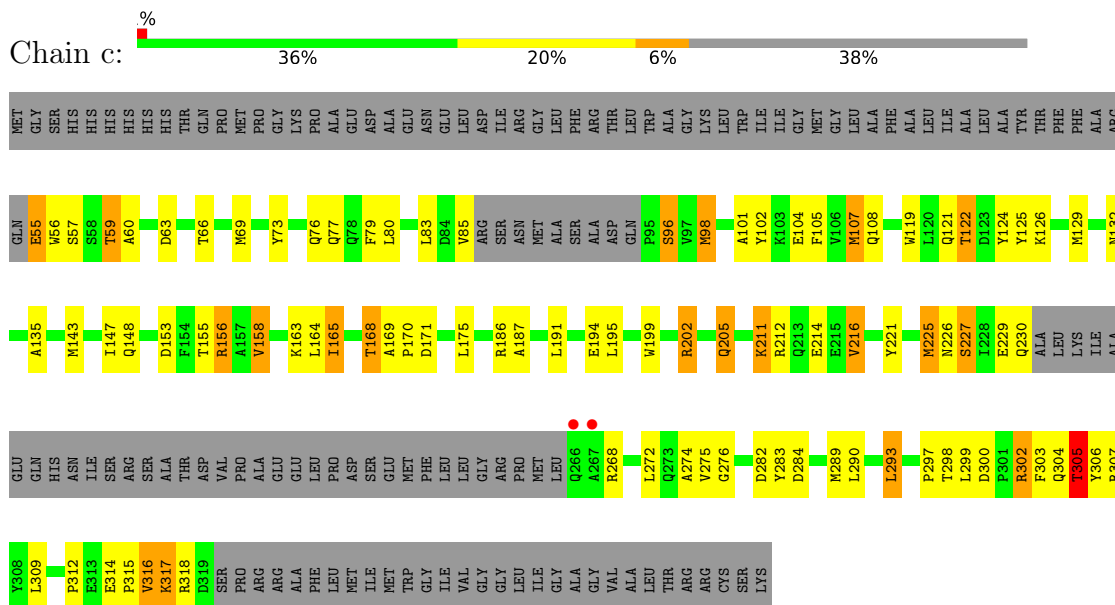


• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

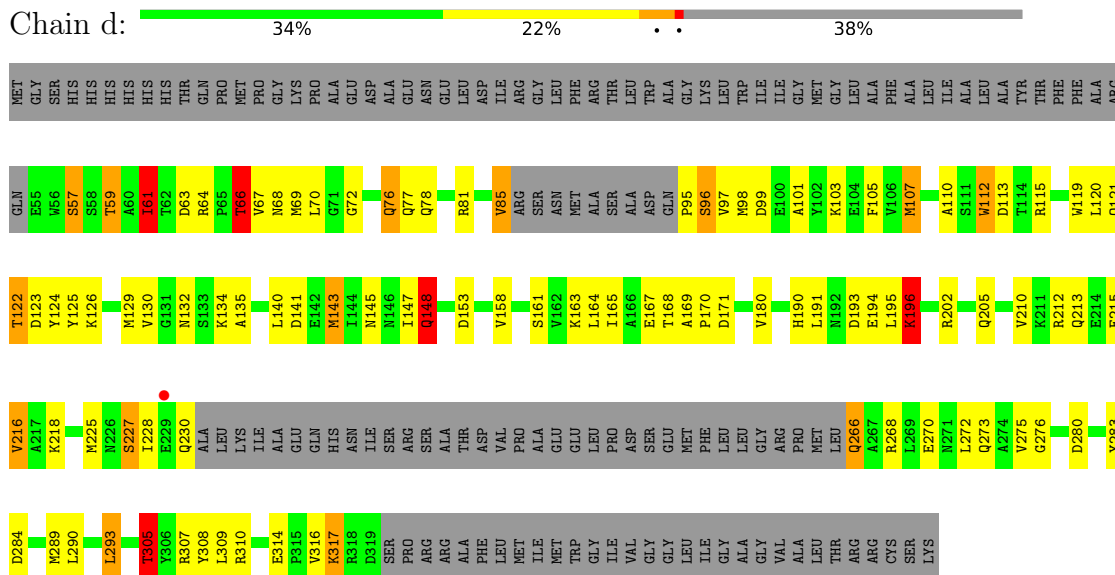




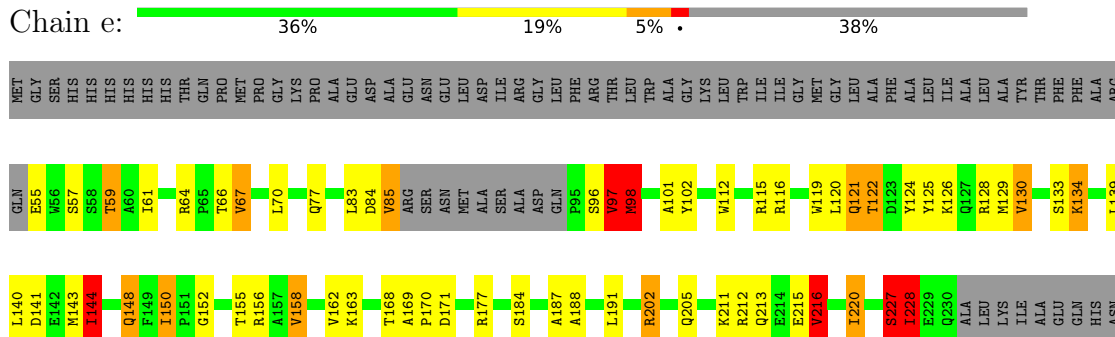
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

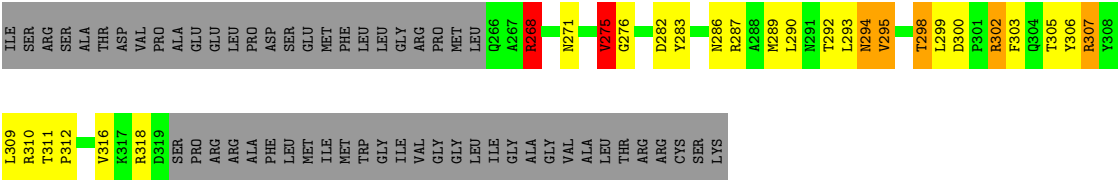


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

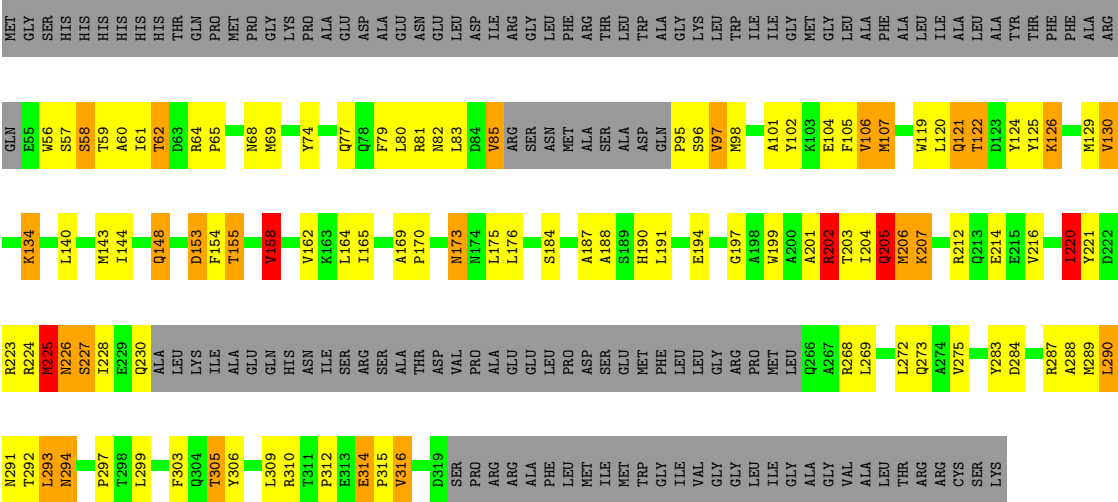
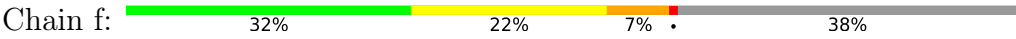


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE





• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 276.85Å 246.31Å 133.20Å<br>90.00° 89.99° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 47.81 – 5.99<br>47.81 – 5.99                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.4 (47.81-5.99)<br>96.3 (47.81-5.99)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.85 (at 6.15Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.9_1692)                            | Depositor        |
| R, $R_{free}$                                                           | 0.234 , 0.245<br>0.257 , 0.261                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2170 reflections (4.81%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 234.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.147                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.20 , 338.3                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction                                             | 0.340 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 57504                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 300.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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     | 0.67         | 1/1830 (0.1%)   | 1.37        | 20/2475 (0.8%)   |
| 1   | B     | 0.73         | 1/1830 (0.1%)   | 1.38        | 24/2475 (1.0%)   |
| 1   | C     | 0.66         | 1/1830 (0.1%)   | 1.28        | 18/2475 (0.7%)   |
| 1   | D     | 0.70         | 1/1830 (0.1%)   | 1.31        | 21/2475 (0.8%)   |
| 1   | E     | 0.80         | 1/1830 (0.1%)   | 1.41        | 28/2475 (1.1%)   |
| 1   | F     | 0.71         | 0/1830          | 1.35        | 16/2475 (0.6%)   |
| 1   | G     | 0.59         | 0/1830          | 1.34        | 22/2475 (0.9%)   |
| 1   | H     | 0.58         | 0/1830          | 1.25        | 14/2475 (0.6%)   |
| 1   | I     | 0.68         | 0/1830          | 1.36        | 29/2475 (1.2%)   |
| 1   | J     | 0.67         | 0/1830          | 1.40        | 28/2475 (1.1%)   |
| 1   | K     | 0.68         | 1/1830 (0.1%)   | 1.41        | 33/2475 (1.3%)   |
| 1   | L     | 0.70         | 0/1830          | 1.43        | 34/2475 (1.4%)   |
| 1   | M     | 0.77         | 0/1830          | 1.49        | 36/2475 (1.5%)   |
| 1   | N     | 0.75         | 2/1830 (0.1%)   | 1.52        | 25/2475 (1.0%)   |
| 1   | O     | 0.74         | 1/1830 (0.1%)   | 1.37        | 28/2475 (1.1%)   |
| 1   | P     | 0.75         | 1/1830 (0.1%)   | 1.46        | 25/2475 (1.0%)   |
| 1   | Q     | 0.66         | 0/1830          | 1.32        | 29/2475 (1.2%)   |
| 1   | R     | 0.77         | 1/1830 (0.1%)   | 1.48        | 37/2475 (1.5%)   |
| 1   | S     | 0.69         | 0/1830          | 1.41        | 28/2475 (1.1%)   |
| 1   | T     | 0.78         | 4/1830 (0.2%)   | 1.47        | 27/2475 (1.1%)   |
| 1   | U     | 0.71         | 1/1830 (0.1%)   | 1.47        | 34/2475 (1.4%)   |
| 1   | V     | 0.66         | 0/1830          | 1.37        | 23/2475 (0.9%)   |
| 1   | W     | 0.73         | 1/1830 (0.1%)   | 1.46        | 33/2475 (1.3%)   |
| 1   | X     | 0.77         | 3/1830 (0.2%)   | 1.48        | 24/2475 (1.0%)   |
| 1   | Y     | 0.75         | 1/1830 (0.1%)   | 1.51        | 38/2475 (1.5%)   |
| 1   | Z     | 0.69         | 0/1830          | 1.42        | 28/2475 (1.1%)   |
| 1   | a     | 0.76         | 1/1830 (0.1%)   | 1.45        | 29/2475 (1.2%)   |
| 1   | b     | 0.80         | 1/1830 (0.1%)   | 1.51        | 39/2475 (1.6%)   |
| 1   | c     | 0.65         | 0/1830          | 1.38        | 25/2475 (1.0%)   |
| 1   | d     | 0.66         | 1/1830 (0.1%)   | 1.44        | 26/2475 (1.1%)   |
| 1   | e     | 0.69         | 2/1830 (0.1%)   | 1.45        | 34/2475 (1.4%)   |
| 1   | f     | 0.74         | 0/1830          | 1.51        | 42/2475 (1.7%)   |
| All | All   | 0.71         | 26/58560 (0.0%) | 1.42        | 897/79200 (1.1%) |

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     | 3                   | 1                   |
| 1   | B     | 1                   | 1                   |
| 1   | F     | 2                   | 0                   |
| 1   | I     | 1                   | 1                   |
| 1   | J     | 1                   | 1                   |
| 1   | L     | 1                   | 0                   |
| 1   | M     | 3                   | 1                   |
| 1   | N     | 1                   | 0                   |
| 1   | O     | 1                   | 0                   |
| 1   | P     | 1                   | 0                   |
| 1   | Q     | 3                   | 0                   |
| 1   | R     | 2                   | 0                   |
| 1   | S     | 0                   | 1                   |
| 1   | T     | 0                   | 1                   |
| 1   | U     | 1                   | 0                   |
| 1   | V     | 0                   | 1                   |
| 1   | W     | 1                   | 1                   |
| 1   | X     | 1                   | 1                   |
| 1   | Y     | 1                   | 0                   |
| 1   | a     | 2                   | 2                   |
| 1   | b     | 1                   | 0                   |
| 1   | c     | 1                   | 0                   |
| 1   | d     | 2                   | 0                   |
| 1   | e     | 3                   | 1                   |
| All | All   | 33                  | 13                  |

All (26) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | O     | 300 | ASP  | CA-C   | 8.68  | 1.63        | 1.52     |
| 1   | X     | 66  | THR  | CB-CG2 | -7.82 | 1.26        | 1.52     |
| 1   | b     | 59  | THR  | CB-CG2 | -7.82 | 1.26        | 1.52     |
| 1   | X     | 66  | THR  | CA-CB  | -7.78 | 1.42        | 1.53     |
| 1   | E     | 189 | SER  | CA-C   | 7.35  | 1.62        | 1.52     |
| 1   | R     | 59  | THR  | CB-CG2 | -6.89 | 1.29        | 1.52     |
| 1   | N     | 142 | GLU  | CA-C   | -6.79 | 1.44        | 1.52     |
| 1   | K     | 218 | LYS  | CG-CD  | 6.72  | 1.72        | 1.52     |
| 1   | T     | 163 | LYS  | CD-CE  | 6.71  | 1.72        | 1.52     |
| 1   | d     | 305 | THR  | CB-CG2 | -6.64 | 1.30        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | T     | 163 | LYS  | CG-CD  | 6.53  | 1.72        | 1.52     |
| 1   | W     | 300 | ASP  | CA-C   | 6.13  | 1.59        | 1.52     |
| 1   | P     | 103 | LYS  | CA-C   | -6.08 | 1.45        | 1.52     |
| 1   | A     | 59  | THR  | CB-CG2 | -6.07 | 1.32        | 1.52     |
| 1   | D     | 143 | MET  | C-O    | -5.72 | 1.17        | 1.24     |
| 1   | e     | 227 | SER  | CA-C   | -5.72 | 1.44        | 1.52     |
| 1   | Y     | 130 | VAL  | CA-C   | 5.60  | 1.60        | 1.52     |
| 1   | e     | 134 | LYS  | CA-C   | -5.39 | 1.46        | 1.52     |
| 1   | T     | 163 | LYS  | CA-C   | 5.31  | 1.59        | 1.52     |
| 1   | C     | 103 | LYS  | CA-C   | 5.29  | 1.59        | 1.52     |
| 1   | X     | 274 | ALA  | CA-CB  | -5.27 | 1.46        | 1.54     |
| 1   | N     | 196 | LYS  | CA-C   | -5.17 | 1.45        | 1.52     |
| 1   | B     | 196 | LYS  | CA-C   | 5.09  | 1.59        | 1.52     |
| 1   | T     | 162 | VAL  | CA-C   | 5.07  | 1.58        | 1.52     |
| 1   | a     | 59  | THR  | CB-CG2 | -5.06 | 1.35        | 1.52     |
| 1   | U     | 207 | LYS  | CD-CE  | 5.05  | 1.67        | 1.52     |

All (897) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | d     | 61  | ILE  | CG1-CB-CG2 | -16.58 | 60.96       | 110.70   |
| 1   | A     | 67  | VAL  | CG1-CB-CG2 | -16.21 | 75.14       | 110.80   |
| 1   | N     | 67  | VAL  | CG1-CB-CG2 | -15.80 | 76.04       | 110.80   |
| 1   | U     | 275 | VAL  | CG1-CB-CG2 | -15.05 | 77.69       | 110.80   |
| 1   | T     | 275 | VAL  | CG1-CB-CG2 | -14.83 | 78.17       | 110.80   |
| 1   | N     | 216 | VAL  | CG1-CB-CG2 | -14.70 | 78.47       | 110.80   |
| 1   | Y     | 210 | VAL  | CG1-CB-CG2 | -14.41 | 79.09       | 110.80   |
| 1   | M     | 156 | ARG  | CA-CB-CG   | 14.07  | 142.25      | 114.10   |
| 1   | G     | 305 | THR  | OG1-CB-CG2 | -13.95 | 81.39       | 109.30   |
| 1   | a     | 210 | VAL  | CG1-CB-CG2 | -13.88 | 80.27       | 110.80   |
| 1   | V     | 106 | VAL  | CG1-CB-CG2 | -13.59 | 80.91       | 110.80   |
| 1   | A     | 106 | VAL  | CG1-CB-CG2 | -13.33 | 81.47       | 110.80   |
| 1   | I     | 311 | THR  | OG1-CB-CG2 | -13.26 | 82.77       | 109.30   |
| 1   | P     | 165 | ILE  | CG1-CB-CG2 | -13.15 | 71.26       | 110.70   |
| 1   | b     | 300 | ASP  | CA-C-N     | -13.14 | 105.76      | 121.00   |
| 1   | b     | 300 | ASP  | C-N-CA     | -13.14 | 105.76      | 121.00   |
| 1   | C     | 97  | VAL  | CG1-CB-CG2 | -13.05 | 82.09       | 110.80   |
| 1   | U     | 97  | VAL  | CG1-CB-CG2 | -12.82 | 82.60       | 110.80   |
| 1   | B     | 122 | THR  | OG1-CB-CG2 | -12.64 | 84.01       | 109.30   |
| 1   | Y     | 295 | VAL  | CG1-CB-CG2 | -12.63 | 83.01       | 110.80   |
| 1   | E     | 298 | THR  | OG1-CB-CG2 | -12.60 | 84.10       | 109.30   |
| 1   | C     | 114 | THR  | OG1-CB-CG2 | -12.48 | 84.34       | 109.30   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | R     | 97  | VAL  | CG1-CB-CG2 | -12.41 | 83.49       | 110.80   |
| 1   | J     | 300 | ASP  | CB-CA-C    | -12.28 | 98.01       | 110.17   |
| 1   | Q     | 97  | VAL  | CG1-CB-CG2 | -12.27 | 83.82       | 110.80   |
| 1   | T     | 226 | ASN  | N-CA-C     | -12.23 | 98.03       | 111.36   |
| 1   | L     | 122 | THR  | OG1-CB-CG2 | -12.02 | 85.26       | 109.30   |
| 1   | Y     | 103 | LYS  | CB-CA-C    | -11.97 | 90.92       | 110.79   |
| 1   | F     | 216 | VAL  | CG1-CB-CG2 | -11.95 | 84.50       | 110.80   |
| 1   | e     | 97  | VAL  | N-CA-C     | 11.89  | 122.73      | 110.72   |
| 1   | A     | 216 | VAL  | CG1-CB-CG2 | -11.86 | 84.71       | 110.80   |
| 1   | I     | 67  | VAL  | N-CA-C     | 11.76  | 121.71      | 110.42   |
| 1   | J     | 205 | GLN  | CA-CB-CG   | 11.76  | 137.61      | 114.10   |
| 1   | E     | 106 | VAL  | N-CA-CB    | 11.75  | 124.30      | 110.55   |
| 1   | G     | 106 | VAL  | CG1-CB-CG2 | -11.68 | 85.10       | 110.80   |
| 1   | a     | 103 | LYS  | CB-CA-C    | -11.61 | 92.65       | 110.88   |
| 1   | Y     | 128 | ARG  | NE-CZ-NH1  | -11.56 | 109.94      | 121.50   |
| 1   | J     | 316 | VAL  | CG1-CB-CG2 | -11.56 | 85.38       | 110.80   |
| 1   | H     | 158 | VAL  | CG1-CB-CG2 | -11.42 | 85.68       | 110.80   |
| 1   | e     | 316 | VAL  | CG1-CB-CG2 | -11.41 | 85.70       | 110.80   |
| 1   | T     | 216 | VAL  | CG1-CB-CG2 | -11.37 | 85.79       | 110.80   |
| 1   | I     | 66  | THR  | OG1-CB-CG2 | -11.29 | 86.71       | 109.30   |
| 1   | W     | 300 | ASP  | CB-CA-C    | 11.18  | 121.23      | 110.17   |
| 1   | e     | 216 | VAL  | CG1-CB-CG2 | -11.14 | 86.29       | 110.80   |
| 1   | Z     | 150 | ILE  | CA-C-N     | -11.03 | 108.73      | 119.76   |
| 1   | Z     | 150 | ILE  | C-N-CA     | -11.03 | 108.73      | 119.76   |
| 1   | N     | 130 | VAL  | CG1-CB-CG2 | -11.01 | 86.57       | 110.80   |
| 1   | Q     | 97  | VAL  | N-CA-C     | 11.01  | 121.84      | 110.72   |
| 1   | Y     | 275 | VAL  | CG1-CB-CG2 | -11.00 | 86.60       | 110.80   |
| 1   | I     | 317 | LYS  | CB-CA-C    | -10.99 | 86.41       | 109.38   |
| 1   | c     | 156 | ARG  | CA-CB-CG   | 10.98  | 136.06      | 114.10   |
| 1   | O     | 298 | THR  | OG1-CB-CG2 | -10.93 | 87.44       | 109.30   |
| 1   | d     | 122 | THR  | OG1-CB-CG2 | -10.89 | 87.53       | 109.30   |
| 1   | R     | 97  | VAL  | N-CA-C     | 10.87  | 121.70      | 110.72   |
| 1   | b     | 97  | VAL  | CG1-CB-CG2 | -10.85 | 86.92       | 110.80   |
| 1   | K     | 211 | LYS  | CB-CA-C    | -10.83 | 93.88       | 110.88   |
| 1   | A     | 150 | ILE  | CG1-CB-CG2 | -10.72 | 78.53       | 110.70   |
| 1   | W     | 61  | ILE  | CG1-CB-CG2 | -10.72 | 78.53       | 110.70   |
| 1   | W     | 298 | THR  | OG1-CB-CG2 | -10.71 | 87.88       | 109.30   |
| 1   | Z     | 150 | ILE  | CG1-CB-CG2 | -10.68 | 78.65       | 110.70   |
| 1   | R     | 216 | VAL  | CG1-CB-CG2 | -10.66 | 87.34       | 110.80   |
| 1   | D     | 275 | VAL  | CG1-CB-CG2 | -10.64 | 87.39       | 110.80   |
| 1   | e     | 134 | LYS  | N-CA-C     | 10.49  | 122.29      | 111.07   |
| 1   | W     | 295 | VAL  | CG1-CB-CG2 | -10.40 | 87.92       | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | K     | 155 | THR  | OG1-CB-CG2 | -10.39 | 88.53       | 109.30   |
| 1   | b     | 61  | ILE  | CG1-CB-CG2 | -10.29 | 79.82       | 110.70   |
| 1   | P     | 316 | VAL  | CG1-CB-CG2 | -10.25 | 88.26       | 110.80   |
| 1   | U     | 107 | MET  | CB-CG-SD   | -10.20 | 82.11       | 112.70   |
| 1   | a     | 272 | LEU  | CB-CA-C    | -10.18 | 93.55       | 110.85   |
| 1   | f     | 207 | LYS  | CA-CB-CG   | 10.17  | 134.44      | 114.10   |
| 1   | M     | 156 | ARG  | CB-CG-CD   | 10.13  | 134.60      | 111.30   |
| 1   | X     | 106 | VAL  | CG1-CB-CG2 | -10.09 | 88.61       | 110.80   |
| 1   | O     | 300 | ASP  | CB-CA-C    | 10.08  | 120.15      | 110.17   |
| 1   | V     | 127 | GLN  | CA-CB-CG   | 10.06  | 134.23      | 114.10   |
| 1   | O     | 296 | GLY  | CA-C-N     | 10.03  | 130.14      | 120.31   |
| 1   | O     | 296 | GLY  | C-N-CA     | 10.03  | 130.14      | 120.31   |
| 1   | B     | 85  | VAL  | CG1-CB-CG2 | -10.01 | 88.78       | 110.80   |
| 1   | D     | 202 | ARG  | CB-CG-CD   | 9.99   | 134.29      | 111.30   |
| 1   | P     | 61  | ILE  | CG1-CB-CG2 | -9.95  | 80.86       | 110.70   |
| 1   | M     | 229 | GLU  | N-CA-C     | 9.91   | 123.01      | 111.11   |
| 1   | X     | 130 | VAL  | N-CA-C     | -9.86  | 103.43      | 112.90   |
| 1   | T     | 122 | THR  | OG1-CB-CG2 | -9.84  | 89.63       | 109.30   |
| 1   | D     | 158 | VAL  | CG1-CB-CG2 | -9.83  | 89.17       | 110.80   |
| 1   | H     | 292 | THR  | OG1-CB-CG2 | -9.83  | 89.64       | 109.30   |
| 1   | Y     | 67  | VAL  | CG1-CB-CG2 | -9.83  | 89.18       | 110.80   |
| 1   | U     | 67  | VAL  | N-CA-C     | 9.82   | 119.85      | 110.42   |
| 1   | X     | 66  | THR  | OG1-CB-CG2 | -9.73  | 89.84       | 109.30   |
| 1   | W     | 58  | SER  | N-CA-C     | -9.61  | 94.67       | 109.95   |
| 1   | R     | 154 | PHE  | N-CA-C     | 9.61   | 124.26      | 112.54   |
| 1   | T     | 210 | VAL  | CG1-CB-CG2 | -9.57  | 89.75       | 110.80   |
| 1   | W     | 207 | LYS  | CA-CB-CG   | 9.55   | 133.21      | 114.10   |
| 1   | G     | 220 | ILE  | CG1-CB-CG2 | -9.52  | 82.14       | 110.70   |
| 1   | N     | 129 | MET  | CA-CB-CG   | 9.51   | 133.12      | 114.10   |
| 1   | N     | 156 | ARG  | CA-CB-CG   | 9.51   | 133.12      | 114.10   |
| 1   | L     | 153 | ASP  | N-CA-C     | -9.49  | 91.38       | 107.80   |
| 1   | e     | 268 | ARG  | CA-CB-CG   | -9.44  | 95.22       | 114.10   |
| 1   | a     | 298 | THR  | OG1-CB-CG2 | -9.43  | 90.44       | 109.30   |
| 1   | D     | 168 | THR  | OG1-CB-CG2 | -9.35  | 90.60       | 109.30   |
| 1   | X     | 210 | VAL  | CG1-CB-CG2 | -9.35  | 90.23       | 110.80   |
| 1   | X     | 62  | THR  | OG1-CB-CG2 | -9.30  | 90.70       | 109.30   |
| 1   | Z     | 226 | ASN  | N-CA-C     | -9.22  | 101.31      | 111.36   |
| 1   | R     | 98  | MET  | CB-CG-SD   | 9.16   | 140.19      | 112.70   |
| 1   | f     | 158 | VAL  | CG1-CB-CG2 | -9.13  | 90.72       | 110.80   |
| 1   | b     | 282 | ASP  | CB-CA-C    | -9.12  | 93.76       | 110.63   |
| 1   | f     | 205 | GLN  | CA-CB-CG   | 9.09   | 132.28      | 114.10   |
| 1   | S     | 227 | SER  | CB-CA-C    | -9.08  | 93.23       | 110.67   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | U     | 62  | THR  | OG1-CB-CG2 | -9.07 | 91.15       | 109.30   |
| 1   | f     | 97  | VAL  | N-CA-C     | 9.05  | 119.86      | 110.72   |
| 1   | b     | 230 | GLN  | CA-CB-CG   | 9.04  | 132.17      | 114.10   |
| 1   | Q     | 317 | LYS  | CA-CB-CG   | 9.01  | 132.13      | 114.10   |
| 1   | c     | 156 | ARG  | N-CA-CB    | -8.98 | 95.76       | 110.40   |
| 1   | B     | 62  | THR  | N-CA-C     | 8.98  | 123.06      | 109.41   |
| 1   | c     | 158 | VAL  | CG1-CB-CG2 | -8.95 | 91.11       | 110.80   |
| 1   | U     | 130 | VAL  | N-CA-C     | -8.93 | 104.32      | 112.90   |
| 1   | E     | 61  | ILE  | CG1-CB-CG2 | -8.93 | 83.92       | 110.70   |
| 1   | a     | 163 | LYS  | CB-CG-CD   | -8.91 | 90.80       | 111.30   |
| 1   | e     | 215 | GLU  | CA-CB-CG   | -8.91 | 96.27       | 114.10   |
| 1   | F     | 144 | ILE  | CG1-CB-CG2 | -8.81 | 84.28       | 110.70   |
| 1   | V     | 220 | ILE  | CG1-CB-CG2 | -8.79 | 84.32       | 110.70   |
| 1   | I     | 205 | GLN  | CB-CA-C    | -8.79 | 97.09       | 110.88   |
| 1   | T     | 163 | LYS  | CA-CB-CG   | 8.78  | 131.66      | 114.10   |
| 1   | H     | 130 | VAL  | CG1-CB-CG2 | -8.77 | 91.50       | 110.80   |
| 1   | D     | 211 | LYS  | CB-CG-CD   | -8.77 | 91.13       | 111.30   |
| 1   | E     | 189 | SER  | CB-CA-C    | 8.77  | 125.34      | 110.79   |
| 1   | F     | 295 | VAL  | N-CA-C     | 8.74  | 120.59      | 110.62   |
| 1   | S     | 68  | ASN  | N-CA-C     | -8.72 | 101.70      | 111.82   |
| 1   | I     | 317 | LYS  | CA-CB-CG   | 8.71  | 131.51      | 114.10   |
| 1   | f     | 153 | ASP  | N-CA-C     | -8.68 | 92.78       | 107.80   |
| 1   | U     | 317 | LYS  | CA-CB-CG   | 8.67  | 131.45      | 114.10   |
| 1   | V     | 289 | MET  | CB-CA-C    | -8.64 | 94.09       | 110.67   |
| 1   | X     | 97  | VAL  | N-CA-C     | 8.63  | 119.44      | 110.72   |
| 1   | U     | 107 | MET  | CB-CA-C    | 8.61  | 124.40      | 110.88   |
| 1   | O     | 122 | THR  | OG1-CB-CG2 | -8.61 | 92.08       | 109.30   |
| 1   | f     | 97  | VAL  | CG1-CB-CG2 | -8.60 | 91.88       | 110.80   |
| 1   | S     | 298 | THR  | OG1-CB-CG2 | -8.59 | 92.11       | 109.30   |
| 1   | S     | 220 | ILE  | CB-CA-C    | -8.56 | 100.59      | 112.14   |
| 1   | R     | 211 | LYS  | CB-CA-C    | 8.53  | 124.28      | 110.88   |
| 1   | S     | 228 | ILE  | CG1-CB-CG2 | -8.53 | 85.12       | 110.70   |
| 1   | M     | 289 | MET  | CB-CG-SD   | -8.52 | 87.13       | 112.70   |
| 1   | G     | 97  | VAL  | N-CA-C     | 8.51  | 120.32      | 110.62   |
| 1   | b     | 268 | ARG  | CB-CG-CD   | 8.46  | 130.76      | 111.30   |
| 1   | K     | 85  | VAL  | CG1-CB-CG2 | -8.43 | 92.25       | 110.80   |
| 1   | K     | 211 | LYS  | CG-CD-CE   | 8.43  | 130.69      | 111.30   |
| 1   | X     | 202 | ARG  | CB-CG-CD   | 8.41  | 130.64      | 111.30   |
| 1   | L     | 66  | THR  | OG1-CB-CG2 | -8.39 | 92.52       | 109.30   |
| 1   | A     | 98  | MET  | CA-CB-CG   | 8.39  | 130.88      | 114.10   |
| 1   | B     | 67  | VAL  | CG1-CB-CG2 | -8.36 | 92.41       | 110.80   |
| 1   | a     | 163 | LYS  | CA-CB-CG   | 8.34  | 130.78      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 211 | LYS  | CB-CG-CD   | 8.33  | 130.45      | 111.30   |
| 1   | G     | 121 | GLN  | N-CA-C     | -8.31 | 102.17      | 113.30   |
| 1   | X     | 229 | GLU  | N-CA-C     | 8.28  | 119.93      | 111.07   |
| 1   | R     | 130 | VAL  | CG1-CB-CG2 | -8.27 | 92.60       | 110.80   |
| 1   | T     | 205 | GLN  | CA-CB-CG   | 8.27  | 130.65      | 114.10   |
| 1   | Y     | 107 | MET  | CA-CB-CG   | 8.20  | 130.50      | 114.10   |
| 1   | c     | 225 | MET  | CG-SD-CE   | -8.16 | 82.94       | 100.90   |
| 1   | Z     | 317 | LYS  | CB-CA-C    | 8.15  | 126.42      | 109.38   |
| 1   | G     | 148 | GLN  | N-CA-CB    | -8.15 | 97.98       | 110.77   |
| 1   | C     | 316 | VAL  | CG1-CB-CG2 | -8.15 | 92.88       | 110.80   |
| 1   | a     | 272 | LEU  | CA-CB-CG   | 8.14  | 144.78      | 116.30   |
| 1   | B     | 61  | ILE  | CG1-CB-CG2 | -8.14 | 86.29       | 110.70   |
| 1   | b     | 316 | VAL  | CG1-CB-CG2 | -8.12 | 92.93       | 110.80   |
| 1   | L     | 295 | VAL  | N-CA-C     | 8.11  | 118.89      | 110.62   |
| 1   | S     | 69  | MET  | CB-CA-C    | -8.10 | 95.65       | 110.63   |
| 1   | b     | 298 | THR  | OG1-CB-CG2 | -8.09 | 93.13       | 109.30   |
| 1   | c     | 216 | VAL  | CG1-CB-CG2 | -8.06 | 93.06       | 110.80   |
| 1   | E     | 106 | VAL  | CB-CA-C    | -8.06 | 101.66      | 111.97   |
| 1   | J     | 300 | ASP  | CA-C-N     | -8.05 | 109.78      | 119.84   |
| 1   | J     | 300 | ASP  | C-N-CA     | -8.05 | 109.78      | 119.84   |
| 1   | c     | 317 | LYS  | CB-CG-CD   | 8.05  | 129.81      | 111.30   |
| 1   | L     | 211 | LYS  | CG-CD-CE   | 8.03  | 129.76      | 111.30   |
| 1   | I     | 107 | MET  | CB-CA-C    | 8.02  | 123.47      | 110.88   |
| 1   | X     | 142 | GLU  | CB-CA-C    | -8.02 | 97.48       | 110.79   |
| 1   | M     | 309 | LEU  | N-CA-C     | -8.01 | 103.64      | 113.41   |
| 1   | c     | 168 | THR  | OG1-CB-CG2 | -7.98 | 93.33       | 109.30   |
| 1   | Z     | 205 | GLN  | CB-CA-C    | 7.97  | 123.40      | 110.88   |
| 1   | b     | 103 | LYS  | CB-CG-CD   | 7.97  | 129.63      | 111.30   |
| 1   | B     | 130 | VAL  | N-CA-C     | -7.97 | 105.37      | 113.10   |
| 1   | Z     | 272 | LEU  | N-CA-C     | -7.96 | 102.69      | 111.36   |
| 1   | J     | 153 | ASP  | N-CA-C     | -7.95 | 93.79       | 107.61   |
| 1   | f     | 126 | LYS  | N-CA-C     | 7.94  | 119.93      | 111.28   |
| 1   | X     | 62  | THR  | N-CA-C     | 7.91  | 122.35      | 109.85   |
| 1   | d     | 66  | THR  | OG1-CB-CG2 | -7.90 | 93.50       | 109.30   |
| 1   | K     | 225 | MET  | CA-CB-CG   | 7.88  | 129.87      | 114.10   |
| 1   | U     | 133 | SER  | N-CA-C     | -7.88 | 102.77      | 111.36   |
| 1   | A     | 147 | ILE  | CG1-CB-CG2 | -7.87 | 87.08       | 110.70   |
| 1   | Y     | 97  | VAL  | CB-CA-C    | -7.86 | 101.37      | 112.22   |
| 1   | P     | 309 | LEU  | N-CA-C     | -7.85 | 103.83      | 113.41   |
| 1   | E     | 266 | GLN  | N-CA-C     | -7.83 | 89.07       | 111.00   |
| 1   | T     | 163 | LYS  | CB-CG-CD   | -7.81 | 93.34       | 111.30   |
| 1   | K     | 225 | MET  | CB-CG-SD   | 7.77  | 136.02      | 112.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | O     | 309 | LEU  | N-CA-C     | -7.77 | 103.93      | 113.41   |
| 1   | Z     | 153 | ASP  | CB-CA-C    | 7.77  | 121.59      | 110.79   |
| 1   | b     | 123 | ASP  | N-CA-C     | 7.75  | 119.73      | 111.28   |
| 1   | e     | 228 | ILE  | CG1-CB-CG2 | -7.75 | 87.45       | 110.70   |
| 1   | M     | 226 | ASN  | N-CA-C     | -7.72 | 102.94      | 111.36   |
| 1   | R     | 58  | SER  | N-CA-C     | -7.72 | 97.67       | 109.95   |
| 1   | M     | 300 | ASP  | CA-C-N     | -7.70 | 112.07      | 121.00   |
| 1   | M     | 300 | ASP  | C-N-CA     | -7.70 | 112.07      | 121.00   |
| 1   | f     | 316 | VAL  | CG1-CB-CG2 | -7.69 | 93.88       | 110.80   |
| 1   | P     | 225 | MET  | CA-CB-CG   | -7.65 | 98.79       | 114.10   |
| 1   | c     | 298 | THR  | OG1-CB-CG2 | -7.65 | 94.01       | 109.30   |
| 1   | X     | 107 | MET  | CB-CG-SD   | -7.64 | 89.78       | 112.70   |
| 1   | Z     | 143 | MET  | CA-CB-CG   | 7.64  | 129.37      | 114.10   |
| 1   | c     | 316 | VAL  | CG1-CB-CG2 | -7.62 | 94.03       | 110.80   |
| 1   | a     | 163 | LYS  | N-CA-CB    | 7.61  | 124.08      | 111.08   |
| 1   | T     | 153 | ASP  | N-CA-C     | -7.58 | 94.68       | 107.80   |
| 1   | W     | 305 | THR  | N-CA-C     | -7.57 | 101.75      | 113.02   |
| 1   | A     | 98  | MET  | CB-CG-SD   | 7.54  | 135.32      | 112.70   |
| 1   | Z     | 296 | GLY  | CA-C-N     | -7.54 | 112.92      | 120.31   |
| 1   | Z     | 296 | GLY  | C-N-CA     | -7.54 | 112.92      | 120.31   |
| 1   | V     | 163 | LYS  | N-CA-CB    | 7.53  | 123.96      | 111.08   |
| 1   | J     | 216 | VAL  | CG1-CB-CG2 | -7.53 | 94.24       | 110.80   |
| 1   | f     | 305 | THR  | OG1-CB-CG2 | -7.53 | 94.25       | 109.30   |
| 1   | W     | 207 | LYS  | CB-CA-C    | -7.53 | 98.30       | 110.79   |
| 1   | V     | 302 | ARG  | CA-CB-CG   | 7.52  | 129.15      | 114.10   |
| 1   | Y     | 97  | VAL  | CG1-CB-CG2 | -7.51 | 94.28       | 110.80   |
| 1   | R     | 74  | TYR  | N-CA-C     | 7.51  | 120.18      | 111.02   |
| 1   | N     | 317 | LYS  | CB-CG-CD   | 7.50  | 128.56      | 111.30   |
| 1   | D     | 204 | ILE  | CG1-CB-CG2 | -7.47 | 88.28       | 110.70   |
| 1   | C     | 144 | ILE  | N-CA-C     | 7.47  | 117.59      | 110.42   |
| 1   | F     | 229 | GLU  | N-CA-C     | 7.46  | 120.36      | 111.33   |
| 1   | I     | 162 | VAL  | N-CA-C     | 7.46  | 119.22      | 108.48   |
| 1   | V     | 229 | GLU  | N-CA-C     | 7.46  | 120.06      | 111.11   |
| 1   | P     | 85  | VAL  | CB-CA-C    | -7.45 | 97.25       | 111.40   |
| 1   | d     | 216 | VAL  | N-CA-C     | -7.44 | 103.27      | 110.42   |
| 1   | M     | 268 | ARG  | CB-CG-CD   | -7.43 | 94.20       | 111.30   |
| 1   | b     | 156 | ARG  | N-CA-C     | -7.43 | 104.19      | 113.18   |
| 1   | T     | 156 | ARG  | CB-CG-CD   | -7.42 | 94.23       | 111.30   |
| 1   | d     | 153 | ASP  | N-CA-C     | -7.42 | 94.97       | 107.80   |
| 1   | f     | 62  | THR  | OG1-CB-CG2 | -7.42 | 94.46       | 109.30   |
| 1   | c     | 156 | ARG  | CB-CA-C    | 7.41  | 125.48      | 109.99   |
| 1   | Q     | 155 | THR  | OG1-CB-CG2 | -7.40 | 94.50       | 109.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | R     | 153 | ASP  | N-CA-C     | -7.40 | 94.74       | 107.61   |
| 1   | B     | 207 | LYS  | N-CA-CB    | 7.39  | 120.99      | 110.12   |
| 1   | O     | 144 | ILE  | CB-CA-C    | 7.37  | 122.09      | 112.14   |
| 1   | J     | 218 | LYS  | CB-CG-CD   | 7.35  | 128.21      | 111.30   |
| 1   | d     | 103 | LYS  | CB-CA-C    | -7.31 | 98.65       | 110.79   |
| 1   | Z     | 143 | MET  | N-CA-CB    | 7.29  | 121.58      | 110.28   |
| 1   | e     | 134 | LYS  | CB-CG-CD   | 7.28  | 128.05      | 111.30   |
| 1   | J     | 154 | PHE  | N-CA-C     | 7.27  | 121.98      | 113.18   |
| 1   | P     | 153 | ASP  | N-CA-C     | -7.27 | 95.23       | 107.80   |
| 1   | d     | 317 | LYS  | CG-CD-CE   | -7.26 | 94.59       | 111.30   |
| 1   | W     | 62  | THR  | N-CA-C     | 7.26  | 121.32      | 109.85   |
| 1   | f     | 107 | MET  | N-CA-CB    | 7.24  | 120.51      | 110.01   |
| 1   | e     | 67  | VAL  | N-CA-C     | 7.23  | 117.36      | 110.42   |
| 1   | D     | 143 | MET  | N-CA-C     | -7.22 | 103.34      | 111.07   |
| 1   | H     | 155 | THR  | N-CA-C     | -7.21 | 104.29      | 113.23   |
| 1   | Y     | 128 | ARG  | NE-CZ-NH2  | 7.20  | 125.68      | 119.20   |
| 1   | N     | 161 | SER  | N-CA-C     | 7.18  | 121.03      | 108.75   |
| 1   | f     | 106 | VAL  | N-CA-C     | 7.18  | 117.90      | 110.36   |
| 1   | R     | 69  | MET  | CB-CG-SD   | -7.17 | 91.18       | 112.70   |
| 1   | Y     | 127 | GLN  | N-CA-C     | -7.16 | 103.80      | 112.54   |
| 1   | O     | 301 | PRO  | N-CA-C     | 7.16  | 123.44      | 114.92   |
| 1   | N     | 142 | GLU  | CB-CA-C    | -7.14 | 98.94       | 110.79   |
| 1   | Y     | 130 | VAL  | N-CA-CB    | -7.13 | 103.06      | 112.26   |
| 1   | G     | 287 | ARG  | CA-CB-CG   | -7.13 | 99.85       | 114.10   |
| 1   | A     | 309 | LEU  | N-CA-C     | -7.10 | 104.75      | 113.41   |
| 1   | X     | 300 | ASP  | CB-CA-C    | -7.10 | 103.14      | 110.17   |
| 1   | N     | 69  | MET  | CB-CG-SD   | 7.08  | 133.93      | 112.70   |
| 1   | d     | 103 | LYS  | N-CA-CB    | 7.07  | 120.51      | 110.12   |
| 1   | b     | 205 | GLN  | CA-CB-CG   | 7.06  | 128.23      | 114.10   |
| 1   | N     | 196 | LYS  | CG-CD-CE   | -7.06 | 95.07       | 111.30   |
| 1   | J     | 218 | LYS  | CG-CD-CE   | -7.05 | 95.08       | 111.30   |
| 1   | M     | 143 | MET  | N-CA-CB    | -7.05 | 99.72       | 110.16   |
| 1   | C     | 196 | LYS  | CB-CG-CD   | -7.04 | 95.10       | 111.30   |
| 1   | f     | 314 | GLU  | CA-C-N     | -7.04 | 112.53      | 119.78   |
| 1   | f     | 314 | GLU  | C-N-CA     | -7.04 | 112.53      | 119.78   |
| 1   | N     | 106 | VAL  | CG1-CB-CG2 | -7.04 | 95.32       | 110.80   |
| 1   | V     | 163 | LYS  | CA-CB-CG   | 7.04  | 128.18      | 114.10   |
| 1   | K     | 121 | GLN  | N-CA-C     | -7.03 | 103.81      | 112.88   |
| 1   | a     | 163 | LYS  | CB-CA-C    | -7.03 | 95.49       | 109.33   |
| 1   | P     | 98  | MET  | CA-CB-CG   | 7.02  | 128.15      | 114.10   |
| 1   | W     | 67  | VAL  | CG1-CB-CG2 | -7.02 | 95.35       | 110.80   |
| 1   | A     | 155 | THR  | N-CA-C     | -7.02 | 103.63      | 111.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | b     | 62  | THR  | N-CA-C     | 7.01  | 120.93      | 109.85   |
| 1   | O     | 300 | ASP  | CA-C-N     | -7.01 | 112.87      | 121.00   |
| 1   | O     | 300 | ASP  | C-N-CA     | -7.01 | 112.87      | 121.00   |
| 1   | Y     | 206 | MET  | CB-CG-SD   | 7.01  | 133.72      | 112.70   |
| 1   | Y     | 97  | VAL  | N-CA-C     | 7.00  | 117.78      | 110.72   |
| 1   | R     | 134 | LYS  | N-CA-C     | 6.99  | 118.55      | 111.07   |
| 1   | N     | 97  | VAL  | N-CA-C     | 6.98  | 117.77      | 110.72   |
| 1   | a     | 66  | THR  | OG1-CB-CG2 | 6.97  | 123.24      | 109.30   |
| 1   | F     | 316 | VAL  | CG1-CB-CG2 | -6.97 | 95.47       | 110.80   |
| 1   | b     | 61  | ILE  | N-CA-C     | 6.97  | 118.34      | 108.17   |
| 1   | J     | 298 | THR  | N-CA-C     | 6.96  | 119.62      | 108.41   |
| 1   | M     | 269 | LEU  | N-CA-C     | -6.96 | 103.62      | 111.07   |
| 1   | e     | 134 | LYS  | CB-CA-C    | -6.95 | 99.97       | 110.88   |
| 1   | G     | 85  | VAL  | CG1-CB-CG2 | -6.93 | 95.56       | 110.80   |
| 1   | J     | 203 | THR  | OG1-CB-CG2 | 6.93  | 123.16      | 109.30   |
| 1   | P     | 103 | LYS  | CA-CB-CG   | 6.93  | 127.96      | 114.10   |
| 1   | N     | 309 | LEU  | N-CA-C     | -6.92 | 104.97      | 113.41   |
| 1   | E     | 98  | MET  | CA-CB-CG   | 6.91  | 127.92      | 114.10   |
| 1   | b     | 59  | THR  | OG1-CB-CG2 | -6.91 | 95.49       | 109.30   |
| 1   | F     | 59  | THR  | OG1-CB-CG2 | 6.89  | 123.08      | 109.30   |
| 1   | K     | 57  | SER  | N-CA-C     | 6.88  | 120.76      | 109.06   |
| 1   | a     | 155 | THR  | OG1-CB-CG2 | -6.88 | 95.54       | 109.30   |
| 1   | C     | 97  | VAL  | N-CA-C     | 6.87  | 117.63      | 110.62   |
| 1   | R     | 69  | MET  | CB-CA-C    | 6.87  | 123.34      | 110.63   |
| 1   | U     | 275 | VAL  | N-CA-C     | 6.87  | 122.04      | 112.50   |
| 1   | f     | 130 | VAL  | CG1-CB-CG2 | -6.86 | 95.70       | 110.80   |
| 1   | X     | 154 | PHE  | N-CA-C     | 6.86  | 121.48      | 113.18   |
| 1   | e     | 133 | SER  | N-CA-C     | -6.86 | 103.88      | 111.36   |
| 1   | A     | 128 | ARG  | N-CA-C     | -6.86 | 104.53      | 113.17   |
| 1   | X     | 311 | THR  | OG1-CB-CG2 | -6.85 | 95.59       | 109.30   |
| 1   | E     | 295 | VAL  | N-CA-C     | 6.84  | 117.59      | 110.62   |
| 1   | P     | 148 | GLN  | N-CA-C     | 6.82  | 119.52      | 108.41   |
| 1   | f     | 74  | TYR  | N-CA-C     | 6.82  | 119.34      | 111.02   |
| 1   | O     | 107 | MET  | CB-CG-SD   | -6.81 | 92.26       | 112.70   |
| 1   | X     | 58  | SER  | N-CA-C     | -6.81 | 99.59       | 110.14   |
| 1   | K     | 148 | GLN  | N-CA-C     | 6.81  | 119.51      | 108.41   |
| 1   | d     | 317 | LYS  | CB-CA-C    | 6.81  | 123.61      | 109.38   |
| 1   | X     | 318 | ARG  | CB-CG-CD   | 6.80  | 126.95      | 111.30   |
| 1   | Z     | 300 | ASP  | CA-C-N     | -6.79 | 111.35      | 119.84   |
| 1   | Z     | 300 | ASP  | C-N-CA     | -6.79 | 111.35      | 119.84   |
| 1   | f     | 154 | PHE  | N-CA-CB    | -6.79 | 99.01       | 110.41   |
| 1   | K     | 162 | VAL  | N-CA-C     | 6.77  | 118.23      | 108.48   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 300 | ASP  | CA-C-N     | -6.75 | 112.72      | 120.89   |
| 1   | E     | 300 | ASP  | C-N-CA     | -6.75 | 112.72      | 120.89   |
| 1   | X     | 63  | ASP  | N-CA-C     | 6.75  | 118.05      | 108.74   |
| 1   | Q     | 298 | THR  | OG1-CB-CG2 | 6.75  | 122.79      | 109.30   |
| 1   | f     | 225 | MET  | CB-CG-SD   | 6.74  | 132.93      | 112.70   |
| 1   | Y     | 68  | ASN  | CA-C-N     | 6.74  | 129.99      | 120.28   |
| 1   | Y     | 68  | ASN  | C-N-CA     | 6.74  | 129.99      | 120.28   |
| 1   | G     | 216 | VAL  | CG1-CB-CG2 | -6.73 | 95.99       | 110.80   |
| 1   | C     | 97  | VAL  | CB-CA-C    | -6.72 | 103.07      | 112.14   |
| 1   | Q     | 73  | TYR  | N-CA-C     | -6.71 | 104.05      | 111.36   |
| 1   | I     | 218 | LYS  | CB-CA-C    | -6.69 | 97.83       | 110.67   |
| 1   | C     | 290 | LEU  | N-CA-C     | -6.69 | 103.99      | 111.28   |
| 1   | H     | 283 | TYR  | N-CA-C     | 6.69  | 118.22      | 111.07   |
| 1   | I     | 218 | LYS  | CG-CD-CE   | -6.68 | 95.94       | 111.30   |
| 1   | P     | 59  | THR  | OG1-CB-CG2 | 6.68  | 122.65      | 109.30   |
| 1   | D     | 216 | VAL  | CG1-CB-CG2 | -6.67 | 96.12       | 110.80   |
| 1   | f     | 58  | SER  | N-CA-C     | -6.67 | 99.80       | 110.14   |
| 1   | P     | 275 | VAL  | CG1-CB-CG2 | -6.67 | 96.14       | 110.80   |
| 1   | V     | 127 | GLN  | N-CA-C     | -6.66 | 105.02      | 113.01   |
| 1   | K     | 128 | ARG  | N-CA-C     | -6.66 | 104.78      | 113.17   |
| 1   | G     | 106 | VAL  | CB-CA-C    | -6.66 | 103.36      | 111.88   |
| 1   | I     | 290 | LEU  | N-CA-C     | -6.64 | 104.04      | 111.28   |
| 1   | F     | 298 | THR  | OG1-CB-CG2 | 6.63  | 122.55      | 109.30   |
| 1   | e     | 59  | THR  | OG1-CB-CG2 | 6.62  | 122.55      | 109.30   |
| 1   | M     | 272 | LEU  | N-CA-C     | -6.62 | 103.55      | 111.69   |
| 1   | I     | 59  | THR  | OG1-CB-CG2 | 6.61  | 122.52      | 109.30   |
| 1   | P     | 103 | LYS  | CG-CD-CE   | -6.61 | 96.09       | 111.30   |
| 1   | f     | 129 | MET  | CB-CG-SD   | -6.61 | 92.89       | 112.70   |
| 1   | f     | 294 | ASN  | N-CA-C     | 6.61  | 119.31      | 111.71   |
| 1   | B     | 62  | THR  | OG1-CB-CG2 | 6.59  | 122.48      | 109.30   |
| 1   | Y     | 103 | LYS  | N-CA-CB    | 6.59  | 119.81      | 110.12   |
| 1   | K     | 123 | ASP  | N-CA-C     | 6.59  | 118.46      | 111.28   |
| 1   | f     | 107 | MET  | CB-CA-C    | -6.58 | 100.55      | 110.88   |
| 1   | M     | 155 | THR  | OG1-CB-CG2 | -6.57 | 96.16       | 109.30   |
| 1   | M     | 225 | MET  | CA-CB-CG   | 6.56  | 127.22      | 114.10   |
| 1   | Z     | 153 | ASP  | N-CA-C     | -6.56 | 96.20       | 107.61   |
| 1   | U     | 107 | MET  | CA-CB-CG   | 6.55  | 127.21      | 114.10   |
| 1   | K     | 207 | LYS  | CA-CB-CG   | 6.55  | 127.20      | 114.10   |
| 1   | H     | 155 | THR  | OG1-CB-CG2 | -6.54 | 96.21       | 109.30   |
| 1   | R     | 107 | MET  | CB-CG-SD   | -6.53 | 93.10       | 112.70   |
| 1   | d     | 59  | THR  | OG1-CB-CG2 | 6.52  | 122.33      | 109.30   |
| 1   | Z     | 216 | VAL  | CG1-CB-CG2 | 6.51  | 125.13      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 309 | LEU  | N-CA-C     | -6.51 | 105.47      | 113.41   |
| 1   | B     | 311 | THR  | CA-C-N     | -6.50 | 113.28      | 119.85   |
| 1   | B     | 311 | THR  | C-N-CA     | -6.50 | 113.28      | 119.85   |
| 1   | a     | 142 | GLU  | CB-CA-C    | -6.49 | 100.03      | 110.79   |
| 1   | Q     | 292 | THR  | OG1-CB-CG2 | 6.48  | 122.26      | 109.30   |
| 1   | T     | 293 | LEU  | N-CA-C     | 6.48  | 118.00      | 111.07   |
| 1   | S     | 224 | ARG  | N-CA-CB    | 6.47  | 120.30      | 110.28   |
| 1   | U     | 165 | ILE  | CG1-CB-CG2 | 6.45  | 130.06      | 110.70   |
| 1   | Y     | 300 | ASP  | CA-C-N     | -6.45 | 113.52      | 121.00   |
| 1   | Y     | 300 | ASP  | C-N-CA     | -6.45 | 113.52      | 121.00   |
| 1   | W     | 275 | VAL  | CG1-CB-CG2 | -6.44 | 96.64       | 110.80   |
| 1   | F     | 121 | GLN  | N-CA-C     | -6.44 | 104.68      | 113.30   |
| 1   | S     | 224 | ARG  | CD-NE-CZ   | 6.42  | 133.39      | 124.40   |
| 1   | X     | 106 | VAL  | N-CA-C     | 6.41  | 117.09      | 110.36   |
| 1   | I     | 148 | GLN  | N-CA-C     | 6.41  | 118.86      | 108.41   |
| 1   | e     | 67  | VAL  | CG1-CB-CG2 | 6.41  | 124.90      | 110.80   |
| 1   | d     | 317 | LYS  | CB-CG-CD   | 6.41  | 126.03      | 111.30   |
| 1   | D     | 305 | THR  | OG1-CB-CG2 | 6.40  | 122.10      | 109.30   |
| 1   | W     | 67  | VAL  | N-CA-C     | 6.40  | 116.56      | 110.42   |
| 1   | D     | 178 | GLN  | N-CA-C     | -6.37 | 104.41      | 111.36   |
| 1   | B     | 316 | VAL  | CG1-CB-CG2 | -6.34 | 96.85       | 110.80   |
| 1   | R     | 98  | MET  | N-CA-CB    | -6.34 | 100.45      | 110.28   |
| 1   | R     | 121 | GLN  | CA-CB-CG   | 6.34  | 126.78      | 114.10   |
| 1   | c     | 59  | THR  | OG1-CB-CG2 | 6.34  | 121.98      | 109.30   |
| 1   | W     | 317 | LYS  | N-CA-CB    | 6.33  | 122.90      | 111.37   |
| 1   | b     | 155 | THR  | OG1-CB-CG2 | -6.33 | 96.63       | 109.30   |
| 1   | N     | 129 | MET  | N-CA-CB    | -6.33 | 100.67      | 109.97   |
| 1   | B     | 74  | TYR  | N-CA-C     | 6.33  | 117.97      | 111.14   |
| 1   | I     | 289 | MET  | CB-CG-SD   | -6.32 | 93.75       | 112.70   |
| 1   | N     | 147 | ILE  | CG1-CB-CG2 | 6.30  | 129.61      | 110.70   |
| 1   | H     | 59  | THR  | OG1-CB-CG2 | 6.30  | 121.90      | 109.30   |
| 1   | S     | 215 | GLU  | N-CA-C     | -6.29 | 104.50      | 111.36   |
| 1   | O     | 67  | VAL  | CG1-CB-CG2 | 6.28  | 124.61      | 110.80   |
| 1   | A     | 67  | VAL  | N-CA-C     | 6.27  | 116.44      | 110.42   |
| 1   | I     | 298 | THR  | OG1-CB-CG2 | 6.26  | 121.83      | 109.30   |
| 1   | e     | 134 | LYS  | CG-CD-CE   | -6.26 | 96.89       | 111.30   |
| 1   | O     | 144 | ILE  | N-CA-C     | -6.26 | 104.23      | 110.62   |
| 1   | e     | 150 | ILE  | CG1-CB-CG2 | 6.26  | 129.47      | 110.70   |
| 1   | W     | 317 | LYS  | N-CA-C     | -6.26 | 99.61       | 109.50   |
| 1   | B     | 196 | LYS  | CB-CA-C    | 6.25  | 121.17      | 110.79   |
| 1   | Y     | 143 | MET  | CB-CG-SD   | 6.25  | 131.46      | 112.70   |
| 1   | O     | 121 | GLN  | N-CA-C     | -6.25 | 104.93      | 113.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | U     | 229 | GLU  | N-CA-C     | 6.24  | 118.89      | 111.33   |
| 1   | F     | 309 | LEU  | N-CA-C     | -6.24 | 106.21      | 113.88   |
| 1   | M     | 66  | THR  | OG1-CB-CG2 | -6.24 | 96.83       | 109.30   |
| 1   | Z     | 317 | LYS  | N-CA-CB    | -6.23 | 100.02      | 111.37   |
| 1   | W     | 133 | SER  | N-CA-C     | -6.23 | 104.57      | 111.36   |
| 1   | G     | 98  | MET  | CA-CB-CG   | -6.22 | 101.66      | 114.10   |
| 1   | Q     | 317 | LYS  | CB-CG-CD   | 6.22  | 125.61      | 111.30   |
| 1   | Z     | 203 | THR  | OG1-CB-CG2 | 6.22  | 121.74      | 109.30   |
| 1   | A     | 106 | VAL  | CB-CA-C    | -6.22 | 103.92      | 111.88   |
| 1   | K     | 97  | VAL  | N-CA-C     | 6.22  | 117.00      | 110.72   |
| 1   | f     | 226 | ASN  | N-CA-C     | -6.21 | 104.60      | 111.36   |
| 1   | L     | 59  | THR  | OG1-CB-CG2 | 6.20  | 121.71      | 109.30   |
| 1   | O     | 295 | VAL  | N-CA-C     | 6.20  | 116.95      | 110.62   |
| 1   | Y     | 69  | MET  | N-CA-CB    | -6.20 | 100.68      | 110.22   |
| 1   | b     | 311 | THR  | OG1-CB-CG2 | 6.19  | 121.69      | 109.30   |
| 1   | L     | 59  | THR  | CA-CB-CG2  | 6.19  | 121.03      | 110.50   |
| 1   | N     | 152 | GLY  | N-CA-C     | 6.19  | 122.70      | 112.30   |
| 1   | Y     | 67  | VAL  | CB-CA-C    | -6.18 | 104.06      | 111.97   |
| 1   | a     | 67  | VAL  | N-CA-C     | 6.17  | 116.34      | 110.42   |
| 1   | e     | 298 | THR  | OG1-CB-CG2 | 6.17  | 121.64      | 109.30   |
| 1   | P     | 273 | GLN  | CA-CB-CG   | 6.17  | 126.44      | 114.10   |
| 1   | c     | 156 | ARG  | CB-CG-CD   | 6.16  | 125.47      | 111.30   |
| 1   | S     | 67  | VAL  | N-CA-C     | 6.16  | 116.33      | 110.42   |
| 1   | S     | 69  | MET  | N-CA-CB    | 6.16  | 119.70      | 110.22   |
| 1   | T     | 317 | LYS  | CB-CG-CD   | 6.15  | 125.45      | 111.30   |
| 1   | d     | 85  | VAL  | CG1-CB-CG2 | 6.15  | 124.33      | 110.80   |
| 1   | L     | 211 | LYS  | CB-CA-C    | -6.15 | 101.22      | 110.88   |
| 1   | K     | 207 | LYS  | CB-CG-CD   | -6.15 | 97.17       | 111.30   |
| 1   | e     | 98  | MET  | CB-CG-SD   | 6.15  | 131.14      | 112.70   |
| 1   | G     | 304 | GLN  | N-CA-C     | -6.14 | 100.56      | 110.32   |
| 1   | L     | 287 | ARG  | N-CA-C     | 6.14  | 117.64      | 111.07   |
| 1   | I     | 161 | SER  | N-CA-C     | 6.13  | 119.23      | 108.75   |
| 1   | Q     | 122 | THR  | CA-CB-CG2  | 6.13  | 120.92      | 110.50   |
| 1   | N     | 289 | MET  | N-CA-C     | -6.12 | 104.72      | 111.82   |
| 1   | M     | 130 | VAL  | CG1-CB-CG2 | 6.12  | 124.27      | 110.80   |
| 1   | K     | 225 | MET  | CB-CA-C    | 6.12  | 121.25      | 110.85   |
| 1   | Q     | 127 | GLN  | N-CA-C     | -6.12 | 105.08      | 112.54   |
| 1   | W     | 74  | TYR  | N-CA-C     | 6.12  | 118.48      | 111.02   |
| 1   | b     | 57  | SER  | N-CA-C     | 6.12  | 119.46      | 109.06   |
| 1   | R     | 309 | LEU  | N-CA-C     | -6.11 | 105.95      | 113.41   |
| 1   | c     | 317 | LYS  | CG-CD-CE   | -6.11 | 97.24       | 111.30   |
| 1   | I     | 106 | VAL  | CG1-CB-CG2 | 6.11  | 124.23      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | R     | 314 | GLU  | CA-C-N     | -6.10 | 113.49      | 119.78   |
| 1   | R     | 314 | GLU  | C-N-CA     | -6.10 | 113.49      | 119.78   |
| 1   | R     | 121 | GLN  | N-CA-C     | -6.10 | 105.12      | 113.30   |
| 1   | S     | 58  | SER  | N-CA-C     | -6.10 | 100.25      | 109.95   |
| 1   | N     | 142 | GLU  | N-CA-CB    | 6.09  | 119.08      | 110.12   |
| 1   | c     | 229 | GLU  | N-CA-C     | 6.09  | 117.58      | 111.07   |
| 1   | U     | 168 | THR  | OG1-CB-CG2 | 6.08  | 121.46      | 109.30   |
| 1   | f     | 148 | GLN  | N-CA-CB    | -6.08 | 101.04      | 110.65   |
| 1   | T     | 62  | THR  | N-CA-C     | 6.08  | 119.45      | 109.85   |
| 1   | T     | 67  | VAL  | CG1-CB-CG2 | 6.08  | 124.17      | 110.80   |
| 1   | C     | 67  | VAL  | CG1-CB-CG2 | 6.07  | 124.16      | 110.80   |
| 1   | a     | 163 | LYS  | CG-CD-CE   | 6.07  | 125.27      | 111.30   |
| 1   | M     | 97  | VAL  | CG1-CB-CG2 | 6.05  | 124.12      | 110.80   |
| 1   | e     | 275 | VAL  | CG1-CB-CG2 | 6.05  | 124.12      | 110.80   |
| 1   | f     | 205 | GLN  | CB-CA-C    | 6.05  | 120.38      | 110.88   |
| 1   | Q     | 204 | ILE  | CG1-CB-CG2 | 6.05  | 128.85      | 110.70   |
| 1   | X     | 105 | PHE  | N-CA-C     | 6.04  | 117.54      | 111.07   |
| 1   | M     | 295 | VAL  | N-CA-C     | 6.04  | 116.78      | 110.62   |
| 1   | c     | 225 | MET  | CB-CA-C    | -6.04 | 100.59      | 110.85   |
| 1   | X     | 127 | GLN  | N-CA-C     | -6.04 | 105.41      | 112.89   |
| 1   | a     | 129 | MET  | CB-CA-C    | 6.03  | 119.97      | 109.65   |
| 1   | U     | 68  | ASN  | N-CA-C     | -6.03 | 104.82      | 111.82   |
| 1   | B     | 144 | ILE  | N-CA-C     | -6.03 | 104.47      | 110.62   |
| 1   | A     | 290 | LEU  | N-CA-C     | -6.03 | 104.71      | 111.28   |
| 1   | Q     | 122 | THR  | OG1-CB-CG2 | 6.02  | 121.35      | 109.30   |
| 1   | Y     | 106 | VAL  | CG1-CB-CG2 | 6.02  | 124.05      | 110.80   |
| 1   | L     | 290 | LEU  | N-CA-C     | -6.02 | 104.72      | 111.28   |
| 1   | b     | 144 | ILE  | CG1-CB-CG2 | 6.01  | 128.74      | 110.70   |
| 1   | f     | 220 | ILE  | CG1-CB-CG2 | 6.01  | 128.74      | 110.70   |
| 1   | A     | 121 | GLN  | N-CA-C     | -6.01 | 105.13      | 112.88   |
| 1   | X     | 153 | ASP  | N-CA-C     | -6.01 | 97.16       | 107.61   |
| 1   | C     | 102 | TYR  | N-CA-C     | 6.00  | 117.83      | 111.28   |
| 1   | R     | 64  | ARG  | CA-C-N     | 6.00  | 127.34      | 119.84   |
| 1   | R     | 64  | ARG  | C-N-CA     | 6.00  | 127.34      | 119.84   |
| 1   | a     | 103 | LYS  | N-CA-CB    | 6.00  | 118.71      | 110.01   |
| 1   | S     | 311 | THR  | OG1-CB-CG2 | 5.99  | 121.28      | 109.30   |
| 1   | a     | 60  | ALA  | N-CA-C     | 5.99  | 118.81      | 109.52   |
| 1   | W     | 300 | ASP  | N-CA-C     | -5.99 | 97.91       | 108.69   |
| 1   | V     | 168 | THR  | OG1-CB-CG2 | 5.99  | 121.27      | 109.30   |
| 1   | e     | 134 | LYS  | CD-CE-NZ   | 5.98  | 131.02      | 111.90   |
| 1   | K     | 226 | ASN  | N-CA-C     | -5.97 | 104.85      | 111.36   |
| 1   | Q     | 142 | GLU  | N-CA-C     | 5.97  | 117.79      | 111.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | V     | 148 | GLN  | N-CA-C     | 5.97  | 118.14      | 108.41   |
| 1   | R     | 153 | ASP  | CB-CA-C    | 5.97  | 119.08      | 110.79   |
| 1   | d     | 59  | THR  | CA-CB-CG2  | 5.96  | 120.64      | 110.50   |
| 1   | J     | 210 | VAL  | CG1-CB-CG2 | 5.96  | 123.92      | 110.80   |
| 1   | M     | 101 | ALA  | N-CA-C     | -5.96 | 104.69      | 111.07   |
| 1   | W     | 122 | THR  | CA-CB-CG2  | 5.96  | 120.64      | 110.50   |
| 1   | R     | 59  | THR  | OG1-CB-CG2 | -5.96 | 97.38       | 109.30   |
| 1   | b     | 122 | THR  | OG1-CB-CG2 | -5.96 | 97.38       | 109.30   |
| 1   | A     | 152 | GLY  | N-CA-C     | 5.95  | 121.61      | 112.51   |
| 1   | E     | 286 | ASN  | N-CA-C     | -5.95 | 104.87      | 111.36   |
| 1   | R     | 228 | ILE  | CG1-CB-CG2 | 5.94  | 128.52      | 110.70   |
| 1   | X     | 155 | THR  | OG1-CB-CG2 | 5.94  | 121.18      | 109.30   |
| 1   | Y     | 309 | LEU  | N-CA-C     | -5.94 | 106.17      | 113.41   |
| 1   | d     | 266 | GLN  | N-CA-C     | -5.93 | 94.39       | 111.00   |
| 1   | M     | 142 | GLU  | CB-CA-C    | -5.93 | 100.95      | 110.79   |
| 1   | P     | 211 | LYS  | CD-CE-NZ   | -5.93 | 92.93       | 111.90   |
| 1   | B     | 70  | LEU  | N-CA-C     | -5.93 | 106.01      | 113.18   |
| 1   | W     | 224 | ARG  | CD-NE-CZ   | 5.93  | 132.70      | 124.40   |
| 1   | W     | 224 | ARG  | NE-CZ-NH2  | -5.92 | 113.87      | 119.20   |
| 1   | V     | 316 | VAL  | N-CA-C     | -5.92 | 104.01      | 112.35   |
| 1   | E     | 226 | ASN  | N-CA-C     | -5.91 | 104.84      | 111.28   |
| 1   | H     | 210 | VAL  | CG1-CB-CG2 | 5.90  | 123.79      | 110.80   |
| 1   | J     | 218 | LYS  | CB-CA-C    | -5.90 | 100.82      | 110.85   |
| 1   | b     | 282 | ASP  | N-CA-C     | 5.90  | 118.49      | 111.71   |
| 1   | Z     | 218 | LYS  | CB-CG-CD   | -5.88 | 97.76       | 111.30   |
| 1   | e     | 309 | LEU  | N-CA-C     | -5.88 | 106.23      | 113.41   |
| 1   | E     | 67  | VAL  | CG1-CB-CG2 | 5.88  | 123.73      | 110.80   |
| 1   | d     | 216 | VAL  | CG1-CB-CG2 | 5.87  | 123.72      | 110.80   |
| 1   | X     | 128 | ARG  | N-CA-C     | -5.87 | 105.78      | 113.17   |
| 1   | B     | 150 | ILE  | CA-C-N     | 5.87  | 126.16      | 119.83   |
| 1   | B     | 150 | ILE  | C-N-CA     | 5.87  | 126.16      | 119.83   |
| 1   | U     | 195 | LEU  | CA-C-N     | 5.87  | 128.46      | 120.54   |
| 1   | U     | 195 | LEU  | C-N-CA     | 5.87  | 128.46      | 120.54   |
| 1   | S     | 223 | ARG  | CA-C-N     | -5.86 | 111.40      | 120.31   |
| 1   | S     | 223 | ARG  | C-N-CA     | -5.86 | 111.40      | 120.31   |
| 1   | M     | 144 | ILE  | CA-CB-CG1  | 5.86  | 120.35      | 110.40   |
| 1   | E     | 162 | VAL  | N-CA-C     | 5.85  | 117.18      | 108.46   |
| 1   | e     | 220 | ILE  | CB-CA-C    | 5.85  | 120.04      | 112.14   |
| 1   | M     | 297 | PRO  | N-CA-C     | 5.85  | 120.47      | 111.57   |
| 1   | f     | 206 | MET  | CA-CB-CG   | 5.84  | 125.78      | 114.10   |
| 1   | K     | 99  | ASP  | N-CA-C     | -5.84 | 104.92      | 111.28   |
| 1   | P     | 165 | ILE  | CB-CA-C    | -5.84 | 102.90      | 110.84   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 227 | SER  | N-CA-C     | 5.83  | 118.58      | 111.82   |
| 1   | W     | 97  | VAL  | CB-CA-C    | -5.83 | 104.17      | 112.22   |
| 1   | G     | 309 | LEU  | N-CA-C     | -5.83 | 106.30      | 113.41   |
| 1   | Y     | 203 | THR  | OG1-CB-CG2 | -5.83 | 97.65       | 109.30   |
| 1   | f     | 206 | MET  | CB-CG-SD   | -5.82 | 95.23       | 112.70   |
| 1   | U     | 300 | ASP  | CA-C-N     | -5.82 | 112.56      | 119.84   |
| 1   | U     | 300 | ASP  | C-N-CA     | -5.82 | 112.56      | 119.84   |
| 1   | D     | 129 | MET  | CB-CA-C    | 5.82  | 120.25      | 109.54   |
| 1   | K     | 211 | LYS  | N-CA-C     | 5.82  | 117.30      | 111.07   |
| 1   | E     | 295 | VAL  | CG1-CB-CG2 | 5.82  | 123.60      | 110.80   |
| 1   | P     | 211 | LYS  | CG-CD-CE   | 5.82  | 124.68      | 111.30   |
| 1   | C     | 216 | VAL  | CG1-CB-CG2 | -5.81 | 98.02       | 110.80   |
| 1   | I     | 59  | THR  | CA-CB-CG2  | 5.81  | 120.38      | 110.50   |
| 1   | a     | 61  | ILE  | CG1-CB-CG2 | 5.80  | 128.11      | 110.70   |
| 1   | D     | 161 | SER  | N-CA-C     | 5.80  | 118.22      | 109.23   |
| 1   | e     | 144 | ILE  | CG1-CB-CG2 | 5.80  | 128.10      | 110.70   |
| 1   | M     | 220 | ILE  | CG1-CB-CG2 | 5.79  | 128.07      | 110.70   |
| 1   | D     | 173 | ASN  | N-CA-C     | 5.79  | 117.28      | 110.97   |
| 1   | f     | 202 | ARG  | CB-CG-CD   | -5.79 | 97.99       | 111.30   |
| 1   | Y     | 141 | ASP  | N-CA-C     | -5.79 | 104.88      | 111.07   |
| 1   | Q     | 144 | ILE  | N-CA-C     | -5.78 | 104.72      | 110.62   |
| 1   | M     | 228 | ILE  | CG1-CB-CG2 | 5.78  | 128.05      | 110.70   |
| 1   | K     | 299 | LEU  | N-CA-C     | 5.78  | 118.16      | 107.99   |
| 1   | T     | 225 | MET  | N-CA-C     | 5.78  | 117.66      | 111.36   |
| 1   | b     | 133 | SER  | CB-CA-C    | 5.78  | 121.27      | 110.70   |
| 1   | Y     | 127 | GLN  | CA-C-N     | -5.77 | 113.02      | 122.54   |
| 1   | Y     | 127 | GLN  | C-N-CA     | -5.77 | 113.02      | 122.54   |
| 1   | L     | 130 | VAL  | CG1-CB-CG2 | 5.76  | 123.47      | 110.80   |
| 1   | I     | 97  | VAL  | N-CA-C     | 5.76  | 116.54      | 110.72   |
| 1   | b     | 161 | SER  | N-CA-C     | 5.76  | 118.60      | 108.75   |
| 1   | G     | 98  | MET  | N-CA-CB    | -5.75 | 101.36      | 110.28   |
| 1   | d     | 148 | GLN  | N-CA-C     | 5.75  | 117.79      | 108.41   |
| 1   | N     | 317 | LYS  | CA-CB-CG   | 5.75  | 125.59      | 114.10   |
| 1   | P     | 98  | MET  | N-CA-CB    | 5.74  | 119.18      | 110.28   |
| 1   | Q     | 62  | THR  | N-CA-C     | 5.74  | 118.92      | 109.85   |
| 1   | R     | 154 | PHE  | N-CA-CB    | -5.74 | 100.85      | 110.39   |
| 1   | H     | 225 | MET  | CA-CB-CG   | -5.74 | 102.62      | 114.10   |
| 1   | V     | 153 | ASP  | N-CA-C     | -5.74 | 97.87       | 107.80   |
| 1   | W     | 299 | LEU  | N-CA-C     | -5.74 | 98.36       | 108.23   |
| 1   | b     | 60  | ALA  | N-CA-C     | 5.74  | 118.41      | 109.52   |
| 1   | O     | 165 | ILE  | CG1-CB-CG2 | 5.74  | 127.91      | 110.70   |
| 1   | Q     | 292 | THR  | CA-CB-CG2  | 5.74  | 120.25      | 110.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | a     | 129 | MET  | N-CA-CB    | -5.73 | 101.54      | 109.97   |
| 1   | R     | 224 | ARG  | CD-NE-CZ   | 5.73  | 132.42      | 124.40   |
| 1   | L     | 220 | ILE  | CG1-CB-CG2 | 5.72  | 127.87      | 110.70   |
| 1   | Z     | 98  | MET  | CB-CA-C    | 5.72  | 122.06      | 110.38   |
| 1   | W     | 121 | GLN  | N-CA-C     | -5.72 | 105.64      | 113.30   |
| 1   | e     | 59  | THR  | CA-CB-CG2  | 5.71  | 120.22      | 110.50   |
| 1   | J     | 147 | ILE  | CG1-CB-CG2 | 5.71  | 127.83      | 110.70   |
| 1   | f     | 85  | VAL  | CG1-CB-CG2 | 5.71  | 123.36      | 110.80   |
| 1   | C     | 103 | LYS  | N-CA-C     | -5.71 | 105.06      | 111.28   |
| 1   | O     | 122 | THR  | CB-CA-C    | 5.71  | 119.16      | 109.75   |
| 1   | V     | 163 | LYS  | CB-CG-CD   | -5.71 | 98.18       | 111.30   |
| 1   | B     | 55  | GLU  | CB-CA-C    | 5.70  | 120.94      | 110.10   |
| 1   | f     | 316 | VAL  | N-CA-C     | -5.70 | 104.31      | 112.35   |
| 1   | E     | 297 | PRO  | N-CA-C     | 5.70  | 121.20      | 111.68   |
| 1   | d     | 101 | ALA  | N-CA-C     | -5.70 | 104.97      | 111.07   |
| 1   | b     | 97  | VAL  | N-CA-C     | 5.70  | 116.47      | 110.72   |
| 1   | S     | 97  | VAL  | CG1-CB-CG2 | 5.70  | 123.33      | 110.80   |
| 1   | R     | 268 | ARG  | NE-CZ-NH1  | -5.69 | 115.81      | 121.50   |
| 1   | Z     | 203 | THR  | CA-CB-CG2  | 5.68  | 120.17      | 110.50   |
| 1   | C     | 292 | THR  | OG1-CB-CG2 | -5.68 | 97.94       | 109.30   |
| 1   | O     | 156 | ARG  | N-CA-C     | 5.68  | 120.27      | 113.23   |
| 1   | G     | 220 | ILE  | CB-CA-C    | -5.68 | 103.06      | 112.26   |
| 1   | S     | 85  | VAL  | CG1-CB-CG2 | 5.68  | 123.30      | 110.80   |
| 1   | O     | 272 | LEU  | N-CA-C     | -5.68 | 105.17      | 111.36   |
| 1   | Q     | 316 | VAL  | N-CA-C     | -5.68 | 104.34      | 112.35   |
| 1   | Q     | 206 | MET  | CB-CG-SD   | -5.68 | 95.67       | 112.70   |
| 1   | J     | 153 | ASP  | CB-CA-C    | 5.67  | 118.67      | 110.79   |
| 1   | a     | 218 | LYS  | CG-CD-CE   | -5.67 | 98.26       | 111.30   |
| 1   | D     | 121 | GLN  | N-CA-C     | -5.67 | 105.57      | 112.88   |
| 1   | T     | 154 | PHE  | N-CA-C     | -5.67 | 106.32      | 113.18   |
| 1   | a     | 107 | MET  | CB-CG-SD   | -5.67 | 95.71       | 112.70   |
| 1   | c     | 165 | ILE  | CG1-CB-CG2 | 5.66  | 127.69      | 110.70   |
| 1   | d     | 196 | LYS  | CA-CB-CG   | 5.66  | 125.43      | 114.10   |
| 1   | W     | 161 | SER  | N-CA-C     | 5.66  | 118.42      | 108.75   |
| 1   | H     | 130 | VAL  | N-CA-C     | -5.65 | 107.62      | 113.10   |
| 1   | c     | 156 | ARG  | CD-NE-CZ   | 5.65  | 132.31      | 124.40   |
| 1   | K     | 228 | ILE  | CA-C-N     | 5.65  | 127.85      | 120.28   |
| 1   | K     | 228 | ILE  | C-N-CA     | 5.65  | 127.85      | 120.28   |
| 1   | Z     | 289 | MET  | CB-CG-SD   | 5.65  | 129.64      | 112.70   |
| 1   | J     | 133 | SER  | N-CA-C     | -5.64 | 105.21      | 111.36   |
| 1   | L     | 67  | VAL  | CG1-CB-CG2 | 5.63  | 123.19      | 110.80   |
| 1   | M     | 121 | GLN  | N-CA-C     | -5.63 | 105.75      | 113.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | U     | 62  | THR  | N-CA-C     | 5.63  | 118.75      | 109.85   |
| 1   | F     | 292 | THR  | CA-C-N     | 5.63  | 127.82      | 120.28   |
| 1   | F     | 292 | THR  | C-N-CA     | 5.63  | 127.82      | 120.28   |
| 1   | b     | 98  | MET  | CA-CB-CG   | -5.63 | 102.84      | 114.10   |
| 1   | b     | 268 | ARG  | CG-CD-NE   | -5.63 | 99.62       | 112.00   |
| 1   | G     | 155 | THR  | OG1-CB-CG2 | 5.63  | 120.55      | 109.30   |
| 1   | Z     | 98  | MET  | CB-CG-SD   | 5.62  | 129.57      | 112.70   |
| 1   | P     | 305 | THR  | OG1-CB-CG2 | 5.62  | 120.54      | 109.30   |
| 1   | F     | 298 | THR  | CA-CB-CG2  | 5.61  | 120.04      | 110.50   |
| 1   | b     | 272 | LEU  | N-CA-C     | -5.61 | 105.24      | 111.36   |
| 1   | M     | 156 | ARG  | N-CA-C     | -5.61 | 105.94      | 112.89   |
| 1   | Y     | 67  | VAL  | N-CA-C     | 5.61  | 115.80      | 110.42   |
| 1   | f     | 206 | MET  | N-CA-CB    | 5.60  | 118.97      | 110.28   |
| 1   | J     | 275 | VAL  | CG1-CB-CG2 | -5.60 | 98.48       | 110.80   |
| 1   | e     | 85  | VAL  | CG1-CB-CG2 | 5.60  | 123.12      | 110.80   |
| 1   | b     | 68  | ASN  | N-CA-C     | -5.60 | 105.33      | 111.82   |
| 1   | Y     | 61  | ILE  | CG1-CB-CG2 | 5.60  | 127.49      | 110.70   |
| 1   | D     | 198 | ALA  | N-CA-C     | -5.59 | 104.81      | 111.69   |
| 1   | L     | 298 | THR  | CA-C-N     | -5.59 | 114.19      | 122.41   |
| 1   | L     | 298 | THR  | C-N-CA     | -5.59 | 114.19      | 122.41   |
| 1   | f     | 106 | VAL  | CG1-CB-CG2 | 5.58  | 123.08      | 110.80   |
| 1   | T     | 101 | ALA  | N-CA-C     | -5.58 | 105.10      | 111.07   |
| 1   | J     | 66  | THR  | OG1-CB-CG2 | -5.58 | 98.15       | 109.30   |
| 1   | B     | 62  | THR  | CA-CB-OG1  | 5.57  | 117.96      | 109.60   |
| 1   | A     | 61  | ILE  | CG1-CB-CG2 | 5.57  | 127.42      | 110.70   |
| 1   | K     | 309 | LEU  | N-CA-C     | -5.57 | 106.61      | 113.41   |
| 1   | e     | 318 | ARG  | N-CA-C     | 5.57  | 117.52      | 110.33   |
| 1   | M     | 206 | MET  | CB-CG-SD   | -5.57 | 96.00       | 112.70   |
| 1   | S     | 77  | GLN  | CB-CA-C    | -5.57 | 101.39      | 110.85   |
| 1   | Y     | 155 | THR  | OG1-CB-CG2 | 5.56  | 120.42      | 109.30   |
| 1   | R     | 226 | ASN  | N-CA-C     | -5.56 | 105.30      | 111.36   |
| 1   | D     | 130 | VAL  | CG1-CB-CG2 | 5.55  | 123.02      | 110.80   |
| 1   | E     | 299 | LEU  | CB-CG-CD2  | 5.55  | 127.36      | 110.70   |
| 1   | d     | 163 | LYS  | CB-CG-CD   | -5.55 | 98.53       | 111.30   |
| 1   | a     | 61  | ILE  | N-CA-C     | 5.54  | 116.26      | 108.17   |
| 1   | T     | 57  | SER  | N-CA-C     | 5.54  | 118.49      | 109.24   |
| 1   | K     | 97  | VAL  | CG1-CB-CG2 | 5.53  | 122.97      | 110.80   |
| 1   | C     | 300 | ASP  | CA-C-N     | -5.53 | 114.59      | 121.00   |
| 1   | C     | 300 | ASP  | C-N-CA     | -5.53 | 114.59      | 121.00   |
| 1   | I     | 148 | GLN  | CA-CB-CG   | -5.53 | 103.04      | 114.10   |
| 1   | b     | 67  | VAL  | N-CA-C     | 5.53  | 115.73      | 110.42   |
| 1   | U     | 314 | GLU  | CA-C-N     | -5.53 | 114.09      | 119.78   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | U     | 314 | GLU  | C-N-CA     | -5.53 | 114.09      | 119.78   |
| 1   | L     | 211 | LYS  | CD-CE-NZ   | -5.53 | 94.22       | 111.90   |
| 1   | T     | 203 | THR  | OG1-CB-CG2 | 5.53  | 120.35      | 109.30   |
| 1   | F     | 297 | PRO  | N-CA-C     | 5.52  | 119.69      | 111.41   |
| 1   | V     | 302 | ARG  | CB-CA-C    | -5.52 | 100.07      | 110.01   |
| 1   | M     | 67  | VAL  | N-CA-C     | 5.52  | 115.72      | 110.42   |
| 1   | U     | 223 | ARG  | N-CA-C     | 5.52  | 116.97      | 111.07   |
| 1   | d     | 107 | MET  | CB-CA-C    | -5.51 | 102.00      | 110.81   |
| 1   | D     | 81  | ARG  | N-CA-C     | -5.51 | 105.29      | 112.23   |
| 1   | Y     | 292 | THR  | CA-CB-CG2  | 5.51  | 119.86      | 110.50   |
| 1   | Y     | 98  | MET  | CA-CB-CG   | 5.50  | 125.10      | 114.10   |
| 1   | e     | 97  | VAL  | CG1-CB-CG2 | -5.50 | 98.70       | 110.80   |
| 1   | a     | 316 | VAL  | CG1-CB-CG2 | 5.50  | 122.89      | 110.80   |
| 1   | E     | 62  | THR  | N-CA-C     | 5.49  | 118.03      | 109.52   |
| 1   | I     | 149 | PHE  | N-CA-C     | 5.49  | 118.76      | 109.76   |
| 1   | T     | 204 | ILE  | CG1-CB-CG2 | 5.49  | 127.17      | 110.70   |
| 1   | C     | 194 | GLU  | N-CA-C     | -5.49 | 105.30      | 111.28   |
| 1   | L     | 311 | THR  | N-CA-C     | -5.49 | 102.72      | 110.29   |
| 1   | O     | 57  | SER  | N-CA-C     | 5.48  | 118.39      | 109.24   |
| 1   | e     | 130 | VAL  | CG1-CB-CG2 | 5.48  | 122.86      | 110.80   |
| 1   | R     | 300 | ASP  | CA-C-N     | -5.48 | 112.99      | 119.84   |
| 1   | R     | 300 | ASP  | C-N-CA     | -5.48 | 112.99      | 119.84   |
| 1   | d     | 305 | THR  | OG1-CB-CG2 | -5.47 | 98.35       | 109.30   |
| 1   | A     | 147 | ILE  | N-CA-CB    | -5.47 | 104.56      | 111.46   |
| 1   | E     | 301 | PRO  | N-CA-C     | -5.47 | 107.03      | 114.80   |
| 1   | b     | 296 | GLY  | CA-C-N     | -5.47 | 114.95      | 120.31   |
| 1   | b     | 296 | GLY  | C-N-CA     | -5.47 | 114.95      | 120.31   |
| 1   | P     | 220 | ILE  | CB-CA-C    | 5.46  | 119.52      | 112.14   |
| 1   | U     | 143 | MET  | CG-SD-CE   | -5.46 | 88.88       | 100.90   |
| 1   | M     | 144 | ILE  | CG1-CB-CG2 | 5.46  | 127.09      | 110.70   |
| 1   | L     | 226 | ASN  | N-CA-C     | -5.46 | 105.41      | 111.36   |
| 1   | P     | 55  | GLU  | N-CA-C     | -5.46 | 95.72       | 111.00   |
| 1   | Z     | 153 | ASP  | N-CA-CB    | 5.46  | 119.06      | 110.71   |
| 1   | U     | 316 | VAL  | N-CA-C     | -5.46 | 104.66      | 112.35   |
| 1   | Q     | 295 | VAL  | N-CA-C     | -5.45 | 105.06      | 110.62   |
| 1   | U     | 268 | ARG  | CA-CB-CG   | -5.45 | 103.20      | 114.10   |
| 1   | S     | 266 | GLN  | N-CA-C     | -5.45 | 95.74       | 111.00   |
| 1   | B     | 97  | VAL  | N-CA-C     | 5.45  | 115.65      | 110.42   |
| 1   | c     | 85  | VAL  | CG1-CB-CG2 | 5.45  | 122.79      | 110.80   |
| 1   | S     | 73  | TYR  | N-CA-C     | 5.45  | 117.30      | 111.36   |
| 1   | L     | 196 | LYS  | CB-CA-C    | -5.45 | 101.70      | 110.74   |
| 1   | R     | 210 | VAL  | CG1-CB-CG2 | 5.45  | 122.78      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | f     | 158 | VAL  | N-CA-CB    | 5.44  | 116.65      | 110.72   |
| 1   | M     | 220 | ILE  | CB-CA-C    | 5.44  | 119.48      | 112.14   |
| 1   | c     | 153 | ASP  | N-CA-C     | -5.43 | 98.40       | 107.80   |
| 1   | T     | 196 | LYS  | CA-CB-CG   | 5.42  | 124.94      | 114.10   |
| 1   | D     | 177 | ARG  | N-CA-C     | 5.42  | 116.87      | 111.07   |
| 1   | Q     | 122 | THR  | CA-CB-OG1  | 5.42  | 117.73      | 109.60   |
| 1   | f     | 309 | LEU  | N-CA-C     | -5.42 | 106.80      | 113.41   |
| 1   | L     | 98  | MET  | CB-CG-SD   | 5.42  | 128.95      | 112.70   |
| 1   | N     | 156 | ARG  | CB-CA-C    | 5.42  | 120.73      | 109.95   |
| 1   | f     | 155 | THR  | N-CA-C     | -5.41 | 105.38      | 111.28   |
| 1   | R     | 317 | LYS  | CA-CB-CG   | -5.41 | 103.28      | 114.10   |
| 1   | e     | 295 | VAL  | CG1-CB-CG2 | 5.41  | 122.70      | 110.80   |
| 1   | F     | 228 | ILE  | CB-CA-C    | -5.40 | 104.77      | 112.22   |
| 1   | I     | 130 | VAL  | CG1-CB-CG2 | 5.40  | 122.68      | 110.80   |
| 1   | L     | 309 | LEU  | N-CA-C     | -5.40 | 106.82      | 113.41   |
| 1   | d     | 143 | MET  | CB-CG-SD   | 5.40  | 128.90      | 112.70   |
| 1   | L     | 218 | LYS  | CG-CD-CE   | 5.39  | 123.70      | 111.30   |
| 1   | F     | 74  | TYR  | N-CA-C     | 5.39  | 117.01      | 111.03   |
| 1   | W     | 108 | GLN  | N-CA-C     | 5.39  | 117.15      | 111.28   |
| 1   | J     | 205 | GLN  | CB-CG-CD   | 5.38  | 121.75      | 112.60   |
| 1   | Q     | 298 | THR  | CA-CB-OG1  | 5.38  | 117.68      | 109.60   |
| 1   | F     | 59  | THR  | CA-CB-CG2  | 5.37  | 119.63      | 110.50   |
| 1   | L     | 195 | LEU  | N-CA-C     | -5.36 | 105.12      | 110.97   |
| 1   | c     | 156 | ARG  | CG-CD-NE   | -5.36 | 100.20      | 112.00   |
| 1   | C     | 62  | THR  | N-CA-C     | 5.36  | 118.01      | 109.81   |
| 1   | L     | 69  | MET  | N-CA-CB    | -5.35 | 101.97      | 110.22   |
| 1   | I     | 206 | MET  | CB-CA-C    | 5.35  | 120.95      | 110.67   |
| 1   | T     | 205 | GLN  | CB-CA-C    | 5.35  | 119.28      | 110.88   |
| 1   | G     | 112 | TRP  | N-CA-C     | 5.35  | 116.79      | 111.07   |
| 1   | d     | 112 | TRP  | N-CA-C     | 5.34  | 116.91      | 111.14   |
| 1   | O     | 299 | LEU  | N-CA-C     | -5.34 | 99.04       | 108.23   |
| 1   | X     | 102 | TYR  | N-CA-C     | -5.34 | 105.54      | 111.36   |
| 1   | D     | 222 | ASP  | N-CA-C     | -5.34 | 105.46      | 111.28   |
| 1   | Q     | 220 | ILE  | CG1-CB-CG2 | 5.34  | 126.71      | 110.70   |
| 1   | O     | 98  | MET  | CA-CB-CG   | 5.33  | 124.77      | 114.10   |
| 1   | H     | 148 | GLN  | N-CA-C     | 5.33  | 117.35      | 108.02   |
| 1   | M     | 182 | PHE  | N-CA-C     | 5.33  | 116.77      | 111.07   |
| 1   | G     | 206 | MET  | CB-CA-C    | 5.32  | 120.89      | 110.67   |
| 1   | L     | 272 | LEU  | N-CA-C     | -5.31 | 105.57      | 111.36   |
| 1   | M     | 224 | ARG  | N-CA-C     | 5.31  | 117.98      | 111.82   |
| 1   | B     | 62  | THR  | CA-CB-CG2  | 5.31  | 119.53      | 110.50   |
| 1   | J     | 218 | LYS  | CD-CE-NZ   | 5.31  | 128.90      | 111.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 85  | VAL  | CG1-CB-CG2 | 5.31  | 122.48      | 110.80   |
| 1   | a     | 66  | THR  | CA-CB-OG1  | 5.31  | 117.56      | 109.60   |
| 1   | J     | 205 | GLN  | CB-CA-C    | -5.30 | 102.56      | 110.88   |
| 1   | V     | 127 | GLN  | CB-CG-CD   | -5.30 | 103.59      | 112.60   |
| 1   | O     | 299 | LEU  | CA-C-N     | -5.30 | 112.54      | 121.76   |
| 1   | O     | 299 | LEU  | C-N-CA     | -5.30 | 112.54      | 121.76   |
| 1   | L     | 156 | ARG  | CB-CG-CD   | 5.30  | 123.48      | 111.30   |
| 1   | S     | 296 | GLY  | CA-C-N     | -5.30 | 115.12      | 120.31   |
| 1   | S     | 296 | GLY  | C-N-CA     | -5.30 | 115.12      | 120.31   |
| 1   | a     | 123 | ASP  | N-CA-C     | 5.30  | 117.05      | 111.28   |
| 1   | N     | 69  | MET  | N-CA-C     | -5.29 | 105.62      | 111.71   |
| 1   | J     | 211 | LYS  | CG-CD-CE   | -5.29 | 99.13       | 111.30   |
| 1   | b     | 224 | ARG  | CB-CA-C    | -5.29 | 100.51      | 110.67   |
| 1   | Q     | 67  | VAL  | CG1-CB-CG2 | 5.29  | 122.43      | 110.80   |
| 1   | L     | 143 | MET  | CA-CB-CG   | 5.28  | 124.67      | 114.10   |
| 1   | c     | 225 | MET  | CB-CG-SD   | 5.28  | 128.55      | 112.70   |
| 1   | U     | 64  | ARG  | CA-C-N     | 5.28  | 126.44      | 119.84   |
| 1   | U     | 64  | ARG  | C-N-CA     | 5.28  | 126.44      | 119.84   |
| 1   | W     | 119 | TRP  | N-CA-C     | -5.28 | 105.53      | 111.28   |
| 1   | a     | 314 | GLU  | CA-C-N     | -5.27 | 114.35      | 119.78   |
| 1   | a     | 314 | GLU  | C-N-CA     | -5.27 | 114.35      | 119.78   |
| 1   | E     | 124 | TYR  | N-CA-C     | 5.27  | 117.45      | 111.02   |
| 1   | J     | 203 | THR  | CA-CB-OG1  | 5.27  | 117.50      | 109.60   |
| 1   | S     | 224 | ARG  | CA-C-N     | -5.27 | 113.22      | 120.28   |
| 1   | S     | 224 | ARG  | C-N-CA     | -5.27 | 113.22      | 120.28   |
| 1   | V     | 55  | GLU  | CB-CA-C    | 5.27  | 120.11      | 110.10   |
| 1   | K     | 173 | ASN  | N-CA-C     | 5.26  | 116.71      | 110.97   |
| 1   | L     | 85  | VAL  | CG1-CB-CG2 | 5.26  | 122.38      | 110.80   |
| 1   | U     | 219 | ALA  | N-CA-C     | -5.26 | 105.62      | 111.36   |
| 1   | A     | 225 | MET  | N-CA-C     | -5.26 | 105.72      | 111.82   |
| 1   | G     | 155 | THR  | N-CA-C     | -5.26 | 106.01      | 112.90   |
| 1   | H     | 121 | GLN  | N-CA-C     | -5.26 | 106.54      | 113.17   |
| 1   | M     | 225 | MET  | CB-CG-SD   | -5.26 | 96.92       | 112.70   |
| 1   | f     | 173 | ASN  | N-CA-C     | 5.26  | 116.70      | 110.97   |
| 1   | J     | 225 | MET  | CB-CG-SD   | -5.26 | 96.93       | 112.70   |
| 1   | W     | 229 | GLU  | N-CA-C     | 5.26  | 116.69      | 111.07   |
| 1   | T     | 163 | LYS  | CG-CD-CE   | 5.25  | 123.39      | 111.30   |
| 1   | B     | 152 | GLY  | CA-C-N     | -5.25 | 114.65      | 122.74   |
| 1   | B     | 152 | GLY  | C-N-CA     | -5.25 | 114.65      | 122.74   |
| 1   | U     | 67  | VAL  | CB-CA-C    | -5.25 | 105.25      | 111.97   |
| 1   | c     | 107 | MET  | CB-CA-C    | -5.25 | 102.64      | 110.88   |
| 1   | N     | 287 | ARG  | N-CA-C     | 5.25  | 116.68      | 111.07   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 129 | MET  | CB-CG-SD   | -5.23 | 97.00       | 112.70   |
| 1   | V     | 272 | LEU  | N-CA-C     | -5.23 | 105.66      | 111.36   |
| 1   | W     | 274 | ALA  | N-CA-C     | -5.23 | 107.57      | 114.31   |
| 1   | T     | 156 | ARG  | N-CA-C     | -5.22 | 106.42      | 112.89   |
| 1   | f     | 287 | ARG  | N-CA-C     | 5.22  | 116.66      | 111.07   |
| 1   | Y     | 292 | THR  | OG1-CB-CG2 | 5.22  | 119.74      | 109.30   |
| 1   | e     | 162 | VAL  | N-CA-C     | 5.21  | 115.99      | 108.48   |
| 1   | Q     | 121 | GLN  | N-CA-C     | -5.21 | 106.32      | 113.30   |
| 1   | e     | 294 | ASN  | N-CA-C     | 5.21  | 116.96      | 111.28   |
| 1   | d     | 123 | ASP  | N-CA-C     | 5.21  | 116.95      | 111.28   |
| 1   | E     | 70  | LEU  | N-CA-C     | -5.20 | 106.88      | 113.18   |
| 1   | J     | 297 | PRO  | N-CA-C     | 5.20  | 119.48      | 111.57   |
| 1   | Q     | 85  | VAL  | CG1-CB-CG2 | 5.20  | 122.25      | 110.80   |
| 1   | W     | 64  | ARG  | CB-CG-CD   | 5.20  | 123.26      | 111.30   |
| 1   | P     | 173 | ASN  | N-CA-C     | 5.20  | 116.64      | 110.97   |
| 1   | U     | 97  | VAL  | N-CA-C     | 5.19  | 115.97      | 110.72   |
| 1   | A     | 303 | PHE  | N-CA-C     | 5.19  | 118.28      | 109.76   |
| 1   | V     | 309 | LEU  | N-CA-C     | -5.19 | 107.08      | 113.41   |
| 1   | J     | 203 | THR  | CA-CB-CG2  | 5.18  | 119.31      | 110.50   |
| 1   | P     | 272 | LEU  | N-CA-C     | -5.18 | 105.71      | 111.36   |
| 1   | S     | 311 | THR  | CA-CB-CG2  | 5.18  | 119.31      | 110.50   |
| 1   | G     | 295 | VAL  | N-CA-C     | -5.18 | 104.58      | 111.05   |
| 1   | Y     | 85  | VAL  | CG1-CB-CG2 | 5.18  | 122.19      | 110.80   |
| 1   | N     | 302 | ARG  | N-CA-CB    | 5.17  | 118.36      | 110.44   |
| 1   | K     | 211 | LYS  | CD-CE-NZ   | -5.17 | 95.35       | 111.90   |
| 1   | U     | 97  | VAL  | CB-CA-C    | -5.17 | 105.08      | 112.22   |
| 1   | V     | 168 | THR  | CA-CB-CG2  | 5.17  | 119.30      | 110.50   |
| 1   | G     | 302 | ARG  | N-CA-C     | 5.17  | 117.00      | 111.36   |
| 1   | Q     | 292 | THR  | CA-CB-OG1  | 5.17  | 117.35      | 109.60   |
| 1   | W     | 122 | THR  | CA-CB-OG1  | 5.17  | 117.35      | 109.60   |
| 1   | S     | 98  | MET  | CB-CG-SD   | 5.17  | 128.19      | 112.70   |
| 1   | T     | 228 | ILE  | N-CA-C     | 5.16  | 119.63      | 112.35   |
| 1   | V     | 83  | LEU  | N-CA-C     | 5.16  | 120.23      | 113.88   |
| 1   | f     | 154 | PHE  | N-CA-C     | 5.16  | 119.42      | 113.18   |
| 1   | W     | 67  | VAL  | CB-CA-C    | -5.16 | 105.37      | 111.97   |
| 1   | O     | 289 | MET  | CB-CG-SD   | -5.15 | 97.25       | 112.70   |
| 1   | R     | 96  | SER  | CA-C-N     | 5.15  | 127.74      | 120.42   |
| 1   | R     | 96  | SER  | C-N-CA     | 5.15  | 127.74      | 120.42   |
| 1   | Z     | 85  | VAL  | CG1-CB-CG2 | 5.15  | 122.13      | 110.80   |
| 1   | W     | 215 | GLU  | N-CA-C     | -5.14 | 105.75      | 111.36   |
| 1   | S     | 158 | VAL  | CG1-CB-CG2 | 5.14  | 122.11      | 110.80   |
| 1   | b     | 106 | VAL  | N-CA-C     | 5.14  | 115.76      | 110.36   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Y     | 64  | ARG  | N-CA-C     | 5.14  | 116.99      | 109.84   |
| 1   | b     | 229 | GLU  | N-CA-CB    | 5.14  | 117.67      | 110.12   |
| 1   | e     | 97  | VAL  | CB-CA-C    | -5.14 | 105.13      | 112.22   |
| 1   | V     | 106 | VAL  | CB-CA-C    | -5.13 | 105.31      | 111.88   |
| 1   | c     | 305 | THR  | N-CA-C     | -5.13 | 105.38      | 113.02   |
| 1   | f     | 134 | LYS  | CD-CE-NZ   | 5.13  | 128.31      | 111.90   |
| 1   | K     | 156 | ARG  | CA-CB-CG   | -5.13 | 103.84      | 114.10   |
| 1   | b     | 298 | THR  | CA-CB-CG2  | -5.13 | 101.78      | 110.50   |
| 1   | Y     | 103 | LYS  | CA-CB-CG   | 5.13  | 124.35      | 114.10   |
| 1   | c     | 186 | ARG  | N-CA-C     | 5.12  | 116.94      | 111.36   |
| 1   | d     | 266 | GLN  | CA-CB-CG   | 5.12  | 124.35      | 114.10   |
| 1   | T     | 163 | LYS  | CD-CE-NZ   | -5.12 | 95.51       | 111.90   |
| 1   | G     | 289 | MET  | N-CA-C     | -5.12 | 105.78      | 111.36   |
| 1   | L     | 123 | ASP  | N-CA-C     | 5.12  | 116.86      | 111.28   |
| 1   | B     | 161 | SER  | N-CA-C     | 5.12  | 117.16      | 109.23   |
| 1   | D     | 125 | TYR  | N-CA-C     | 5.12  | 116.54      | 111.07   |
| 1   | O     | 225 | MET  | N-CA-C     | -5.12 | 105.78      | 111.36   |
| 1   | a     | 66  | THR  | CA-CB-CG2  | 5.12  | 119.20      | 110.50   |
| 1   | e     | 276 | GLY  | CA-C-N     | -5.12 | 114.68      | 119.85   |
| 1   | e     | 276 | GLY  | C-N-CA     | -5.12 | 114.68      | 119.85   |
| 1   | f     | 82  | ASN  | N-CA-C     | -5.12 | 107.06      | 113.15   |
| 1   | I     | 61  | ILE  | N-CA-C     | 5.11  | 115.64      | 108.17   |
| 1   | N     | 162 | VAL  | N-CA-C     | 5.11  | 115.84      | 108.48   |
| 1   | P     | 57  | SER  | N-CA-C     | 5.11  | 117.78      | 109.24   |
| 1   | P     | 107 | MET  | CB-CG-SD   | -5.11 | 97.37       | 112.70   |
| 1   | H     | 126 | LYS  | N-CA-C     | 5.11  | 116.85      | 111.28   |
| 1   | c     | 107 | MET  | CB-CG-SD   | -5.11 | 97.38       | 112.70   |
| 1   | Z     | 98  | MET  | CA-CB-CG   | 5.10  | 124.31      | 114.10   |
| 1   | J     | 309 | LEU  | N-CA-C     | -5.10 | 107.19      | 113.41   |
| 1   | Y     | 74  | TYR  | N-CA-C     | 5.10  | 117.24      | 111.02   |
| 1   | E     | 98  | MET  | CB-CG-SD   | 5.10  | 127.99      | 112.70   |
| 1   | E     | 308 | TYR  | N-CA-C     | 5.10  | 117.86      | 109.76   |
| 1   | Z     | 64  | ARG  | N-CA-C     | 5.09  | 116.92      | 109.84   |
| 1   | Q     | 289 | MET  | CB-CG-SD   | -5.09 | 97.44       | 112.70   |
| 1   | L     | 157 | ALA  | N-CA-C     | -5.08 | 106.38      | 112.58   |
| 1   | T     | 60  | ALA  | N-CA-C     | 5.08  | 117.39      | 109.52   |
| 1   | K     | 76  | GLN  | N-CA-C     | -5.07 | 105.45      | 111.69   |
| 1   | W     | 272 | LEU  | N-CA-C     | -5.07 | 105.45      | 111.69   |
| 1   | I     | 147 | ILE  | CG1-CB-CG2 | 5.07  | 125.91      | 110.70   |
| 1   | I     | 225 | MET  | CB-CG-SD   | 5.07  | 127.91      | 112.70   |
| 1   | U     | 102 | TYR  | N-CA-C     | -5.07 | 105.83      | 111.36   |
| 1   | Z     | 158 | VAL  | N-CA-C     | -5.07 | 100.47      | 108.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Q     | 316 | VAL  | CA-C-N     | -5.07 | 114.72      | 122.62   |
| 1   | Q     | 316 | VAL  | C-N-CA     | -5.07 | 114.72      | 122.62   |
| 1   | e     | 156 | ARG  | CG-CD-NE   | -5.07 | 100.85      | 112.00   |
| 1   | b     | 163 | LYS  | CB-CG-CD   | 5.06  | 122.95      | 111.30   |
| 1   | L     | 150 | ILE  | CA-C-N     | -5.06 | 114.70      | 119.76   |
| 1   | L     | 150 | ILE  | C-N-CA     | -5.06 | 114.70      | 119.76   |
| 1   | M     | 114 | THR  | OG1-CB-CG2 | 5.06  | 119.42      | 109.30   |
| 1   | E     | 123 | ASP  | N-CA-C     | 5.06  | 116.79      | 111.28   |
| 1   | O     | 300 | ASP  | N-CA-C     | -5.05 | 99.59       | 108.69   |
| 1   | N     | 98  | MET  | CA-CB-CG   | -5.05 | 104.00      | 114.10   |
| 1   | R     | 218 | LYS  | N-CA-C     | 5.05  | 117.68      | 111.82   |
| 1   | L     | 59  | THR  | CA-CB-OG1  | 5.05  | 117.17      | 109.60   |
| 1   | S     | 225 | MET  | CG-SD-CE   | -5.05 | 89.80       | 100.90   |
| 1   | d     | 57  | SER  | N-CA-C     | 5.04  | 117.66      | 109.24   |
| 1   | H     | 85  | VAL  | CG1-CB-CG2 | 5.04  | 121.89      | 110.80   |
| 1   | a     | 69  | MET  | N-CA-C     | -5.04 | 105.91      | 111.71   |
| 1   | E     | 133 | SER  | N-CA-C     | -5.04 | 105.87      | 111.36   |
| 1   | K     | 165 | ILE  | N-CA-C     | 5.03  | 116.21      | 108.71   |
| 1   | V     | 74  | TYR  | N-CA-C     | 5.03  | 117.16      | 111.02   |
| 1   | f     | 121 | GLN  | N-CA-C     | -5.03 | 106.39      | 112.88   |
| 1   | M     | 230 | GLN  | CA-CB-CG   | 5.03  | 124.16      | 114.10   |
| 1   | E     | 106 | VAL  | CA-CB-CG2  | 5.03  | 118.95      | 110.40   |
| 1   | E     | 302 | ARG  | CA-CB-CG   | 5.02  | 124.14      | 114.10   |
| 1   | I     | 57  | SER  | N-CA-C     | 5.01  | 117.58      | 109.06   |
| 1   | K     | 314 | GLU  | CA-C-N     | -5.01 | 114.62      | 119.78   |
| 1   | K     | 314 | GLU  | C-N-CA     | -5.01 | 114.62      | 119.78   |
| 1   | C     | 311 | THR  | N-CA-C     | -5.01 | 103.76      | 110.07   |
| 1   | R     | 211 | LYS  | CA-CB-CG   | 5.01  | 124.12      | 114.10   |
| 1   | U     | 180 | VAL  | CG1-CB-CG2 | 5.01  | 121.82      | 110.80   |
| 1   | A     | 97  | VAL  | N-CA-C     | 5.01  | 115.78      | 110.72   |
| 1   | D     | 303 | PHE  | N-CA-C     | -5.01 | 103.92      | 110.53   |
| 1   | O     | 126 | LYS  | CB-CA-C    | 5.01  | 119.10      | 110.79   |
| 1   | E     | 229 | GLU  | N-CA-C     | 5.01  | 117.12      | 111.11   |
| 1   | b     | 268 | ARG  | N-CA-C     | 5.01  | 117.47      | 111.71   |
| 1   | L     | 57  | SER  | N-CA-C     | 5.00  | 117.56      | 109.06   |

All (33) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 59  | THR  | CB   |
| 1   | A     | 168 | THR  | CB   |
| 1   | A     | 305 | THR  | CB   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | B     | 62  | THR  | CB   |
| 1   | F     | 59  | THR  | CB   |
| 1   | F     | 298 | THR  | CB   |
| 1   | I     | 59  | THR  | CB   |
| 1   | J     | 203 | THR  | CB   |
| 1   | L     | 59  | THR  | CB   |
| 1   | M     | 144 | ILE  | CB   |
| 1   | M     | 220 | ILE  | CB   |
| 1   | M     | 228 | ILE  | CB   |
| 1   | N     | 147 | ILE  | CB   |
| 1   | O     | 144 | ILE  | CB   |
| 1   | P     | 220 | ILE  | CB   |
| 1   | Q     | 122 | THR  | CB   |
| 1   | Q     | 292 | THR  | CB   |
| 1   | Q     | 298 | THR  | CB   |
| 1   | R     | 59  | THR  | CB   |
| 1   | R     | 298 | THR  | CB   |
| 1   | U     | 155 | THR  | CB   |
| 1   | W     | 122 | THR  | CB   |
| 1   | X     | 66  | THR  | CB   |
| 1   | Y     | 292 | THR  | CB   |
| 1   | a     | 59  | THR  | CB   |
| 1   | a     | 66  | THR  | CB   |
| 1   | b     | 59  | THR  | CB   |
| 1   | c     | 165 | ILE  | CB   |
| 1   | d     | 59  | THR  | CB   |
| 1   | d     | 305 | THR  | CB   |
| 1   | e     | 59  | THR  | CB   |
| 1   | e     | 144 | ILE  | CB   |
| 1   | e     | 220 | ILE  | CB   |

All (13) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 215 | GLU  | Sidechain |
| 1   | B     | 279 | PHE  | Sidechain |
| 1   | I     | 148 | GLN  | Sidechain |
| 1   | J     | 300 | ASP  | Sidechain |
| 1   | M     | 148 | GLN  | Sidechain |
| 1   | S     | 273 | GLN  | Sidechain |
| 1   | T     | 280 | ASP  | Sidechain |
| 1   | V     | 148 | GLN  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | W     | 142 | GLU  | Sidechain |
| 1   | X     | 300 | ASP  | Sidechain |
| 1   | a     | 148 | GLN  | Sidechain |
| 1   | a     | 266 | GLN  | Sidechain |
| 1   | e     | 84  | ASP  | Sidechain |

## 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     | 1797  | 0        | 1748     | 68      | 0            |
| 1   | B     | 1797  | 0        | 1748     | 76      | 0            |
| 1   | C     | 1797  | 0        | 1748     | 52      | 0            |
| 1   | D     | 1797  | 0        | 1748     | 73      | 1            |
| 1   | E     | 1797  | 0        | 1748     | 54      | 0            |
| 1   | F     | 1797  | 0        | 1748     | 87      | 0            |
| 1   | G     | 1797  | 0        | 1748     | 70      | 0            |
| 1   | H     | 1797  | 0        | 1748     | 79      | 0            |
| 1   | I     | 1797  | 0        | 1748     | 54      | 0            |
| 1   | J     | 1797  | 0        | 1748     | 64      | 0            |
| 1   | K     | 1797  | 0        | 1748     | 60      | 0            |
| 1   | L     | 1797  | 0        | 1748     | 65      | 1            |
| 1   | M     | 1797  | 0        | 1748     | 70      | 0            |
| 1   | N     | 1797  | 0        | 1748     | 59      | 0            |
| 1   | O     | 1797  | 0        | 1748     | 62      | 0            |
| 1   | P     | 1797  | 0        | 1748     | 78      | 0            |
| 1   | Q     | 1797  | 0        | 1748     | 62      | 0            |
| 1   | R     | 1797  | 0        | 1748     | 62      | 0            |
| 1   | S     | 1797  | 0        | 1748     | 81      | 0            |
| 1   | T     | 1797  | 0        | 1747     | 81      | 0            |
| 1   | U     | 1797  | 0        | 1748     | 84      | 0            |
| 1   | V     | 1797  | 0        | 1748     | 61      | 0            |
| 1   | W     | 1797  | 0        | 1748     | 78      | 0            |
| 1   | X     | 1797  | 0        | 1748     | 64      | 0            |
| 1   | Y     | 1797  | 0        | 1748     | 64      | 0            |
| 1   | Z     | 1797  | 0        | 1748     | 67      | 0            |
| 1   | a     | 1797  | 0        | 1748     | 68      | 0            |
| 1   | b     | 1797  | 0        | 1748     | 81      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | c     | 1797  | 0        | 1748     | 64      | 0            |
| 1   | d     | 1797  | 0        | 1748     | 67      | 0            |
| 1   | e     | 1797  | 0        | 1748     | 63      | 0            |
| 1   | f     | 1797  | 0        | 1748     | 85      | 0            |
| All | All   | 57504 | 0        | 55935    | 2019    | 1            |

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 18.

All (2019) 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:T:96:SER:OG   | 1:T:98:MET:SD    | 1.93                     | 1.26              |
| 1:G:125:TYR:HD1 | 1:G:143:MET:HE3  | 1.09                     | 1.16              |
| 1:B:225:MET:HE1 | 1:B:273:GLN:HG2  | 1.24                     | 1.10              |
| 1:T:196:LYS:HG3 | 1:T:299:LEU:HD21 | 1.38                     | 1.04              |
| 1:Q:105:PHE:HB2 | 1:Q:305:THR:HG23 | 1.35                     | 1.03              |
| 1:X:126:LYS:HA  | 1:X:129:MET:HG3  | 1.40                     | 1.01              |
| 1:S:96:SER:OG   | 1:S:98:MET:SD    | 2.20                     | 0.99              |
| 1:M:105:PHE:HB2 | 1:M:305:THR:HG23 | 1.45                     | 0.98              |
| 1:W:194:GLU:OE2 | 1:X:66:THR:OG1   | 1.84                     | 0.96              |
| 1:G:125:TYR:CD1 | 1:G:143:MET:HE3  | 2.01                     | 0.96              |
| 1:A:98:MET:H    | 1:A:98:MET:HE3   | 1.29                     | 0.95              |
| 1:U:126:LYS:HA  | 1:U:129:MET:HG3  | 1.46                     | 0.95              |
| 1:E:211:LYS:HE3 | 1:E:211:LYS:HA   | 1.44                     | 0.95              |
| 1:W:61:ILE:HB   | 1:W:310:ARG:HB3  | 1.46                     | 0.95              |
| 1:P:187:ALA:HB3 | 1:P:305:THR:HG21 | 1.48                     | 0.95              |
| 1:b:61:ILE:HB   | 1:b:310:ARG:HB3  | 1.46                     | 0.95              |
| 1:A:61:ILE:HG13 | 1:A:310:ARG:HB3  | 1.50                     | 0.93              |
| 1:J:211:LYS:HA  | 1:J:211:LYS:HE3  | 1.50                     | 0.93              |
| 1:P:105:PHE:HB2 | 1:P:305:THR:HG23 | 1.48                     | 0.93              |
| 1:B:105:PHE:HB2 | 1:B:305:THR:HG23 | 1.49                     | 0.93              |
| 1:e:268:ARG:HG2 | 1:e:268:ARG:HH11 | 1.34                     | 0.92              |
| 1:Z:72:GLY:O    | 1:Z:76:GLN:NE2   | 2.01                     | 0.92              |
| 1:P:83:LEU:HB3  | 1:P:202:ARG:HH11 | 1.33                     | 0.91              |
| 1:E:61:ILE:HB   | 1:E:310:ARG:HB3  | 1.52                     | 0.91              |
| 1:J:64:ARG:HD3  | 1:J:99:ASP:HA    | 1.51                     | 0.90              |
| 1:R:107:MET:HE3 | 1:S:309:LEU:HD22 | 1.50                     | 0.90              |
| 1:d:61:ILE:HB   | 1:d:310:ARG:HB3  | 1.53                     | 0.90              |
| 1:U:230:GLN:OE1 | 1:U:230:GLN:N    | 2.04                     | 0.89              |
| 1:T:98:MET:SD   | 1:T:98:MET:N     | 2.45                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:126:LYS:HA   | 1:A:129:MET:HG3  | 1.55                     | 0.89              |
| 1:M:230:GLN:OE1  | 1:M:230:GLN:N    | 2.06                     | 0.88              |
| 1:F:98:MET:SD    | 1:F:98:MET:N     | 2.47                     | 0.88              |
| 1:f:105:PHE:HB2  | 1:f:305:THR:HG23 | 1.55                     | 0.88              |
| 1:F:290:LEU:O    | 1:F:294:ASN:ND2  | 2.05                     | 0.88              |
| 1:a:207:LYS:HE3  | 1:a:294:ASN:HD21 | 1.35                     | 0.87              |
| 1:G:200:ALA:O    | 1:O:302:ARG:NH2  | 2.07                     | 0.87              |
| 1:K:225:MET:HA   | 1:K:272:LEU:HD21 | 1.55                     | 0.87              |
| 1:D:187:ALA:HB3  | 1:D:305:THR:HG21 | 1.54                     | 0.87              |
| 1:K:105:PHE:HB2  | 1:K:305:THR:HG23 | 1.57                     | 0.87              |
| 1:S:105:PHE:HB2  | 1:S:305:THR:HG23 | 1.55                     | 0.87              |
| 1:H:207:LYS:HG3  | 1:H:290:LEU:HD21 | 1.55                     | 0.86              |
| 1:P:203:THR:O    | 1:P:207:LYS:HG3  | 1.74                     | 0.86              |
| 1:F:187:ALA:HB3  | 1:F:305:THR:HG21 | 1.57                     | 0.86              |
| 1:B:225:MET:CE   | 1:B:273:GLN:HG2  | 2.05                     | 0.86              |
| 1:D:105:PHE:HB2  | 1:D:305:THR:HG23 | 1.56                     | 0.85              |
| 1:E:300:ASP:OD1  | 1:E:302:ARG:NH1  | 2.10                     | 0.85              |
| 1:J:202:ARG:HH21 | 1:J:205:GLN:HG2  | 1.41                     | 0.85              |
| 1:J:271:ASN:O    | 1:J:275:VAL:HG23 | 1.75                     | 0.85              |
| 1:E:275:VAL:HG13 | 1:E:276:GLY:H    | 1.42                     | 0.84              |
| 1:c:168:THR:OG1  | 1:c:171:ASP:OD2  | 1.95                     | 0.84              |
| 1:f:187:ALA:HB3  | 1:f:305:THR:HG21 | 1.59                     | 0.84              |
| 1:L:72:GLY:O     | 1:L:76:GLN:HG3   | 1.78                     | 0.83              |
| 1:V:225:MET:HE1  | 1:V:273:GLN:HG3  | 1.59                     | 0.82              |
| 1:G:122:THR:HG22 | 1:G:125:TYR:H    | 1.44                     | 0.82              |
| 1:S:68:ASN:HD22  | 1:S:68:ASN:H     | 1.25                     | 0.82              |
| 1:A:69:MET:HE1   | 1:A:307:ARG:HB3  | 1.62                     | 0.82              |
| 1:D:180:VAL:HG21 | 1:D:308:TYR:OH   | 1.80                     | 0.82              |
| 1:U:66:THR:OG1   | 1:U:69:MET:HE3   | 1.80                     | 0.82              |
| 1:b:229:GLU:HG3  | 1:b:269:LEU:HD11 | 1.62                     | 0.81              |
| 1:O:107:MET:HE3  | 1:P:63:ASP:OD2   | 1.80                     | 0.81              |
| 1:Z:227:SER:HB2  | 1:a:275:VAL:HG23 | 1.61                     | 0.81              |
| 1:f:202:ARG:HH21 | 1:f:205:GLN:NE2  | 1.78                     | 0.81              |
| 1:C:105:PHE:HB2  | 1:C:305:THR:HG23 | 1.62                     | 0.81              |
| 1:U:134:LYS:NZ   | 1:V:316:VAL:O    | 2.13                     | 0.80              |
| 1:E:98:MET:HE3   | 1:E:98:MET:H     | 1.46                     | 0.80              |
| 1:K:70:LEU:HD11  | 1:K:98:MET:HB3   | 1.63                     | 0.80              |
| 1:V:177:ARG:NH2  | 1:V:312:PRO:O    | 2.15                     | 0.80              |
| 1:T:199:TRP:NE1  | 1:T:293:LEU:O    | 2.10                     | 0.80              |
| 1:R:224:ARG:O    | 1:R:228:ILE:HG13 | 1.81                     | 0.80              |
| 1:A:105:PHE:HB2  | 1:A:305:THR:HG23 | 1.62                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:316:VAL:O    | 1:X:134:LYS:NZ   | 2.14                     | 0.80              |
| 1:I:105:PHE:HB2  | 1:I:305:THR:HG23 | 1.62                     | 0.80              |
| 1:L:105:PHE:HB2  | 1:L:305:THR:HG23 | 1.64                     | 0.80              |
| 1:P:83:LEU:HB3   | 1:P:202:ARG:NH1  | 1.96                     | 0.80              |
| 1:L:185:GLN:O    | 1:L:189:SER:OG   | 2.00                     | 0.79              |
| 1:Z:105:PHE:HB2  | 1:Z:305:THR:HG23 | 1.62                     | 0.79              |
| 1:T:187:ALA:HB3  | 1:T:305:THR:HG21 | 1.64                     | 0.79              |
| 1:F:61:ILE:HG12  | 1:F:161:SER:HB3  | 1.64                     | 0.79              |
| 1:X:81:ARG:NH1   | 1:X:95:PRO:O     | 2.15                     | 0.79              |
| 1:Z:271:ASN:O    | 1:Z:275:VAL:HG23 | 1.83                     | 0.79              |
| 1:P:72:GLY:O     | 1:P:76:GLN:HG3   | 1.83                     | 0.79              |
| 1:E:105:PHE:HB2  | 1:E:305:THR:HG23 | 1.65                     | 0.78              |
| 1:J:202:ARG:NH2  | 1:J:205:GLN:HG2  | 1.99                     | 0.78              |
| 1:T:202:ARG:HE   | 1:T:205:GLN:HG3  | 1.50                     | 0.77              |
| 1:b:163:LYS:HG2  | 1:b:164:LEU:N    | 1.99                     | 0.77              |
| 1:K:225:MET:HB2  | 1:K:272:LEU:HD11 | 1.66                     | 0.77              |
| 1:f:202:ARG:HH21 | 1:f:205:GLN:HE21 | 1.31                     | 0.77              |
| 1:U:96:SER:OG    | 1:U:98:MET:HG2   | 1.85                     | 0.77              |
| 1:B:225:MET:HE1  | 1:B:273:GLN:CG   | 2.09                     | 0.76              |
| 1:A:98:MET:HE3   | 1:A:98:MET:N     | 1.99                     | 0.76              |
| 1:B:117:GLU:OE1  | 1:B:186:ARG:NH1  | 2.17                     | 0.76              |
| 1:D:225:MET:HE1  | 1:D:273:GLN:HA   | 1.66                     | 0.76              |
| 1:W:173:ASN:OD1  | 1:W:177:ARG:NE   | 2.17                     | 0.76              |
| 1:G:125:TYR:HD1  | 1:G:143:MET:CE   | 1.95                     | 0.76              |
| 1:c:187:ALA:HB3  | 1:c:305:THR:HG21 | 1.65                     | 0.76              |
| 1:C:132:ASN:HD22 | 1:C:135:ALA:H    | 1.32                     | 0.76              |
| 1:Z:228:ILE:HD12 | 1:Z:272:LEU:HD22 | 1.68                     | 0.76              |
| 1:V:300:ASP:OD1  | 1:V:302:ARG:HD3  | 1.85                     | 0.75              |
| 1:W:105:PHE:HB2  | 1:W:305:THR:HG22 | 1.68                     | 0.75              |
| 1:W:207:LYS:NZ   | 1:W:294:ASN:HD21 | 1.83                     | 0.75              |
| 1:W:74:TYR:HE1   | 1:W:98:MET:HE1   | 1.52                     | 0.75              |
| 1:G:204:ILE:HD12 | 1:O:302:ARG:CZ   | 2.16                     | 0.75              |
| 1:Q:69:MET:HE1   | 1:Q:307:ARG:HB3  | 1.66                     | 0.75              |
| 1:U:132:ASN:HD22 | 1:U:135:ALA:H    | 1.32                     | 0.75              |
| 1:S:68:ASN:H     | 1:S:68:ASN:ND2   | 1.81                     | 0.75              |
| 1:Y:61:ILE:HG13  | 1:Y:310:ARG:HB3  | 1.69                     | 0.75              |
| 1:A:292:THR:HG21 | 1:H:212:ARG:HD3  | 1.70                     | 0.74              |
| 1:L:119:TRP:CE2  | 1:L:143:MET:HB3  | 2.22                     | 0.74              |
| 1:T:105:PHE:HB2  | 1:T:305:THR:HG23 | 1.70                     | 0.74              |
| 1:P:228:ILE:HD12 | 1:P:272:LEU:HD22 | 1.67                     | 0.74              |
| 1:I:98:MET:N     | 1:I:98:MET:SD    | 2.61                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:203:THR:HG23 | 1:J:293:LEU:HB3  | 1.70                     | 0.74              |
| 1:M:206:MET:HE3  | 1:M:286:ASN:HB3  | 1.69                     | 0.74              |
| 1:U:139:LEU:HG   | 1:U:143:MET:HE3  | 1.69                     | 0.74              |
| 1:V:227:SER:HB2  | 1:W:275:VAL:HG23 | 1.70                     | 0.74              |
| 1:d:70:LEU:HD11  | 1:d:98:MET:HG2   | 1.70                     | 0.73              |
| 1:a:61:ILE:HG13  | 1:a:310:ARG:HB3  | 1.69                     | 0.73              |
| 1:e:140:LEU:O    | 1:e:144:ILE:HG13 | 1.88                     | 0.73              |
| 1:H:213:GLN:HE22 | 1:H:286:ASN:HD22 | 1.36                     | 0.73              |
| 1:S:68:ASN:HD22  | 1:S:68:ASN:N     | 1.83                     | 0.73              |
| 1:T:196:LYS:CG   | 1:T:299:LEU:HD21 | 2.17                     | 0.73              |
| 1:G:200:ALA:C    | 1:O:302:ARG:HH22 | 1.96                     | 0.73              |
| 1:b:80:LEU:HD12  | 1:b:195:LEU:HD12 | 1.70                     | 0.73              |
| 1:A:316:VAL:HG23 | 1:A:317:LYS:HD3  | 1.70                     | 0.73              |
| 1:H:105:PHE:HB2  | 1:H:305:THR:HG23 | 1.71                     | 0.73              |
| 1:a:202:ARG:NH2  | 1:a:205:GLN:OE1  | 2.21                     | 0.73              |
| 1:A:70:LEU:HD11  | 1:A:98:MET:HB3   | 1.69                     | 0.73              |
| 1:A:60:ALA:HB2   | 1:A:312:PRO:HG3  | 1.71                     | 0.72              |
| 1:E:64:ARG:NE    | 1:E:99:ASP:OD1   | 2.20                     | 0.72              |
| 1:Q:187:ALA:HB3  | 1:Q:305:THR:HG21 | 1.70                     | 0.72              |
| 1:F:122:THR:HG22 | 1:F:125:TYR:H    | 1.54                     | 0.72              |
| 1:a:132:ASN:HD22 | 1:a:135:ALA:H    | 1.36                     | 0.72              |
| 1:b:64:ARG:NE    | 1:b:99:ASP:OD1   | 2.23                     | 0.72              |
| 1:O:228:ILE:HD13 | 1:O:268:ARG:HB3  | 1.70                     | 0.72              |
| 1:F:74:TYR:CE1   | 1:F:98:MET:HE1   | 2.25                     | 0.72              |
| 1:F:105:PHE:HB2  | 1:F:305:THR:HG23 | 1.72                     | 0.72              |
| 1:H:199:TRP:CD1  | 1:H:297:PRO:HD3  | 2.25                     | 0.72              |
| 1:U:63:ASP:OD1   | 1:U:64:ARG:HG2   | 1.90                     | 0.71              |
| 1:J:115:ARG:HG2  | 1:J:147:ILE:HD12 | 1.73                     | 0.71              |
| 1:I:207:LYS:HG3  | 1:I:290:LEU:HD11 | 1.73                     | 0.71              |
| 1:c:107:MET:HE2  | 1:d:63:ASP:OD2   | 1.90                     | 0.71              |
| 1:Y:307:ARG:NH2  | 1:f:107:MET:SD   | 2.63                     | 0.71              |
| 1:C:318:ARG:H    | 1:C:318:ARG:HD2  | 1.56                     | 0.71              |
| 1:I:152:GLY:N    | 1:I:160:ASP:OD2  | 2.20                     | 0.71              |
| 1:Z:81:ARG:NH1   | 1:Z:95:PRO:O     | 2.22                     | 0.71              |
| 1:B:187:ALA:HB3  | 1:B:305:THR:HG21 | 1.70                     | 0.71              |
| 1:N:60:ALA:HB2   | 1:N:312:PRO:HG3  | 1.71                     | 0.71              |
| 1:K:132:ASN:HD22 | 1:K:135:ALA:H    | 1.38                     | 0.71              |
| 1:M:103:LYS:O    | 1:M:107:MET:HG2  | 1.90                     | 0.71              |
| 1:S:225:MET:HE1  | 1:S:273:GLN:HG3  | 1.70                     | 0.71              |
| 1:S:212:ARG:HG2  | 1:T:288:ALA:HB1  | 1.73                     | 0.71              |
| 1:W:207:LYS:HZ3  | 1:W:294:ASN:HD21 | 1.39                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:77:GLN:HG2   | 1:e:97:VAL:HG11  | 1.73                     | 0.71              |
| 1:C:187:ALA:HB3  | 1:C:305:THR:HG21 | 1.72                     | 0.70              |
| 1:H:210:VAL:HG22 | 1:H:286:ASN:HB3  | 1.73                     | 0.70              |
| 1:P:203:THR:HG22 | 1:P:207:LYS:HE3  | 1.72                     | 0.70              |
| 1:X:119:TRP:CE2  | 1:X:143:MET:HB3  | 2.26                     | 0.70              |
| 1:U:132:ASN:ND2  | 1:U:135:ALA:H    | 1.89                     | 0.70              |
| 1:L:57:SER:HB2   | 1:L:163:LYS:HE3  | 1.73                     | 0.70              |
| 1:S:225:MET:HA   | 1:S:272:LEU:HD21 | 1.73                     | 0.70              |
| 1:J:96:SER:OG    | 1:J:98:MET:HE2   | 1.91                     | 0.70              |
| 1:W:124:TYR:CG   | 1:W:175:LEU:HD11 | 2.26                     | 0.70              |
| 1:W:164:LEU:HB2  | 1:W:176:LEU:HD13 | 1.72                     | 0.70              |
| 1:W:202:ARG:NH2  | 1:W:205:GLN:OE1  | 2.24                     | 0.70              |
| 1:J:105:PHE:HB2  | 1:J:305:THR:HG23 | 1.74                     | 0.70              |
| 1:O:212:ARG:HH11 | 1:P:292:THR:HG21 | 1.57                     | 0.70              |
| 1:E:98:MET:HE3   | 1:E:98:MET:N     | 2.07                     | 0.70              |
| 1:Z:211:LYS:HA   | 1:Z:211:LYS:HE3  | 1.73                     | 0.70              |
| 1:X:80:LEU:HD23  | 1:X:83:LEU:HD12  | 1.73                     | 0.70              |
| 1:D:98:MET:SD    | 1:D:98:MET:N     | 2.59                     | 0.70              |
| 1:T:287:ARG:NH2  | 1:b:295:VAL:O    | 2.25                     | 0.70              |
| 1:A:224:ARG:HA   | 1:A:227:SER:OG   | 1.92                     | 0.69              |
| 1:F:210:VAL:HA   | 1:F:213:GLN:HE21 | 1.55                     | 0.69              |
| 1:G:210:VAL:HA   | 1:G:213:GLN:HE21 | 1.55                     | 0.69              |
| 1:Z:70:LEU:HD11  | 1:Z:98:MET:HB3   | 1.73                     | 0.69              |
| 1:P:61:ILE:HB    | 1:P:310:ARG:HB3  | 1.74                     | 0.69              |
| 1:B:141:ASP:HA   | 1:B:144:ILE:HD12 | 1.73                     | 0.69              |
| 1:P:119:TRP:NE1  | 1:P:143:MET:O    | 2.25                     | 0.69              |
| 1:T:83:LEU:HB3   | 1:T:202:ARG:HH11 | 1.57                     | 0.69              |
| 1:a:105:PHE:HB2  | 1:a:305:THR:HG23 | 1.74                     | 0.69              |
| 1:f:80:LEU:HD23  | 1:f:83:LEU:HD12  | 1.74                     | 0.69              |
| 1:d:113:ASP:OD2  | 1:e:311:THR:OG1  | 2.09                     | 0.69              |
| 1:A:307:ARG:HH22 | 1:H:104:GLU:CD   | 2.01                     | 0.69              |
| 1:J:122:THR:HG23 | 1:J:125:TYR:H    | 1.57                     | 0.69              |
| 1:J:194:GLU:OE2  | 1:K:68:ASN:ND2   | 2.25                     | 0.69              |
| 1:Q:304:GLN:NE2  | 1:Q:306:TYR:O    | 2.24                     | 0.69              |
| 1:U:80:LEU:HD23  | 1:U:83:LEU:HD12  | 1.73                     | 0.69              |
| 1:R:194:GLU:OE2  | 1:S:68:ASN:ND2   | 2.26                     | 0.69              |
| 1:T:295:VAL:HG21 | 1:b:300:ASP:HB2  | 1.73                     | 0.69              |
| 1:V:316:VAL:HG23 | 1:V:317:LYS:HD3  | 1.74                     | 0.69              |
| 1:H:147:ILE:HG12 | 1:H:164:LEU:HD12 | 1.75                     | 0.68              |
| 1:U:83:LEU:HB3   | 1:U:202:ARG:HH11 | 1.58                     | 0.68              |
| 1:J:64:ARG:CD    | 1:J:99:ASP:HA    | 2.24                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:106:VAL:HG13 | 1:R:149:PHE:CZ   | 2.29                     | 0.68              |
| 1:E:132:ASN:HD22 | 1:E:135:ALA:H    | 1.40                     | 0.68              |
| 1:G:300:ASP:OD1  | 1:G:302:ARG:NH1  | 2.27                     | 0.68              |
| 1:Y:60:ALA:HB2   | 1:Y:312:PRO:HG3  | 1.76                     | 0.68              |
| 1:b:76:GLN:OE1   | 1:b:298:THR:N    | 2.23                     | 0.68              |
| 1:d:64:ARG:HE    | 1:d:99:ASP:HA    | 1.57                     | 0.68              |
| 1:R:80:LEU:HD23  | 1:R:83:LEU:HD12  | 1.73                     | 0.68              |
| 1:b:134:LYS:NZ   | 1:c:316:VAL:O    | 2.25                     | 0.68              |
| 1:C:213:GLN:HE22 | 1:C:286:ASN:HD22 | 1.40                     | 0.67              |
| 1:K:210:VAL:HG13 | 1:K:283:TYR:HE1  | 1.57                     | 0.67              |
| 1:M:132:ASN:HD22 | 1:M:135:ALA:H    | 1.42                     | 0.67              |
| 1:T:294:ASN:CB   | 1:b:298:THR:HG21 | 2.22                     | 0.67              |
| 1:D:228:ILE:HD12 | 1:D:272:LEU:HD22 | 1.75                     | 0.67              |
| 1:K:60:ALA:HB2   | 1:K:312:PRO:HG3  | 1.76                     | 0.67              |
| 1:J:211:LYS:HE3  | 1:J:211:LYS:CA   | 2.21                     | 0.67              |
| 1:L:96:SER:OG    | 1:L:98:MET:HG2   | 1.95                     | 0.67              |
| 1:T:207:LYS:HE3  | 1:T:294:ASN:HD21 | 1.58                     | 0.67              |
| 1:d:70:LEU:CD1   | 1:d:98:MET:HG2   | 2.25                     | 0.67              |
| 1:B:60:ALA:HB2   | 1:B:312:PRO:HG3  | 1.77                     | 0.67              |
| 1:E:185:GLN:HA   | 1:E:185:GLN:HE21 | 1.59                     | 0.67              |
| 1:T:156:ARG:HB3  | 1:T:158:VAL:HG23 | 1.76                     | 0.67              |
| 1:d:107:MET:HE2  | 1:e:307:ARG:HH12 | 1.59                     | 0.67              |
| 1:b:224:ARG:HB3  | 1:b:272:LEU:HD21 | 1.77                     | 0.67              |
| 1:T:295:VAL:CG2  | 1:b:300:ASP:HB2  | 2.24                     | 0.67              |
| 1:V:173:ASN:OD1  | 1:V:177:ARG:NE   | 2.26                     | 0.67              |
| 1:F:128:ARG:HB3  | 1:F:139:LEU:HD21 | 1.75                     | 0.67              |
| 1:N:173:ASN:OD1  | 1:N:177:ARG:NE   | 2.26                     | 0.67              |
| 1:P:207:LYS:HE2  | 1:P:294:ASN:HD21 | 1.60                     | 0.67              |
| 1:M:96:SER:OG    | 1:M:98:MET:HG2   | 1.95                     | 0.67              |
| 1:I:177:ARG:NH2  | 1:I:312:PRO:O    | 2.28                     | 0.67              |
| 1:R:112:TRP:HB3  | 1:S:310:ARG:HB2  | 1.77                     | 0.67              |
| 1:T:292:THR:HG22 | 1:b:302:ARG:HH12 | 1.59                     | 0.67              |
| 1:W:97:VAL:HB    | 1:W:98:MET:HE2   | 1.77                     | 0.67              |
| 1:X:207:LYS:HE3  | 1:X:294:ASN:HD21 | 1.59                     | 0.67              |
| 1:f:224:ARG:O    | 1:f:228:ILE:HG13 | 1.95                     | 0.67              |
| 1:T:63:ASP:OD1   | 1:T:64:ARG:HG2   | 1.95                     | 0.67              |
| 1:f:216:VAL:O    | 1:f:220:ILE:HG13 | 1.94                     | 0.67              |
| 1:S:187:ALA:HB3  | 1:S:305:THR:HG21 | 1.77                     | 0.66              |
| 1:H:207:LYS:HE3  | 1:H:294:ASN:HD21 | 1.61                     | 0.66              |
| 1:R:164:LEU:HB2  | 1:R:176:LEU:HD13 | 1.76                     | 0.66              |
| 1:R:177:ARG:NH2  | 1:R:312:PRO:O    | 2.27                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:168:THR:OG1  | 1:D:171:ASP:OD2  | 2.11                     | 0.66              |
| 1:E:69:MET:HB3   | 1:E:304:GLN:HB3  | 1.77                     | 0.66              |
| 1:d:72:GLY:O     | 1:d:76:GLN:HG3   | 1.95                     | 0.66              |
| 1:f:83:LEU:HB3   | 1:f:202:ARG:HH11 | 1.61                     | 0.66              |
| 1:S:224:ARG:HA   | 1:S:227:SER:OG   | 1.96                     | 0.66              |
| 1:G:200:ALA:HB1  | 1:O:302:ARG:HH12 | 1.60                     | 0.66              |
| 1:N:202:ARG:NH2  | 1:N:205:GLN:OE1  | 2.28                     | 0.66              |
| 1:Q:216:VAL:O    | 1:Q:220:ILE:HG13 | 1.95                     | 0.66              |
| 1:V:128:ARG:HD3  | 1:V:143:MET:HE1  | 1.77                     | 0.66              |
| 1:L:83:LEU:HB3   | 1:L:202:ARG:HH11 | 1.61                     | 0.66              |
| 1:C:288:ALA:O    | 1:C:291:ASN:HB2  | 1.96                     | 0.66              |
| 1:F:283:TYR:CZ   | 1:F:287:ARG:HD3  | 2.30                     | 0.66              |
| 1:T:177:ARG:NH2  | 1:T:312:PRO:O    | 2.29                     | 0.66              |
| 1:G:128:ARG:HE   | 1:G:167:GLU:CD   | 2.04                     | 0.66              |
| 1:L:187:ALA:HB3  | 1:L:305:THR:HG21 | 1.78                     | 0.66              |
| 1:M:83:LEU:HD21  | 1:M:289:MET:HE2  | 1.78                     | 0.66              |
| 1:M:216:VAL:O    | 1:M:220:ILE:HG13 | 1.95                     | 0.65              |
| 1:S:225:MET:HB2  | 1:S:272:LEU:HD11 | 1.78                     | 0.65              |
| 1:Y:141:ASP:HA   | 1:Y:144:ILE:HD12 | 1.78                     | 0.65              |
| 1:D:126:LYS:O    | 1:D:129:MET:HG2  | 1.95                     | 0.65              |
| 1:N:126:LYS:O    | 1:N:129:MET:HG3  | 1.96                     | 0.65              |
| 1:J:202:ARG:HH21 | 1:J:205:GLN:CG   | 2.09                     | 0.65              |
| 1:D:76:GLN:NE2   | 1:D:298:THR:O    | 2.21                     | 0.65              |
| 1:F:64:ARG:HE    | 1:F:99:ASP:HA    | 1.59                     | 0.65              |
| 1:E:70:LEU:HB2   | 1:E:74:TYR:HB2   | 1.78                     | 0.65              |
| 1:N:64:ARG:HE    | 1:N:99:ASP:HA    | 1.61                     | 0.65              |
| 1:O:202:ARG:NH2  | 1:O:205:GLN:OE1  | 2.30                     | 0.65              |
| 1:f:164:LEU:HB2  | 1:f:176:LEU:HD13 | 1.78                     | 0.65              |
| 1:M:114:THR:HG23 | 1:M:186:ARG:HD3  | 1.77                     | 0.65              |
| 1:R:64:ARG:HB3   | 1:R:102:TYR:HB2  | 1.79                     | 0.65              |
| 1:A:66:THR:HG21  | 1:H:190:HIS:HE1  | 1.62                     | 0.65              |
| 1:R:122:THR:HG22 | 1:R:125:TYR:H    | 1.61                     | 0.65              |
| 1:U:211:LYS:HA   | 1:U:211:LYS:HE3  | 1.78                     | 0.65              |
| 1:R:105:PHE:HB2  | 1:R:305:THR:HG23 | 1.79                     | 0.65              |
| 1:N:61:ILE:HB    | 1:N:310:ARG:HB3  | 1.79                     | 0.64              |
| 1:J:223:ARG:HH12 | 1:K:284:ASP:CG   | 2.06                     | 0.64              |
| 1:S:226:ASN:OD1  | 1:S:230:GLN:NE2  | 2.30                     | 0.64              |
| 1:W:132:ASN:HB3  | 1:W:135:ALA:HB3  | 1.78                     | 0.64              |
| 1:H:139:LEU:HD11 | 1:H:143:MET:HE3  | 1.79                     | 0.64              |
| 1:M:112:TRP:HB3  | 1:N:310:ARG:HB2  | 1.78                     | 0.64              |
| 1:M:122:THR:HG22 | 1:M:125:TYR:H    | 1.62                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:56:TRP:HB3   | 1:c:315:PRO:HG2  | 1.79                     | 0.64              |
| 1:F:177:ARG:NH2  | 1:F:312:PRO:O    | 2.31                     | 0.64              |
| 1:H:210:VAL:CG2  | 1:H:286:ASN:HB3  | 2.27                     | 0.64              |
| 1:T:223:ARG:HH12 | 1:U:284:ASP:CG   | 2.04                     | 0.64              |
| 1:B:61:ILE:HG22  | 1:B:309:LEU:HB2  | 1.80                     | 0.64              |
| 1:F:210:VAL:HG11 | 1:F:290:LEU:HD12 | 1.80                     | 0.64              |
| 1:K:202:ARG:NH2  | 1:K:205:GLN:OE1  | 2.28                     | 0.64              |
| 1:L:60:ALA:HB2   | 1:L:312:PRO:HG3  | 1.80                     | 0.64              |
| 1:R:173:ASN:OD1  | 1:R:177:ARG:NE   | 2.27                     | 0.64              |
| 1:Z:64:ARG:HG2   | 1:Z:102:TYR:CG   | 2.32                     | 0.64              |
| 1:Z:190:HIS:CE1  | 1:a:66:THR:HG21  | 2.33                     | 0.64              |
| 1:I:124:TYR:OH   | 1:I:167:GLU:N    | 2.31                     | 0.64              |
| 1:W:58:SER:HB2   | 1:W:176:LEU:HD23 | 1.79                     | 0.64              |
| 1:A:66:THR:HG21  | 1:H:190:HIS:CE1  | 2.32                     | 0.64              |
| 1:H:141:ASP:HA   | 1:H:144:ILE:HD12 | 1.79                     | 0.64              |
| 1:H:302:ARG:HH22 | 1:O:186:ARG:HG2  | 1.61                     | 0.64              |
| 1:c:226:ASN:OD1  | 1:c:230:GLN:NE2  | 2.30                     | 0.64              |
| 1:d:66:THR:H     | 1:d:69:MET:HB2   | 1.63                     | 0.64              |
| 1:C:132:ASN:ND2  | 1:C:135:ALA:H    | 1.95                     | 0.64              |
| 1:D:223:ARG:HH12 | 1:E:284:ASP:CG   | 2.06                     | 0.64              |
| 1:N:177:ARG:NH2  | 1:N:312:PRO:O    | 2.31                     | 0.63              |
| 1:W:124:TYR:CD2  | 1:W:175:LEU:HD11 | 2.33                     | 0.63              |
| 1:d:61:ILE:HG22  | 1:d:309:LEU:HB2  | 1.81                     | 0.63              |
| 1:f:56:TRP:O     | 1:f:165:ILE:HA   | 1.99                     | 0.63              |
| 1:O:112:TRP:CZ2  | 1:O:144:ILE:HD12 | 2.33                     | 0.63              |
| 1:O:122:THR:O    | 1:O:126:LYS:HG2  | 1.97                     | 0.63              |
| 1:b:69:MET:CG    | 1:b:304:GLN:HB3  | 2.28                     | 0.63              |
| 1:V:64:ARG:HE    | 1:V:99:ASP:HA    | 1.63                     | 0.63              |
| 1:H:210:VAL:HA   | 1:H:213:GLN:HE21 | 1.63                     | 0.63              |
| 1:V:230:GLN:OE1  | 1:V:230:GLN:N    | 2.30                     | 0.63              |
| 1:V:225:MET:HE1  | 1:V:273:GLN:CG   | 2.26                     | 0.63              |
| 1:b:69:MET:HG2   | 1:b:304:GLN:HB3  | 1.81                     | 0.63              |
| 1:I:58:SER:OG    | 1:I:313:GLU:O    | 2.16                     | 0.63              |
| 1:T:223:ARG:NH1  | 1:U:284:ASP:OD2  | 2.29                     | 0.63              |
| 1:G:196:LYS:HE2  | 1:O:298:THR:HG22 | 1.79                     | 0.63              |
| 1:N:66:THR:OG1   | 1:N:69:MET:HE2   | 1.97                     | 0.63              |
| 1:b:96:SER:OG    | 1:b:98:MET:HG2   | 1.99                     | 0.63              |
| 1:F:182:PHE:CE2  | 1:F:186:ARG:HD2  | 2.34                     | 0.62              |
| 1:F:290:LEU:HD22 | 1:F:294:ASN:HD21 | 1.64                     | 0.62              |
| 1:K:61:ILE:HB    | 1:K:310:ARG:HB3  | 1.80                     | 0.62              |
| 1:M:111:SER:HB3  | 1:M:114:THR:OG1  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:66:THR:HG21  | 1:X:190:HIS:CE1  | 2.34                     | 0.62              |
| 1:G:196:LYS:NZ   | 1:O:296:GLY:O    | 2.32                     | 0.62              |
| 1:H:74:TYR:CE1   | 1:H:98:MET:HE1   | 2.33                     | 0.62              |
| 1:P:205:GLN:HG3  | 1:P:206:MET:N    | 2.14                     | 0.62              |
| 1:Q:119:TRP:NE1  | 1:Q:143:MET:O    | 2.32                     | 0.62              |
| 1:Z:190:HIS:NE2  | 1:a:66:THR:HG21  | 2.14                     | 0.62              |
| 1:F:74:TYR:HE1   | 1:F:98:MET:HE1   | 1.64                     | 0.62              |
| 1:X:67:VAL:HG22  | 1:X:98:MET:HE1   | 1.81                     | 0.62              |
| 1:Z:223:ARG:NH2  | 1:a:284:ASP:OD1  | 2.17                     | 0.62              |
| 1:c:105:PHE:HB2  | 1:c:305:THR:HG23 | 1.81                     | 0.62              |
| 1:M:122:THR:CG2  | 1:M:125:TYR:H    | 2.12                     | 0.62              |
| 1:X:206:MET:O    | 1:X:210:VAL:HG22 | 1.99                     | 0.62              |
| 1:a:101:ALA:HA   | 1:a:191:LEU:HD11 | 1.80                     | 0.62              |
| 1:D:119:TRP:CD2  | 1:D:143:MET:HG3  | 2.35                     | 0.62              |
| 1:H:116:ARG:HG3  | 1:H:144:ILE:HD11 | 1.81                     | 0.62              |
| 1:J:74:TYR:OH    | 1:J:78:GLN:NE2   | 2.33                     | 0.62              |
| 1:Q:63:ASP:OD2   | 1:Q:64:ARG:N     | 2.29                     | 0.62              |
| 1:Z:226:ASN:O    | 1:Z:230:GLN:HG3  | 1.99                     | 0.62              |
| 1:F:125:TYR:HA   | 1:F:143:MET:HE1  | 1.80                     | 0.62              |
| 1:Y:119:TRP:CE2  | 1:Y:143:MET:HB3  | 2.35                     | 0.62              |
| 1:G:302:ARG:HH21 | 1:N:215:GLU:CD   | 2.06                     | 0.62              |
| 1:H:126:LYS:HA   | 1:H:129:MET:SD   | 2.40                     | 0.62              |
| 1:Q:98:MET:N     | 1:Q:98:MET:SD    | 2.72                     | 0.62              |
| 1:U:83:LEU:O     | 1:U:202:ARG:NH1  | 2.33                     | 0.62              |
| 1:e:119:TRP:NE1  | 1:e:143:MET:O    | 2.33                     | 0.62              |
| 1:Q:83:LEU:HB3   | 1:Q:202:ARG:HH11 | 1.65                     | 0.61              |
| 1:Z:96:SER:OG    | 1:Z:98:MET:SD    | 2.58                     | 0.61              |
| 1:f:204:ILE:O    | 1:f:207:LYS:HB2  | 1.99                     | 0.61              |
| 1:I:119:TRP:NE1  | 1:I:143:MET:O    | 2.33                     | 0.61              |
| 1:W:58:SER:HG    | 1:W:172:ALA:C    | 2.07                     | 0.61              |
| 1:E:266:GLN:O    | 1:E:266:GLN:HG2  | 1.99                     | 0.61              |
| 1:F:187:ALA:CB   | 1:F:305:THR:HG21 | 2.30                     | 0.61              |
| 1:H:113:ASP:O    | 1:H:117:GLU:HG3  | 2.00                     | 0.61              |
| 1:I:141:ASP:HA   | 1:I:144:ILE:HD12 | 1.82                     | 0.61              |
| 1:K:228:ILE:HD12 | 1:K:272:LEU:HD22 | 1.82                     | 0.61              |
| 1:T:72:GLY:O     | 1:T:76:GLN:HG3   | 2.00                     | 0.61              |
| 1:A:177:ARG:NH2  | 1:A:312:PRO:O    | 2.32                     | 0.61              |
| 1:G:126:LYS:HA   | 1:G:129:MET:HE2  | 1.82                     | 0.61              |
| 1:J:63:ASP:HB2   | 1:J:309:LEU:HD11 | 1.83                     | 0.61              |
| 1:O:229:GLU:HG3  | 1:O:269:LEU:HD11 | 1.83                     | 0.61              |
| 1:V:206:MET:HE2  | 1:V:289:MET:HG2  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:96:SER:OG    | 1:Y:98:MET:HE2   | 2.00                     | 0.61              |
| 1:b:168:THR:OG1  | 1:b:171:ASP:OD2  | 2.12                     | 0.61              |
| 1:A:152:GLY:HA2  | 1:A:158:VAL:HG12 | 1.81                     | 0.61              |
| 1:I:141:ASP:O    | 1:I:145:ASN:ND2  | 2.33                     | 0.61              |
| 1:K:227:SER:HB2  | 1:L:275:VAL:HG23 | 1.82                     | 0.61              |
| 1:e:152:GLY:HA2  | 1:e:158:VAL:HG12 | 1.82                     | 0.61              |
| 1:C:83:LEU:HD21  | 1:C:289:MET:SD   | 2.41                     | 0.61              |
| 1:E:177:ARG:NH2  | 1:E:312:PRO:O    | 2.25                     | 0.61              |
| 1:H:164:LEU:HB2  | 1:H:176:LEU:HD13 | 1.82                     | 0.61              |
| 1:T:80:LEU:HD12  | 1:T:195:LEU:HD12 | 1.81                     | 0.61              |
| 1:Y:124:TYR:OH   | 1:Y:167:GLU:N    | 2.28                     | 0.61              |
| 1:b:58:SER:OG    | 1:b:172:ALA:C    | 2.44                     | 0.61              |
| 1:J:70:LEU:HD11  | 1:J:98:MET:HB3   | 1.81                     | 0.61              |
| 1:S:177:ARG:NH2  | 1:S:312:PRO:O    | 2.34                     | 0.61              |
| 1:Y:105:PHE:HB2  | 1:Y:305:THR:HG23 | 1.83                     | 0.61              |
| 1:f:59:THR:HB    | 1:f:310:ARG:CZ   | 2.31                     | 0.61              |
| 1:f:101:ALA:HA   | 1:f:191:LEU:HD11 | 1.83                     | 0.60              |
| 1:B:177:ARG:NH2  | 1:B:312:PRO:O    | 2.34                     | 0.60              |
| 1:G:76:GLN:NE2   | 1:G:298:THR:H    | 1.99                     | 0.60              |
| 1:K:225:MET:HE2  | 1:K:225:MET:O    | 2.00                     | 0.60              |
| 1:P:139:LEU:O    | 1:P:143:MET:HG2  | 2.01                     | 0.60              |
| 1:V:202:ARG:NH2  | 1:V:205:GLN:OE1  | 2.34                     | 0.60              |
| 1:c:79:PHE:HE2   | 1:c:293:LEU:HD13 | 1.66                     | 0.60              |
| 1:X:105:PHE:HB2  | 1:X:305:THR:HG23 | 1.83                     | 0.60              |
| 1:Y:122:THR:HG22 | 1:Y:125:TYR:H    | 1.67                     | 0.60              |
| 1:D:108:GLN:HG3  | 1:D:187:ALA:HB2  | 1.82                     | 0.60              |
| 1:E:98:MET:H     | 1:E:98:MET:CE    | 2.14                     | 0.60              |
| 1:I:60:ALA:HB2   | 1:I:312:PRO:HG3  | 1.84                     | 0.60              |
| 1:a:132:ASN:ND2  | 1:a:135:ALA:H    | 1.99                     | 0.60              |
| 1:e:119:TRP:CD2  | 1:e:143:MET:HB3  | 2.37                     | 0.60              |
| 1:f:202:ARG:NH2  | 1:f:205:GLN:HE21 | 2.00                     | 0.60              |
| 1:D:190:HIS:NE2  | 1:E:66:THR:HG21  | 2.17                     | 0.60              |
| 1:D:228:ILE:HG21 | 1:D:269:LEU:HA   | 1.82                     | 0.60              |
| 1:F:184:SER:HB2  | 1:F:306:TYR:CE1  | 2.36                     | 0.60              |
| 1:G:67:VAL:HG22  | 1:G:98:MET:HE1   | 1.84                     | 0.60              |
| 1:J:124:TYR:O    | 1:J:128:ARG:NH1  | 2.28                     | 0.60              |
| 1:L:112:TRP:HB3  | 1:M:310:ARG:HB2  | 1.84                     | 0.60              |
| 1:W:74:TYR:CE1   | 1:W:98:MET:HE1   | 2.34                     | 0.60              |
| 1:E:132:ASN:ND2  | 1:E:135:ALA:H    | 1.99                     | 0.60              |
| 1:E:168:THR:OG1  | 1:E:171:ASP:OD2  | 2.19                     | 0.60              |
| 1:R:227:SER:HB2  | 1:S:275:VAL:HG23 | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:73:TYR:CZ    | 1:L:191:LEU:HB3  | 2.37                     | 0.60              |
| 1:P:187:ALA:CB   | 1:P:305:THR:HG21 | 2.29                     | 0.60              |
| 1:Y:152:GLY:HA2  | 1:Y:158:VAL:HG12 | 1.83                     | 0.60              |
| 1:a:210:VAL:HG21 | 1:a:290:LEU:HD12 | 1.83                     | 0.60              |
| 1:B:77:GLN:HG2   | 1:B:97:VAL:HG13  | 1.84                     | 0.59              |
| 1:E:268:ARG:HA   | 1:E:271:ASN:HB2  | 1.82                     | 0.59              |
| 1:I:316:VAL:HG23 | 1:I:317:LYS:HD2  | 1.84                     | 0.59              |
| 1:M:225:MET:HE1  | 1:M:273:GLN:HA   | 1.84                     | 0.59              |
| 1:T:292:THR:HG22 | 1:b:302:ARG:NH1  | 2.17                     | 0.59              |
| 1:F:268:ARG:HA   | 1:F:271:ASN:HB2  | 1.83                     | 0.59              |
| 1:F:290:LEU:HD22 | 1:F:294:ASN:ND2  | 2.17                     | 0.59              |
| 1:M:132:ASN:ND2  | 1:M:135:ALA:H    | 2.00                     | 0.59              |
| 1:U:66:THR:HG1   | 1:U:69:MET:HE3   | 1.66                     | 0.59              |
| 1:Z:126:LYS:HG2  | 1:Z:129:MET:HE2  | 1.84                     | 0.59              |
| 1:A:227:SER:HB3  | 1:B:275:VAL:HG22 | 1.85                     | 0.59              |
| 1:J:210:VAL:HA   | 1:J:213:GLN:HE21 | 1.67                     | 0.59              |
| 1:Z:173:ASN:OD1  | 1:Z:177:ARG:NE   | 2.35                     | 0.59              |
| 1:A:228:ILE:HD12 | 1:A:272:LEU:HD22 | 1.85                     | 0.59              |
| 1:S:73:TYR:CE1   | 1:S:191:LEU:HB3  | 2.37                     | 0.59              |
| 1:Y:122:THR:CG2  | 1:Y:125:TYR:H    | 2.14                     | 0.59              |
| 1:B:61:ILE:HB    | 1:B:310:ARG:HB3  | 1.85                     | 0.59              |
| 1:E:123:ASP:HB3  | 1:E:127:GLN:HE21 | 1.68                     | 0.59              |
| 1:K:69:MET:SD    | 1:K:307:ARG:HB3  | 2.43                     | 0.59              |
| 1:d:107:MET:HE2  | 1:e:307:ARG:NH1  | 2.16                     | 0.59              |
| 1:M:224:ARG:O    | 1:M:228:ILE:HG13 | 2.02                     | 0.59              |
| 1:Z:126:LYS:O    | 1:Z:129:MET:HG3  | 2.03                     | 0.59              |
| 1:f:122:THR:O    | 1:f:126:LYS:HG3  | 2.03                     | 0.59              |
| 1:M:275:VAL:HG13 | 1:M:276:GLY:H    | 1.67                     | 0.59              |
| 1:N:122:THR:HG22 | 1:N:125:TYR:H    | 1.68                     | 0.59              |
| 1:O:119:TRP:CE3  | 1:O:122:THR:HG21 | 2.37                     | 0.59              |
| 1:U:122:THR:HG22 | 1:U:125:TYR:H    | 1.67                     | 0.59              |
| 1:a:207:LYS:HE3  | 1:a:294:ASN:ND2  | 2.13                     | 0.59              |
| 1:e:83:LEU:HD21  | 1:e:289:MET:HE2  | 1.84                     | 0.59              |
| 1:e:120:LEU:HD21 | 1:e:140:LEU:HD22 | 1.85                     | 0.59              |
| 1:A:169:ALA:HB3  | 1:A:170:PRO:HD3  | 1.85                     | 0.59              |
| 1:B:119:TRP:NE1  | 1:B:143:MET:O    | 2.35                     | 0.59              |
| 1:L:103:LYS:O    | 1:L:107:MET:HG3  | 2.03                     | 0.59              |
| 1:L:223:ARG:O    | 1:L:227:SER:OG   | 2.20                     | 0.59              |
| 1:e:268:ARG:HG2  | 1:e:268:ARG:NH1  | 2.07                     | 0.59              |
| 1:F:61:ILE:HG22  | 1:F:309:LEU:HB2  | 1.85                     | 0.59              |
| 1:G:227:SER:HB2  | 1:H:275:VAL:HG23 | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:56:TRP:HB3   | 1:R:315:PRO:HG2  | 1.85                     | 0.59              |
| 1:P:207:LYS:HG2  | 1:P:290:LEU:HD21 | 1.85                     | 0.59              |
| 1:C:225:MET:HG3  | 1:C:272:LEU:HD21 | 1.84                     | 0.58              |
| 1:L:80:LEU:HD21  | 1:L:199:TRP:HA   | 1.85                     | 0.58              |
| 1:I:164:LEU:HB2  | 1:I:176:LEU:HD13 | 1.84                     | 0.58              |
| 1:O:217:ALA:HA   | 1:O:220:ILE:HD12 | 1.84                     | 0.58              |
| 1:d:225:MET:HE1  | 1:d:273:GLN:HG3  | 1.84                     | 0.58              |
| 1:d:227:SER:HB2  | 1:e:275:VAL:HG23 | 1.84                     | 0.58              |
| 1:H:203:THR:HA   | 1:H:293:LEU:HD23 | 1.83                     | 0.58              |
| 1:a:104:GLU:CD   | 1:b:307:ARG:HH22 | 2.10                     | 0.58              |
| 1:f:214:GLU:HG3  | 1:f:283:TYR:CE1  | 2.38                     | 0.58              |
| 1:b:140:LEU:O    | 1:b:144:ILE:HG13 | 2.03                     | 0.58              |
| 1:d:202:ARG:NH2  | 1:d:205:GLN:OE1  | 2.35                     | 0.58              |
| 1:B:72:GLY:C     | 1:B:76:GLN:HE21  | 2.11                     | 0.58              |
| 1:W:56:TRP:O     | 1:W:165:ILE:HA   | 2.04                     | 0.58              |
| 1:Y:69:MET:HE2   | 1:Y:304:GLN:HB3  | 1.85                     | 0.58              |
| 1:K:212:ARG:HH11 | 1:L:292:THR:HG21 | 1.69                     | 0.58              |
| 1:P:76:GLN:NE2   | 1:P:298:THR:O    | 2.36                     | 0.58              |
| 1:S:212:ARG:O    | 1:S:216:VAL:HG23 | 2.04                     | 0.58              |
| 1:c:202:ARG:NH2  | 1:c:205:GLN:OE1  | 2.37                     | 0.58              |
| 1:I:223:ARG:NH2  | 1:J:284:ASP:OD1  | 2.26                     | 0.58              |
| 1:W:58:SER:HB2   | 1:W:176:LEU:CD2  | 2.33                     | 0.58              |
| 1:Z:316:VAL:HG23 | 1:Z:317:LYS:HG2  | 1.85                     | 0.58              |
| 1:D:58:SER:OG    | 1:D:313:GLU:O    | 2.22                     | 0.58              |
| 1:F:73:TYR:CZ    | 1:F:191:LEU:HB3  | 2.38                     | 0.58              |
| 1:J:64:ARG:HG2   | 1:J:102:TYR:CB   | 2.33                     | 0.58              |
| 1:J:66:THR:H     | 1:J:69:MET:HB2   | 1.68                     | 0.58              |
| 1:M:212:ARG:O    | 1:M:216:VAL:HG23 | 2.04                     | 0.58              |
| 1:Q:177:ARG:NH2  | 1:Q:312:PRO:O    | 2.36                     | 0.58              |
| 1:V:164:LEU:HB2  | 1:V:176:LEU:HD13 | 1.85                     | 0.58              |
| 1:Y:79:PHE:O     | 1:Y:83:LEU:HG    | 2.03                     | 0.58              |
| 1:Z:122:THR:HG22 | 1:Z:125:TYR:H    | 1.68                     | 0.58              |
| 1:e:122:THR:HG22 | 1:e:125:TYR:H    | 1.68                     | 0.58              |
| 1:C:107:MET:HE3  | 1:D:307:ARG:HH21 | 1.68                     | 0.57              |
| 1:W:57:SER:HA    | 1:W:164:LEU:O    | 2.04                     | 0.57              |
| 1:X:136:ASP:O    | 1:X:140:LEU:HB2  | 2.03                     | 0.57              |
| 1:T:294:ASN:HB2  | 1:b:298:THR:HG21 | 1.85                     | 0.57              |
| 1:b:130:VAL:HG23 | 1:b:132:ASN:H    | 1.69                     | 0.57              |
| 1:D:205:GLN:HG3  | 1:D:206:MET:N    | 2.19                     | 0.57              |
| 1:I:122:THR:HG22 | 1:I:125:TYR:H    | 1.70                     | 0.57              |
| 1:Q:122:THR:CG2  | 1:Q:124:TYR:HB3  | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:162:VAL:HG13 | 1:R:176:LEU:HD11 | 1.86                     | 0.57              |
| 1:N:283:TYR:CZ   | 1:N:287:ARG:HD3  | 2.38                     | 0.57              |
| 1:U:169:ALA:HB1  | 1:U:314:GLU:HG2  | 1.85                     | 0.57              |
| 1:Y:187:ALA:HB3  | 1:Y:305:THR:HG21 | 1.86                     | 0.57              |
| 1:e:268:ARG:HH11 | 1:e:268:ARG:CG   | 2.14                     | 0.57              |
| 1:M:187:ALA:HB3  | 1:M:305:THR:HG21 | 1.86                     | 0.57              |
| 1:T:104:GLU:CD   | 1:U:307:ARG:HH22 | 2.12                     | 0.57              |
| 1:U:55:GLU:O     | 1:U:318:ARG:HG2  | 2.05                     | 0.57              |
| 1:d:124:TYR:OH   | 1:d:167:GLU:HG3  | 2.04                     | 0.57              |
| 1:H:124:TYR:OH   | 1:H:167:GLU:HG3  | 2.05                     | 0.57              |
| 1:M:124:TYR:CE1  | 1:M:143:MET:HE2  | 2.39                     | 0.57              |
| 1:Y:56:TRP:CE3   | 1:Y:169:ALA:HB2  | 2.40                     | 0.57              |
| 1:E:187:ALA:HB3  | 1:E:305:THR:HG21 | 1.85                     | 0.57              |
| 1:Q:122:THR:HG23 | 1:Q:124:TYR:HB3  | 1.86                     | 0.57              |
| 1:V:168:THR:OG1  | 1:V:170:PRO:HD2  | 2.04                     | 0.57              |
| 1:X:56:TRP:CZ2   | 1:X:318:ARG:HD2  | 2.40                     | 0.57              |
| 1:M:168:THR:OG1  | 1:M:171:ASP:OD2  | 2.19                     | 0.57              |
| 1:O:124:TYR:CG   | 1:O:175:LEU:HD11 | 2.39                     | 0.57              |
| 1:U:122:THR:CG2  | 1:U:125:TYR:H    | 2.17                     | 0.57              |
| 1:f:216:VAL:HG12 | 1:f:220:ILE:HD11 | 1.87                     | 0.57              |
| 1:K:56:TRP:CE3   | 1:K:169:ALA:HB2  | 2.39                     | 0.57              |
| 1:P:202:ARG:HE   | 1:P:205:GLN:HG2  | 1.70                     | 0.57              |
| 1:f:119:TRP:NE1  | 1:f:143:MET:O    | 2.38                     | 0.57              |
| 1:A:226:ASN:O    | 1:A:230:GLN:HG3  | 2.05                     | 0.57              |
| 1:I:148:GLN:HE21 | 1:I:148:GLN:N    | 2.03                     | 0.57              |
| 1:W:115:ARG:HD3  | 1:W:147:ILE:HB   | 1.87                     | 0.57              |
| 1:b:61:ILE:HG22  | 1:b:309:LEU:HB2  | 1.85                     | 0.57              |
| 1:L:76:GLN:NE2   | 1:L:298:THR:OG1  | 2.37                     | 0.56              |
| 1:M:119:TRP:NE1  | 1:M:143:MET:O    | 2.38                     | 0.56              |
| 1:P:63:ASP:O     | 1:P:307:ARG:N    | 2.28                     | 0.56              |
| 1:P:199:TRP:NE1  | 1:P:293:LEU:O    | 2.29                     | 0.56              |
| 1:Q:105:PHE:HB2  | 1:Q:305:THR:CG2  | 2.23                     | 0.56              |
| 1:R:56:TRP:CE3   | 1:R:169:ALA:HB2  | 2.40                     | 0.56              |
| 1:R:61:ILE:HB    | 1:R:310:ARG:HB3  | 1.87                     | 0.56              |
| 1:D:199:TRP:CD2  | 1:D:297:PRO:HD3  | 2.40                     | 0.56              |
| 1:L:196:LYS:HG3  | 1:L:299:LEU:HD21 | 1.87                     | 0.56              |
| 1:S:164:LEU:HB2  | 1:S:176:LEU:HD13 | 1.86                     | 0.56              |
| 1:X:164:LEU:HB2  | 1:X:176:LEU:HD13 | 1.87                     | 0.56              |
| 1:Y:152:GLY:N    | 1:Y:160:ASP:OD2  | 2.28                     | 0.56              |
| 1:b:199:TRP:NE1  | 1:b:296:GLY:HA2  | 2.20                     | 0.56              |
| 1:d:190:HIS:CE1  | 1:e:66:THR:HG21  | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:120:LEU:O    | 1:F:126:LYS:HE2  | 2.05                     | 0.56              |
| 1:F:188:ALA:HA   | 1:F:303:PHE:CZ   | 2.40                     | 0.56              |
| 1:K:132:ASN:ND2  | 1:K:135:ALA:H    | 2.01                     | 0.56              |
| 1:P:69:MET:O     | 1:P:303:PHE:HB2  | 2.06                     | 0.56              |
| 1:W:118:PHE:O    | 1:W:122:THR:OG1  | 2.14                     | 0.56              |
| 1:e:271:ASN:O    | 1:e:275:VAL:HG12 | 2.05                     | 0.56              |
| 1:C:122:THR:O    | 1:C:126:LYS:HG3  | 2.05                     | 0.56              |
| 1:X:132:ASN:HB3  | 1:X:135:ALA:HB3  | 1.88                     | 0.56              |
| 1:Y:66:THR:HG21  | 1:f:190:HIS:NE2  | 2.20                     | 0.56              |
| 1:C:152:GLY:N    | 1:C:160:ASP:OD2  | 2.20                     | 0.56              |
| 1:D:56:TRP:CE3   | 1:D:169:ALA:HB2  | 2.40                     | 0.56              |
| 1:F:64:ARG:O     | 1:F:307:ARG:HG2  | 2.05                     | 0.56              |
| 1:Q:66:THR:HB    | 1:X:194:GLU:CD   | 2.31                     | 0.56              |
| 1:X:283:TYR:CZ   | 1:X:287:ARG:HD3  | 2.41                     | 0.56              |
| 1:D:74:TYR:CE1   | 1:D:98:MET:HE1   | 2.41                     | 0.56              |
| 1:G:105:PHE:HB2  | 1:G:305:THR:HG22 | 1.87                     | 0.56              |
| 1:M:269:LEU:O    | 1:M:273:GLN:HB2  | 2.05                     | 0.56              |
| 1:Q:124:TYR:OH   | 1:Q:167:GLU:N    | 2.37                     | 0.56              |
| 1:U:115:ARG:HD3  | 1:U:147:ILE:HB   | 1.87                     | 0.56              |
| 1:Y:177:ARG:NH2  | 1:Y:312:PRO:O    | 2.38                     | 0.56              |
| 1:M:139:LEU:O    | 1:M:143:MET:HG3  | 2.06                     | 0.56              |
| 1:a:129:MET:HG2  | 1:a:136:ASP:CG   | 2.30                     | 0.56              |
| 1:a:194:GLU:OE2  | 1:b:67:VAL:HG23  | 2.05                     | 0.56              |
| 1:c:96:SER:OG    | 1:c:98:MET:SD    | 2.63                     | 0.56              |
| 1:O:118:PHE:O    | 1:O:122:THR:HB   | 2.06                     | 0.56              |
| 1:O:123:ASP:HA   | 1:O:126:LYS:HG3  | 1.87                     | 0.56              |
| 1:S:77:GLN:HB3   | 1:S:97:VAL:HG11  | 1.88                     | 0.56              |
| 1:Z:104:GLU:OE1  | 1:a:307:ARG:NH2  | 2.38                     | 0.56              |
| 1:b:55:GLU:N     | 1:b:166:ALA:O    | 2.39                     | 0.56              |
| 1:b:190:HIS:NE2  | 1:c:66:THR:HG21  | 2.20                     | 0.56              |
| 1:A:119:TRP:CZ2  | 1:A:143:MET:HG2  | 2.41                     | 0.56              |
| 1:A:141:ASP:HA   | 1:A:144:ILE:HD12 | 1.88                     | 0.56              |
| 1:C:122:THR:HG22 | 1:C:125:TYR:H    | 1.71                     | 0.56              |
| 1:D:107:MET:HE1  | 1:E:63:ASP:OD2   | 2.06                     | 0.56              |
| 1:I:128:ARG:HE   | 1:I:167:GLU:CD   | 2.14                     | 0.56              |
| 1:J:223:ARG:NH2  | 1:K:284:ASP:OD1  | 2.33                     | 0.56              |
| 1:Q:65:PRO:HD2   | 1:Q:102:TYR:HB2  | 1.88                     | 0.56              |
| 1:X:122:THR:HG22 | 1:X:125:TYR:H    | 1.71                     | 0.56              |
| 1:Z:64:ARG:HG2   | 1:Z:102:TYR:CD2  | 2.40                     | 0.56              |
| 1:Z:79:PHE:O     | 1:Z:83:LEU:HG    | 2.06                     | 0.56              |
| 1:A:211:LYS:HA   | 1:A:211:LYS:HE3  | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:192:ASN:HB3  | 1:C:299:LEU:HD22 | 1.88                     | 0.56              |
| 1:a:76:GLN:NE2   | 1:a:298:THR:H    | 2.04                     | 0.56              |
| 1:c:83:LEU:HD21  | 1:c:289:MET:HE2  | 1.87                     | 0.56              |
| 1:H:124:TYR:OH   | 1:H:167:GLU:N    | 2.37                     | 0.55              |
| 1:U:173:ASN:OD1  | 1:U:177:ARG:NE   | 2.38                     | 0.55              |
| 1:d:57:SER:HB3   | 1:d:165:ILE:HG12 | 1.88                     | 0.55              |
| 1:e:122:THR:CG2  | 1:e:124:TYR:HB3  | 2.36                     | 0.55              |
| 1:L:190:HIS:NE2  | 1:M:66:THR:HG21  | 2.21                     | 0.55              |
| 1:B:182:PHE:CE2  | 1:B:186:ARG:HD2  | 2.41                     | 0.55              |
| 1:D:76:GLN:OE1   | 1:D:298:THR:N    | 2.38                     | 0.55              |
| 1:L:152:GLY:HA2  | 1:L:158:VAL:HG12 | 1.87                     | 0.55              |
| 1:U:120:LEU:HD23 | 1:U:125:TYR:HE2  | 1.69                     | 0.55              |
| 1:V:56:TRP:HE3   | 1:V:315:PRO:HG2  | 1.71                     | 0.55              |
| 1:V:96:SER:HB3   | 1:V:99:ASP:OD2   | 2.06                     | 0.55              |
| 1:W:58:SER:OG    | 1:W:172:ALA:C    | 2.50                     | 0.55              |
| 1:c:101:ALA:HA   | 1:c:191:LEU:HD11 | 1.88                     | 0.55              |
| 1:L:76:GLN:HB3   | 1:L:195:LEU:HD11 | 1.88                     | 0.55              |
| 1:O:194:GLU:OE2  | 1:P:67:VAL:HG23  | 2.07                     | 0.55              |
| 1:a:206:MET:HE2  | 1:a:209:GLN:OE1  | 2.05                     | 0.55              |
| 1:B:69:MET:O     | 1:B:303:PHE:HB2  | 2.07                     | 0.55              |
| 1:B:269:LEU:O    | 1:B:273:GLN:HG3  | 2.05                     | 0.55              |
| 1:D:79:PHE:CE2   | 1:D:83:LEU:HD11  | 2.42                     | 0.55              |
| 1:D:300:ASP:O    | 1:D:303:PHE:HD2  | 1.89                     | 0.55              |
| 1:J:223:ARG:NH1  | 1:K:284:ASP:OD2  | 2.29                     | 0.55              |
| 1:R:96:SER:OG    | 1:R:98:MET:HG3   | 2.05                     | 0.55              |
| 1:U:132:ASN:HD22 | 1:U:135:ALA:N    | 2.01                     | 0.55              |
| 1:W:169:ALA:C    | 1:W:314:GLU:HG2  | 2.31                     | 0.55              |
| 1:W:229:GLU:HG3  | 1:W:269:LEU:HD11 | 1.89                     | 0.55              |
| 1:e:202:ARG:NH2  | 1:e:205:GLN:OE1  | 2.38                     | 0.55              |
| 1:B:210:VAL:HA   | 1:B:213:GLN:HE21 | 1.71                     | 0.55              |
| 1:T:292:THR:CG2  | 1:b:302:ARG:HH22 | 2.18                     | 0.55              |
| 1:T:295:VAL:HA   | 1:b:72:GLY:HA3   | 1.88                     | 0.55              |
| 1:K:63:ASP:HB2   | 1:K:309:LEU:HD11 | 1.88                     | 0.55              |
| 1:U:180:VAL:HG11 | 1:U:308:TYR:OH   | 2.06                     | 0.55              |
| 1:f:221:TYR:OH   | 1:f:273:GLN:HA   | 2.07                     | 0.55              |
| 1:A:152:GLY:HA2  | 1:A:158:VAL:CG1  | 2.37                     | 0.55              |
| 1:G:204:ILE:HD12 | 1:O:302:ARG:NE   | 2.21                     | 0.55              |
| 1:R:110:ALA:HB2  | 1:R:149:PHE:CD2  | 2.41                     | 0.55              |
| 1:e:77:GLN:CG    | 1:e:97:VAL:HG11  | 2.36                     | 0.55              |
| 1:R:79:PHE:O     | 1:R:83:LEU:HG    | 2.06                     | 0.55              |
| 1:T:139:LEU:O    | 1:T:143:MET:HG3  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:212:ARG:O    | 1:c:216:VAL:HG23 | 2.06                     | 0.55              |
| 1:f:60:ALA:HB2   | 1:f:312:PRO:HG3  | 1.89                     | 0.55              |
| 1:G:301:PRO:HD2  | 1:G:302:ARG:HD2  | 1.89                     | 0.55              |
| 1:N:64:ARG:HH21  | 1:N:99:ASP:HB3   | 1.71                     | 0.55              |
| 1:T:79:PHE:O     | 1:T:83:LEU:HG    | 2.06                     | 0.55              |
| 1:X:124:TYR:OH   | 1:X:167:GLU:HG3  | 2.07                     | 0.55              |
| 1:Y:70:LEU:HD11  | 1:Y:98:MET:HB3   | 1.88                     | 0.55              |
| 1:a:105:PHE:HB2  | 1:a:305:THR:CG2  | 2.37                     | 0.55              |
| 1:F:64:ARG:HA    | 1:F:102:TYR:HB2  | 1.89                     | 0.54              |
| 1:I:122:THR:HG23 | 1:I:124:TYR:HB3  | 1.89                     | 0.54              |
| 1:R:224:ARG:HG2  | 1:R:228:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:230:GLN:OE1  | 1:B:274:ALA:HB1  | 2.07                     | 0.54              |
| 1:M:122:THR:HG23 | 1:M:124:TYR:HB3  | 1.88                     | 0.54              |
| 1:P:141:ASP:HA   | 1:P:144:ILE:HD12 | 1.89                     | 0.54              |
| 1:d:316:VAL:HG23 | 1:d:317:LYS:HG3  | 1.88                     | 0.54              |
| 1:C:107:MET:HE3  | 1:D:307:ARG:NH2  | 2.22                     | 0.54              |
| 1:F:73:TYR:CE1   | 1:F:191:LEU:HB3  | 2.42                     | 0.54              |
| 1:I:61:ILE:HB    | 1:I:310:ARG:HB3  | 1.90                     | 0.54              |
| 1:P:207:LYS:CE   | 1:P:294:ASN:HD21 | 2.20                     | 0.54              |
| 1:S:122:THR:HG22 | 1:S:125:TYR:H    | 1.70                     | 0.54              |
| 1:c:126:LYS:HA   | 1:c:129:MET:HG3  | 1.88                     | 0.54              |
| 1:c:216:VAL:HG13 | 1:d:284:ASP:HB3  | 1.90                     | 0.54              |
| 1:e:227:SER:HB2  | 1:f:275:VAL:HG23 | 1.87                     | 0.54              |
| 1:R:141:ASP:HA   | 1:R:144:ILE:HD12 | 1.88                     | 0.54              |
| 1:S:122:THR:CG2  | 1:S:125:TYR:H    | 2.20                     | 0.54              |
| 1:H:152:GLY:N    | 1:H:160:ASP:OD2  | 2.30                     | 0.54              |
| 1:J:64:ARG:HD3   | 1:J:99:ASP:CA    | 2.30                     | 0.54              |
| 1:M:83:LEU:HD21  | 1:M:289:MET:CE   | 2.38                     | 0.54              |
| 1:N:107:MET:HE1  | 1:O:307:ARG:NH1  | 2.22                     | 0.54              |
| 1:O:300:ASP:OD1  | 1:O:302:ARG:NH1  | 2.30                     | 0.54              |
| 1:R:56:TRP:HE3   | 1:R:315:PRO:HG2  | 1.72                     | 0.54              |
| 1:X:125:TYR:O    | 1:X:129:MET:N    | 2.40                     | 0.54              |
| 1:Z:78:GLN:HG2   | 1:Z:97:VAL:HG21  | 1.89                     | 0.54              |
| 1:d:110:ALA:O    | 1:d:115:ARG:NH2  | 2.40                     | 0.54              |
| 1:A:153:ASP:H    | 1:A:158:VAL:HG12 | 1.73                     | 0.54              |
| 1:F:104:GLU:HG2  | 1:F:191:LEU:HG   | 1.90                     | 0.54              |
| 1:Q:213:GLN:HE22 | 1:Q:283:TYR:HA   | 1.71                     | 0.54              |
| 1:F:128:ARG:CB   | 1:F:139:LEU:HD21 | 2.38                     | 0.54              |
| 1:I:122:THR:O    | 1:I:126:LYS:HG3  | 2.08                     | 0.54              |
| 1:S:74:TYR:HD1   | 1:S:97:VAL:CG2   | 2.20                     | 0.54              |
| 1:W:83:LEU:HD21  | 1:W:289:MET:HE2  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:116:ARG:HG3  | 1:W:140:LEU:HD21 | 1.90                     | 0.54              |
| 1:X:122:THR:CG2  | 1:X:125:TYR:H    | 2.20                     | 0.54              |
| 1:c:98:MET:SD    | 1:c:98:MET:N     | 2.74                     | 0.54              |
| 1:B:68:ASN:H     | 1:B:68:ASN:HD22  | 1.56                     | 0.54              |
| 1:F:119:TRP:CE3  | 1:F:122:THR:HG21 | 2.43                     | 0.54              |
| 1:G:187:ALA:CB   | 1:G:305:THR:HG21 | 2.38                     | 0.54              |
| 1:G:200:ALA:HB1  | 1:O:302:ARG:NH1  | 2.22                     | 0.54              |
| 1:H:213:GLN:NE2  | 1:H:286:ASN:HD22 | 2.04                     | 0.54              |
| 1:K:226:ASN:O    | 1:K:230:GLN:HG3  | 2.08                     | 0.54              |
| 1:T:200:ALA:O    | 1:T:204:ILE:HG12 | 2.07                     | 0.54              |
| 1:T:292:THR:HG22 | 1:b:302:ARG:HH22 | 1.72                     | 0.54              |
| 1:U:128:ARG:HB3  | 1:U:139:LEU:HD21 | 1.90                     | 0.54              |
| 1:e:57:SER:CB    | 1:e:163:LYS:HE2  | 2.37                     | 0.54              |
| 1:I:310:ARG:HB2  | 1:P:112:TRP:HB3  | 1.89                     | 0.54              |
| 1:N:122:THR:CG2  | 1:N:125:TYR:H    | 2.21                     | 0.54              |
| 1:T:300:ASP:OD1  | 1:T:302:ARG:HB2  | 2.07                     | 0.54              |
| 1:E:169:ALA:HB3  | 1:E:170:PRO:HD3  | 1.90                     | 0.54              |
| 1:F:108:GLN:HG3  | 1:F:187:ALA:HB2  | 1.90                     | 0.54              |
| 1:H:56:TRP:CE3   | 1:H:169:ALA:HB2  | 2.43                     | 0.54              |
| 1:T:199:TRP:NE1  | 1:T:296:GLY:HA2  | 2.23                     | 0.54              |
| 1:C:122:THR:CG2  | 1:C:125:TYR:H    | 2.19                     | 0.53              |
| 1:C:168:THR:OG1  | 1:C:171:ASP:OD2  | 2.26                     | 0.53              |
| 1:F:83:LEU:C     | 1:F:85:VAL:H     | 2.15                     | 0.53              |
| 1:H:119:TRP:CD2  | 1:H:143:MET:HB3  | 2.43                     | 0.53              |
| 1:H:225:MET:HE1  | 1:H:273:GLN:NE2  | 2.23                     | 0.53              |
| 1:K:169:ALA:HB3  | 1:K:170:PRO:HD3  | 1.90                     | 0.53              |
| 1:L:66:THR:OG1   | 1:L:69:MET:HG3   | 2.08                     | 0.53              |
| 1:M:126:LYS:HA   | 1:M:129:MET:HG3  | 1.89                     | 0.53              |
| 1:T:76:GLN:NE2   | 1:T:298:THR:O    | 2.41                     | 0.53              |
| 1:V:61:ILE:HB    | 1:V:310:ARG:HB3  | 1.89                     | 0.53              |
| 1:e:125:TYR:HA   | 1:e:143:MET:HE1  | 1.89                     | 0.53              |
| 1:I:83:LEU:HB3   | 1:I:202:ARG:HH11 | 1.74                     | 0.53              |
| 1:K:80:LEU:HD23  | 1:K:83:LEU:HD12  | 1.90                     | 0.53              |
| 1:L:104:GLU:CD   | 1:M:307:ARG:HH22 | 2.16                     | 0.53              |
| 1:T:202:ARG:HH21 | 1:T:205:GLN:NE2  | 2.06                     | 0.53              |
| 1:U:227:SER:HB2  | 1:V:275:VAL:HG23 | 1.90                     | 0.53              |
| 1:Z:185:GLN:NE2  | 1:Z:301:PRO:O    | 2.35                     | 0.53              |
| 1:e:112:TRP:HB3  | 1:f:310:ARG:HB2  | 1.89                     | 0.53              |
| 1:e:283:TYR:OH   | 1:e:287:ARG:NH1  | 2.42                     | 0.53              |
| 1:G:119:TRP:O    | 1:G:125:TYR:HB3  | 2.08                     | 0.53              |
| 1:K:210:VAL:HG13 | 1:K:283:TYR:CE1  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:106:VAL:HG13 | 1:L:149:PHE:CZ   | 2.44                     | 0.53              |
| 1:L:288:ALA:O    | 1:L:291:ASN:HB2  | 2.08                     | 0.53              |
| 1:P:206:MET:SD   | 1:P:289:MET:HG3  | 2.48                     | 0.53              |
| 1:Z:80:LEU:HD23  | 1:Z:83:LEU:HD12  | 1.90                     | 0.53              |
| 1:a:112:TRP:HB3  | 1:b:310:ARG:HB2  | 1.88                     | 0.53              |
| 1:A:124:TYR:OH   | 1:A:167:GLU:HG3  | 2.08                     | 0.53              |
| 1:A:226:ASN:OD1  | 1:A:230:GLN:NE2  | 2.40                     | 0.53              |
| 1:F:184:SER:HA   | 1:F:305:THR:HG22 | 1.89                     | 0.53              |
| 1:L:96:SER:HB3   | 1:L:99:ASP:OD2   | 2.09                     | 0.53              |
| 1:U:76:GLN:HE22  | 1:U:297:PRO:HA   | 1.72                     | 0.53              |
| 1:W:57:SER:CB    | 1:W:163:LYS:HE2  | 2.39                     | 0.53              |
| 1:e:57:SER:HB2   | 1:e:163:LYS:HE2  | 1.90                     | 0.53              |
| 1:e:122:THR:O    | 1:e:126:LYS:HG3  | 2.09                     | 0.53              |
| 1:X:288:ALA:O    | 1:X:292:THR:OG1  | 2.26                     | 0.53              |
| 1:F:96:SER:O     | 1:F:100:GLU:HG2  | 2.08                     | 0.53              |
| 1:P:163:LYS:HE3  | 1:P:165:ILE:HD12 | 1.91                     | 0.53              |
| 1:Q:143:MET:HA   | 1:Q:146:ASN:HB2  | 1.91                     | 0.53              |
| 1:U:169:ALA:HB3  | 1:U:170:PRO:HD3  | 1.91                     | 0.53              |
| 1:W:119:TRP:CE2  | 1:W:143:MET:HB3  | 2.43                     | 0.53              |
| 1:W:300:ASP:OD1  | 1:W:302:ARG:HD3  | 2.09                     | 0.53              |
| 1:d:64:ARG:O     | 1:d:307:ARG:HG2  | 2.08                     | 0.53              |
| 1:G:143:MET:HA   | 1:G:146:ASN:HB2  | 1.91                     | 0.53              |
| 1:Q:152:GLY:HA2  | 1:Q:158:VAL:HG12 | 1.90                     | 0.53              |
| 1:U:61:ILE:HB    | 1:U:310:ARG:HB3  | 1.91                     | 0.53              |
| 1:W:122:THR:HG22 | 1:W:125:TYR:H    | 1.72                     | 0.53              |
| 1:a:70:LEU:HD11  | 1:a:98:MET:HB3   | 1.91                     | 0.53              |
| 1:F:266:GLN:HE21 | 1:F:269:LEU:HD23 | 1.72                     | 0.53              |
| 1:U:120:LEU:HD23 | 1:U:125:TYR:CE2  | 2.43                     | 0.53              |
| 1:W:108:GLN:HG3  | 1:W:187:ALA:HB2  | 1.90                     | 0.53              |
| 1:X:124:TYR:OH   | 1:X:167:GLU:N    | 2.39                     | 0.53              |
| 1:d:105:PHE:HB2  | 1:d:305:THR:HG23 | 1.91                     | 0.53              |
| 1:A:224:ARG:HA   | 1:A:227:SER:HG   | 1.71                     | 0.53              |
| 1:B:57:SER:CB    | 1:B:163:LYS:HE2  | 2.39                     | 0.53              |
| 1:C:199:TRP:CD1  | 1:C:297:PRO:HD3  | 2.43                     | 0.53              |
| 1:F:105:PHE:CZ   | 1:F:109:LEU:HD13 | 2.44                     | 0.53              |
| 1:I:275:VAL:HG23 | 1:P:227:SER:HB2  | 1.91                     | 0.53              |
| 1:L:64:ARG:NE    | 1:L:99:ASP:OD1   | 2.42                     | 0.53              |
| 1:a:283:TYR:CZ   | 1:a:287:ARG:HD3  | 2.44                     | 0.53              |
| 1:f:122:THR:CG2  | 1:f:125:TYR:H    | 2.22                     | 0.53              |
| 1:F:212:ARG:O    | 1:F:216:VAL:HG23 | 2.09                     | 0.53              |
| 1:S:73:TYR:CZ    | 1:S:191:LEU:HB3  | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:122:THR:CG2  | 1:U:124:TYR:HB3  | 2.39                     | 0.53              |
| 1:b:81:ARG:NH1   | 1:b:95:PRO:O     | 2.38                     | 0.53              |
| 1:K:56:TRP:CD1   | 1:K:168:THR:HA   | 2.43                     | 0.52              |
| 1:Q:300:ASP:OD1  | 1:Q:302:ARG:HD3  | 2.09                     | 0.52              |
| 1:R:124:TYR:HH   | 1:R:167:GLU:H    | 1.56                     | 0.52              |
| 1:S:194:GLU:HA   | 1:S:194:GLU:OE2  | 2.09                     | 0.52              |
| 1:V:152:GLY:HA2  | 1:V:158:VAL:HG12 | 1.90                     | 0.52              |
| 1:c:83:LEU:HB3   | 1:c:202:ARG:HH11 | 1.73                     | 0.52              |
| 1:I:83:LEU:HD21  | 1:I:289:MET:HE3  | 1.91                     | 0.52              |
| 1:J:206:MET:HE3  | 1:J:289:MET:HG2  | 1.90                     | 0.52              |
| 1:O:168:THR:OG1  | 1:O:171:ASP:OD2  | 2.25                     | 0.52              |
| 1:P:202:ARG:HH21 | 1:P:205:GLN:NE2  | 2.07                     | 0.52              |
| 1:S:122:THR:CG2  | 1:S:124:TYR:HB3  | 2.39                     | 0.52              |
| 1:U:202:ARG:NH2  | 1:U:205:GLN:OE1  | 2.42                     | 0.52              |
| 1:d:119:TRP:NE1  | 1:d:143:MET:O    | 2.42                     | 0.52              |
| 1:e:122:THR:CG2  | 1:e:125:TYR:H    | 2.21                     | 0.52              |
| 1:f:69:MET:O     | 1:f:303:PHE:HB2  | 2.10                     | 0.52              |
| 1:M:140:LEU:O    | 1:M:144:ILE:HG13 | 2.08                     | 0.52              |
| 1:M:206:MET:HE3  | 1:M:286:ASN:CB   | 2.36                     | 0.52              |
| 1:U:119:TRP:CE2  | 1:U:143:MET:HB3  | 2.43                     | 0.52              |
| 1:X:152:GLY:HA2  | 1:X:158:VAL:HG12 | 1.91                     | 0.52              |
| 1:f:194:GLU:HA   | 1:f:194:GLU:OE2  | 2.10                     | 0.52              |
| 1:K:155:THR:HB   | 1:K:156:ARG:HD2  | 1.90                     | 0.52              |
| 1:R:125:TYR:HD1  | 1:R:143:MET:SD   | 2.32                     | 0.52              |
| 1:T:207:LYS:CE   | 1:T:294:ASN:HD21 | 2.20                     | 0.52              |
| 1:a:55:GLU:O     | 1:a:319:ASP:N    | 2.32                     | 0.52              |
| 1:c:194:GLU:OE2  | 1:d:67:VAL:HG23  | 2.09                     | 0.52              |
| 1:A:221:TYR:CE1  | 1:A:272:LEU:HG   | 2.45                     | 0.52              |
| 1:C:73:TYR:CZ    | 1:C:191:LEU:HB3  | 2.44                     | 0.52              |
| 1:J:187:ALA:HB3  | 1:J:305:THR:HG21 | 1.91                     | 0.52              |
| 1:Q:66:THR:HG21  | 1:X:190:HIS:NE2  | 2.23                     | 0.52              |
| 1:S:275:VAL:HG13 | 1:S:276:GLY:O    | 2.09                     | 0.52              |
| 1:W:115:ARG:HD2  | 1:W:144:ILE:O    | 2.10                     | 0.52              |
| 1:Z:199:TRP:O    | 1:Z:203:THR:OG1  | 2.27                     | 0.52              |
| 1:A:307:ARG:NH2  | 1:H:104:GLU:OE1  | 2.43                     | 0.52              |
| 1:D:266:GLN:HG2  | 1:D:269:LEU:HB3  | 1.92                     | 0.52              |
| 1:L:76:GLN:OE1   | 1:L:298:THR:N    | 2.24                     | 0.52              |
| 1:L:280:ASP:OD2  | 1:L:282:ASP:HB3  | 2.09                     | 0.52              |
| 1:a:168:THR:OG1  | 1:a:171:ASP:OD2  | 2.20                     | 0.52              |
| 1:d:125:TYR:HB2  | 1:d:143:MET:HE3  | 1.91                     | 0.52              |
| 1:B:108:GLN:HG3  | 1:B:187:ALA:HB2  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:203:THR:HA   | 1:I:293:LEU:HD23 | 1.92                     | 0.52              |
| 1:U:63:ASP:OD1   | 1:U:64:ARG:N     | 2.35                     | 0.52              |
| 1:W:212:ARG:O    | 1:W:216:VAL:HG23 | 2.10                     | 0.52              |
| 1:Y:57:SER:HA    | 1:Y:164:LEU:O    | 2.10                     | 0.52              |
| 1:b:141:ASP:HB2  | 1:c:316:VAL:HG11 | 1.92                     | 0.52              |
| 1:d:169:ALA:HB1  | 1:d:314:GLU:HG2  | 1.91                     | 0.52              |
| 1:G:200:ALA:C    | 1:O:302:ARG:NH2  | 2.63                     | 0.52              |
| 1:H:128:ARG:HE   | 1:H:167:GLU:CD   | 2.18                     | 0.52              |
| 1:I:122:THR:CG2  | 1:I:124:TYR:HB3  | 2.40                     | 0.52              |
| 1:J:119:TRP:NE1  | 1:J:147:ILE:HD11 | 2.25                     | 0.52              |
| 1:L:107:MET:HE1  | 1:M:63:ASP:OD2   | 2.10                     | 0.52              |
| 1:M:275:VAL:HG13 | 1:M:276:GLY:N    | 2.24                     | 0.52              |
| 1:N:168:THR:OG1  | 1:N:171:ASP:OD2  | 2.25                     | 0.52              |
| 1:N:213:GLN:NE2  | 1:N:286:ASN:HD22 | 2.08                     | 0.52              |
| 1:Q:199:TRP:CE2  | 1:Q:293:LEU:HD12 | 2.45                     | 0.52              |
| 1:V:164:LEU:HD13 | 1:V:176:LEU:HA   | 1.91                     | 0.52              |
| 1:b:207:LYS:HE3  | 1:b:290:LEU:HD21 | 1.92                     | 0.52              |
| 1:D:122:THR:HG22 | 1:D:125:TYR:H    | 1.75                     | 0.52              |
| 1:F:122:THR:CG2  | 1:F:124:TYR:HB3  | 2.40                     | 0.52              |
| 1:J:121:GLN:O    | 1:J:121:GLN:HG2  | 2.10                     | 0.52              |
| 1:S:182:PHE:CE2  | 1:S:186:ARG:HD2  | 2.45                     | 0.52              |
| 1:U:209:GLN:HA   | 1:U:212:ARG:NH2  | 2.25                     | 0.52              |
| 1:X:57:SER:HA    | 1:X:164:LEU:O    | 2.10                     | 0.52              |
| 1:Z:214:GLU:HA   | 1:Z:279:PHE:HE2  | 1.75                     | 0.52              |
| 1:c:83:LEU:O     | 1:c:202:ARG:NH1  | 2.42                     | 0.52              |
| 1:e:77:GLN:HG2   | 1:e:97:VAL:CG1   | 2.39                     | 0.52              |
| 1:F:64:ARG:HD3   | 1:F:99:ASP:OD1   | 2.10                     | 0.52              |
| 1:F:147:ILE:HG12 | 1:F:164:LEU:HD12 | 1.92                     | 0.52              |
| 1:G:272:LEU:HA   | 1:G:275:VAL:HG12 | 1.91                     | 0.52              |
| 1:H:122:THR:CG2  | 1:H:125:TYR:H    | 2.22                     | 0.52              |
| 1:L:223:ARG:CZ   | 1:M:279:PHE:HB2  | 2.40                     | 0.52              |
| 1:P:184:SER:HB2  | 1:P:306:TYR:CE1  | 2.45                     | 0.52              |
| 1:Y:66:THR:HB    | 1:f:194:GLU:OE2  | 2.10                     | 0.52              |
| 1:c:55:GLU:O     | 1:c:318:ARG:HG2  | 2.09                     | 0.52              |
| 1:H:61:ILE:HG22  | 1:H:309:LEU:HB2  | 1.92                     | 0.51              |
| 1:J:57:SER:HB2   | 1:J:163:LYS:HE2  | 1.92                     | 0.51              |
| 1:S:194:GLU:OE2  | 1:T:66:THR:HB    | 2.10                     | 0.51              |
| 1:W:55:GLU:O     | 1:W:318:ARG:HB2  | 2.09                     | 0.51              |
| 1:Y:221:TYR:CE1  | 1:Y:272:LEU:HG   | 2.44                     | 0.51              |
| 1:C:283:TYR:CZ   | 1:C:287:ARG:HD3  | 2.45                     | 0.51              |
| 1:O:80:LEU:HD12  | 1:O:195:LEU:HD12 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:96:SER:HG    | 1:U:98:MET:HG2   | 1.75                     | 0.51              |
| 1:V:128:ARG:CD   | 1:V:143:MET:HE1  | 2.40                     | 0.51              |
| 1:V:169:ALA:HB3  | 1:V:170:PRO:HD3  | 1.91                     | 0.51              |
| 1:c:63:ASP:HB2   | 1:c:309:LEU:HD11 | 1.92                     | 0.51              |
| 1:C:126:LYS:HA   | 1:C:129:MET:HE2  | 1.92                     | 0.51              |
| 1:C:206:MET:HE3  | 1:C:286:ASN:HA   | 1.91                     | 0.51              |
| 1:C:225:MET:HE1  | 1:C:273:GLN:HE21 | 1.76                     | 0.51              |
| 1:G:116:ARG:HG3  | 1:G:140:LEU:HD21 | 1.92                     | 0.51              |
| 1:G:295:VAL:HA   | 1:N:204:ILE:HD11 | 1.92                     | 0.51              |
| 1:H:119:TRP:NE1  | 1:H:143:MET:O    | 2.43                     | 0.51              |
| 1:H:196:LYS:HD2  | 1:H:299:LEU:CD1  | 2.40                     | 0.51              |
| 1:Q:196:LYS:HD2  | 1:Q:299:LEU:HD21 | 1.91                     | 0.51              |
| 1:S:187:ALA:CB   | 1:S:305:THR:HG21 | 2.39                     | 0.51              |
| 1:e:187:ALA:HB1  | 1:e:305:THR:HG21 | 1.93                     | 0.51              |
| 1:E:66:THR:OG1   | 1:E:69:MET:HE3   | 2.10                     | 0.51              |
| 1:F:105:PHE:CG   | 1:F:306:TYR:HB3  | 2.46                     | 0.51              |
| 1:K:119:TRP:HA   | 1:K:122:THR:HB   | 1.92                     | 0.51              |
| 1:R:122:THR:HG23 | 1:R:124:TYR:HB3  | 1.92                     | 0.51              |
| 1:X:70:LEU:HD11  | 1:X:98:MET:HB3   | 1.90                     | 0.51              |
| 1:Y:301:PRO:HD2  | 1:Y:302:ARG:HH11 | 1.75                     | 0.51              |
| 1:f:269:LEU:O    | 1:f:273:GLN:HB2  | 2.10                     | 0.51              |
| 1:B:187:ALA:CB   | 1:B:305:THR:HG21 | 2.40                     | 0.51              |
| 1:Q:122:THR:O    | 1:Q:126:LYS:HG3  | 2.10                     | 0.51              |
| 1:V:199:TRP:NE1  | 1:V:293:LEU:O    | 2.40                     | 0.51              |
| 1:b:72:GLY:O     | 1:b:76:GLN:HG3   | 2.10                     | 0.51              |
| 1:C:289:MET:HA   | 1:C:292:THR:OG1  | 2.11                     | 0.51              |
| 1:D:164:LEU:HB2  | 1:D:176:LEU:HD13 | 1.92                     | 0.51              |
| 1:e:141:ASP:HA   | 1:e:144:ILE:HD12 | 1.93                     | 0.51              |
| 1:B:72:GLY:O     | 1:B:76:GLN:NE2   | 2.29                     | 0.51              |
| 1:F:119:TRP:HA   | 1:F:122:THR:HB   | 1.92                     | 0.51              |
| 1:L:119:TRP:CD2  | 1:L:143:MET:HB3  | 2.45                     | 0.51              |
| 1:R:81:ARG:NH2   | 1:R:95:PRO:O     | 2.40                     | 0.51              |
| 1:Y:63:ASP:OD2   | 1:Y:64:ARG:HG2   | 2.11                     | 0.51              |
| 1:f:288:ALA:O    | 1:f:291:ASN:HB2  | 2.10                     | 0.51              |
| 1:E:151:PRO:HG3  | 1:F:157:ALA:HB3  | 1.93                     | 0.51              |
| 1:F:69:MET:O     | 1:F:303:PHE:HB2  | 2.11                     | 0.51              |
| 1:F:207:LYS:HG3  | 1:F:290:LEU:HD21 | 1.92                     | 0.51              |
| 1:N:182:PHE:CE2  | 1:N:186:ARG:HD2  | 2.46                     | 0.51              |
| 1:Y:271:ASN:O    | 1:Y:275:VAL:HB   | 2.11                     | 0.51              |
| 1:Z:70:LEU:HD11  | 1:Z:98:MET:CB    | 2.41                     | 0.51              |
| 1:C:125:TYR:HD1  | 1:C:143:MET:SD   | 2.33                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:182:PHE:CE2  | 1:L:186:ARG:HD2  | 2.46                     | 0.51              |
| 1:W:216:VAL:HG22 | 1:X:284:ASP:C    | 2.35                     | 0.51              |
| 1:Z:126:LYS:HA   | 1:Z:129:MET:HE2  | 1.93                     | 0.51              |
| 1:f:225:MET:HE1  | 1:f:273:GLN:CD   | 2.36                     | 0.51              |
| 1:L:73:TYR:CD1   | 1:L:195:LEU:HD22 | 2.46                     | 0.51              |
| 1:S:122:THR:HG23 | 1:S:124:TYR:HB3  | 1.92                     | 0.51              |
| 1:U:125:TYR:CE2  | 1:U:129:MET:SD   | 3.04                     | 0.51              |
| 1:Z:104:GLU:CD   | 1:a:307:ARG:HH22 | 2.19                     | 0.51              |
| 1:a:199:TRP:NE1  | 1:a:296:GLY:HA2  | 2.26                     | 0.51              |
| 1:d:120:LEU:HD21 | 1:d:140:LEU:HD22 | 1.93                     | 0.51              |
| 1:f:83:LEU:HB3   | 1:f:202:ARG:NH1  | 2.24                     | 0.51              |
| 1:f:202:ARG:HE   | 1:f:205:GLN:HE21 | 1.58                     | 0.51              |
| 1:D:81:ARG:NH2   | 1:D:95:PRO:O     | 2.43                     | 0.50              |
| 1:D:213:GLN:HE22 | 1:D:286:ASN:HD22 | 1.59                     | 0.50              |
| 1:F:206:MET:HE3  | 1:F:289:MET:HG2  | 1.93                     | 0.50              |
| 1:R:120:LEU:HG   | 1:R:140:LEU:HD11 | 1.93                     | 0.50              |
| 1:R:283:TYR:CZ   | 1:R:287:ARG:HD3  | 2.46                     | 0.50              |
| 1:S:74:TYR:CD1   | 1:S:97:VAL:CG2   | 2.94                     | 0.50              |
| 1:V:122:THR:HG22 | 1:V:125:TYR:H    | 1.75                     | 0.50              |
| 1:b:169:ALA:HB3  | 1:b:170:PRO:HD3  | 1.92                     | 0.50              |
| 1:e:115:ARG:HB2  | 1:e:144:ILE:HG23 | 1.92                     | 0.50              |
| 1:C:169:ALA:HB3  | 1:C:170:PRO:HD3  | 1.93                     | 0.50              |
| 1:G:58:SER:OG    | 1:G:313:GLU:O    | 2.29                     | 0.50              |
| 1:I:288:ALA:O    | 1:I:291:ASN:HB2  | 2.11                     | 0.50              |
| 1:V:203:THR:O    | 1:V:207:LYS:HB2  | 2.12                     | 0.50              |
| 1:V:210:VAL:HG13 | 1:V:283:TYR:CE1  | 2.46                     | 0.50              |
| 1:E:105:PHE:HB2  | 1:E:305:THR:CG2  | 2.38                     | 0.50              |
| 1:P:202:ARG:NH2  | 1:P:205:GLN:HE21 | 2.09                     | 0.50              |
| 1:S:105:PHE:HB2  | 1:S:305:THR:CG2  | 2.37                     | 0.50              |
| 1:S:198:ALA:HB2  | 1:T:67:VAL:HG21  | 1.93                     | 0.50              |
| 1:Y:122:THR:O    | 1:Y:126:LYS:HG3  | 2.11                     | 0.50              |
| 1:c:226:ASN:CG   | 1:c:230:GLN:HE22 | 2.19                     | 0.50              |
| 1:E:143:MET:O    | 1:E:146:ASN:HB2  | 2.12                     | 0.50              |
| 1:G:229:GLU:HG2  | 1:G:269:LEU:HD11 | 1.92                     | 0.50              |
| 1:H:196:LYS:HD2  | 1:H:299:LEU:HD11 | 1.94                     | 0.50              |
| 1:H:299:LEU:HD12 | 1:O:121:GLN:HE21 | 1.77                     | 0.50              |
| 1:L:177:ARG:NH2  | 1:L:312:PRO:O    | 2.44                     | 0.50              |
| 1:R:139:LEU:O    | 1:R:143:MET:HG3  | 2.11                     | 0.50              |
| 1:W:74:TYR:CZ    | 1:W:78:GLN:HG3   | 2.46                     | 0.50              |
| 1:X:77:GLN:HG3   | 1:X:97:VAL:HG22  | 1.94                     | 0.50              |
| 1:e:134:LYS:NZ   | 1:f:316:VAL:O    | 2.43                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:138:ALA:HB2  | 1:C:316:VAL:HG11 | 1.93                     | 0.50              |
| 1:C:122:THR:HG23 | 1:C:124:TYR:H    | 1.77                     | 0.50              |
| 1:E:76:GLN:NE2   | 1:E:298:THR:H    | 2.10                     | 0.50              |
| 1:E:123:ASP:HB3  | 1:E:127:GLN:NE2  | 2.27                     | 0.50              |
| 1:I:69:MET:HE1   | 1:I:306:TYR:O    | 2.11                     | 0.50              |
| 1:I:168:THR:OG1  | 1:I:171:ASP:OD2  | 2.19                     | 0.50              |
| 1:W:119:TRP:O    | 1:W:125:TYR:HB3  | 2.12                     | 0.50              |
| 1:b:230:GLN:HE21 | 1:c:274:ALA:HB1  | 1.76                     | 0.50              |
| 1:L:196:LYS:HA   | 1:L:297:PRO:HG3  | 1.94                     | 0.50              |
| 1:Q:122:THR:HG22 | 1:Q:125:TYR:H    | 1.76                     | 0.50              |
| 1:S:124:TYR:O    | 1:S:128:ARG:NH1  | 2.40                     | 0.50              |
| 1:Z:122:THR:CG2  | 1:Z:125:TYR:H    | 2.25                     | 0.50              |
| 1:A:57:SER:HA    | 1:A:164:LEU:O    | 2.12                     | 0.50              |
| 1:C:225:MET:O    | 1:C:229:GLU:HG3  | 2.12                     | 0.50              |
| 1:D:64:ARG:NE    | 1:D:99:ASP:OD1   | 2.45                     | 0.50              |
| 1:F:69:MET:HB3   | 1:F:304:GLN:HB3  | 1.94                     | 0.50              |
| 1:M:202:ARG:HH21 | 1:M:205:GLN:CD   | 2.18                     | 0.50              |
| 1:Q:64:ARG:HA    | 1:Q:102:TYR:CD1  | 2.47                     | 0.50              |
| 1:Q:116:ARG:HG3  | 1:Q:140:LEU:HD21 | 1.94                     | 0.50              |
| 1:U:112:TRP:CE2  | 1:U:144:ILE:HG21 | 2.47                     | 0.50              |
| 1:Y:307:ARG:HH22 | 1:f:104:GLU:CD   | 2.20                     | 0.50              |
| 1:c:76:GLN:HE22  | 1:c:297:PRO:HA   | 1.77                     | 0.50              |
| 1:c:104:GLU:O    | 1:c:108:GLN:HG2  | 2.12                     | 0.50              |
| 1:d:63:ASP:OD1   | 1:d:64:ARG:HG2   | 2.11                     | 0.50              |
| 1:A:63:ASP:OD2   | 1:A:64:ARG:N     | 2.40                     | 0.50              |
| 1:B:120:LEU:HD21 | 1:B:140:LEU:HD22 | 1.94                     | 0.50              |
| 1:H:57:SER:HA    | 1:H:164:LEU:O    | 2.11                     | 0.50              |
| 1:Q:70:LEU:HD11  | 1:Q:98:MET:HB3   | 1.93                     | 0.50              |
| 1:R:56:TRP:CD1   | 1:R:168:THR:HA   | 2.47                     | 0.50              |
| 1:R:138:ALA:N    | 1:S:316:VAL:HG11 | 2.27                     | 0.50              |
| 1:Y:107:MET:HE1  | 1:Z:63:ASP:OD2   | 2.12                     | 0.50              |
| 1:A:307:ARG:NH2  | 1:H:107:MET:HE3  | 2.26                     | 0.49              |
| 1:B:118:PHE:CG   | 1:B:179:TYR:HD1  | 2.28                     | 0.49              |
| 1:K:119:TRP:CE3  | 1:K:122:THR:HG21 | 2.47                     | 0.49              |
| 1:M:122:THR:CG2  | 1:M:124:TYR:HB3  | 2.42                     | 0.49              |
| 1:N:56:TRP:CE3   | 1:N:169:ALA:HB2  | 2.47                     | 0.49              |
| 1:P:199:TRP:NE1  | 1:P:296:GLY:HA2  | 2.26                     | 0.49              |
| 1:S:56:TRP:CE3   | 1:S:169:ALA:HB2  | 2.47                     | 0.49              |
| 1:Z:141:ASP:HA   | 1:Z:144:ILE:HD12 | 1.92                     | 0.49              |
| 1:I:122:THR:CG2  | 1:I:125:TYR:H    | 2.26                     | 0.49              |
| 1:M:148:GLN:N    | 1:M:148:GLN:HE21 | 2.09                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:206:MET:HE1  | 1:N:289:MET:HG2  | 1.94                     | 0.49              |
| 1:Q:141:ASP:HA   | 1:Q:144:ILE:HD12 | 1.94                     | 0.49              |
| 1:R:122:THR:CG2  | 1:R:125:TYR:H    | 2.24                     | 0.49              |
| 1:T:271:ASN:O    | 1:T:275:VAL:HB   | 2.12                     | 0.49              |
| 1:c:122:THR:CG2  | 1:c:125:TYR:H    | 2.24                     | 0.49              |
| 1:f:61:ILE:HB    | 1:f:310:ARG:HB3  | 1.95                     | 0.49              |
| 1:B:101:ALA:HA   | 1:B:191:LEU:HD21 | 1.94                     | 0.49              |
| 1:D:103:LYS:O    | 1:D:107:MET:HG3  | 2.11                     | 0.49              |
| 1:G:65:PRO:CB    | 1:G:69:MET:HG2   | 2.41                     | 0.49              |
| 1:K:226:ASN:OD1  | 1:K:230:GLN:NE2  | 2.45                     | 0.49              |
| 1:N:213:GLN:HE22 | 1:N:286:ASN:HD22 | 1.60                     | 0.49              |
| 1:W:97:VAL:HB    | 1:W:98:MET:CE    | 2.41                     | 0.49              |
| 1:B:141:ASP:O    | 1:B:145:ASN:ND2  | 2.46                     | 0.49              |
| 1:F:225:MET:HE3  | 1:F:269:LEU:HD11 | 1.94                     | 0.49              |
| 1:H:132:ASN:HB3  | 1:H:135:ALA:HB3  | 1.95                     | 0.49              |
| 1:O:61:ILE:HB    | 1:O:310:ARG:HB3  | 1.95                     | 0.49              |
| 1:Q:125:TYR:OH   | 1:Q:136:ASP:O    | 2.22                     | 0.49              |
| 1:S:61:ILE:HB    | 1:S:310:ARG:HB3  | 1.93                     | 0.49              |
| 1:S:74:TYR:CD1   | 1:S:97:VAL:HG21  | 2.47                     | 0.49              |
| 1:T:169:ALA:HB3  | 1:T:170:PRO:HD3  | 1.93                     | 0.49              |
| 1:T:292:THR:HG22 | 1:b:302:ARG:NH2  | 2.27                     | 0.49              |
| 1:W:119:TRP:CZ3  | 1:W:175:LEU:HD22 | 2.47                     | 0.49              |
| 1:Z:216:VAL:CG2  | 1:a:285:GLN:HA   | 2.42                     | 0.49              |
| 1:a:83:LEU:HB3   | 1:a:202:ARG:NH1  | 2.27                     | 0.49              |
| 1:A:61:ILE:CG1   | 1:A:310:ARG:HB3  | 2.34                     | 0.49              |
| 1:C:60:ALA:HB2   | 1:C:312:PRO:HG3  | 1.94                     | 0.49              |
| 1:J:152:GLY:HA2  | 1:J:158:VAL:HG12 | 1.94                     | 0.49              |
| 1:K:267:ALA:O    | 1:K:271:ASN:ND2  | 2.45                     | 0.49              |
| 1:U:122:THR:HG23 | 1:U:124:TYR:HB3  | 1.94                     | 0.49              |
| 1:D:70:LEU:HA    | 1:D:303:PHE:CD1  | 2.48                     | 0.49              |
| 1:H:207:LYS:CE   | 1:H:294:ASN:HD21 | 2.23                     | 0.49              |
| 1:P:119:TRP:CD2  | 1:P:143:MET:HB2  | 2.47                     | 0.49              |
| 1:P:203:THR:HA   | 1:P:293:LEU:HD23 | 1.95                     | 0.49              |
| 1:T:114:THR:HG22 | 1:T:179:TYR:CE1  | 2.47                     | 0.49              |
| 1:U:213:GLN:NE2  | 1:U:286:ASN:HD22 | 2.11                     | 0.49              |
| 1:Z:60:ALA:HB2   | 1:Z:312:PRO:HG3  | 1.94                     | 0.49              |
| 1:e:139:LEU:HG   | 1:e:143:MET:HE3  | 1.95                     | 0.49              |
| 1:f:64:ARG:HA    | 1:f:102:TYR:CD1  | 2.47                     | 0.49              |
| 1:C:76:GLN:HE22  | 1:C:298:THR:H    | 1.60                     | 0.49              |
| 1:D:70:LEU:O     | 1:D:73:TYR:HB3   | 2.13                     | 0.49              |
| 1:G:199:TRP:CE2  | 1:G:297:PRO:HD3  | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:223:ARG:HH12 | 1:J:284:ASP:CG   | 2.20                     | 0.49              |
| 1:J:63:ASP:CG    | 1:J:64:ARG:H     | 2.20                     | 0.49              |
| 1:O:169:ALA:HB3  | 1:O:170:PRO:HD3  | 1.94                     | 0.49              |
| 1:Q:56:TRP:CD1   | 1:Q:168:THR:HA   | 2.48                     | 0.49              |
| 1:Q:57:SER:HA    | 1:Q:164:LEU:O    | 2.13                     | 0.49              |
| 1:T:83:LEU:HB3   | 1:T:202:ARG:NH1  | 2.26                     | 0.49              |
| 1:U:76:GLN:NE2   | 1:U:297:PRO:HA   | 2.27                     | 0.49              |
| 1:Y:218:LYS:HE2  | 1:Y:222:ASP:OD2  | 2.12                     | 0.49              |
| 1:Z:74:TYR:CE1   | 1:Z:98:MET:SD    | 3.06                     | 0.49              |
| 1:f:77:GLN:HG2   | 1:f:97:VAL:HG13  | 1.94                     | 0.49              |
| 1:C:230:GLN:OE1  | 1:D:274:ALA:HB1  | 2.13                     | 0.49              |
| 1:J:169:ALA:HB3  | 1:J:170:PRO:HD3  | 1.94                     | 0.49              |
| 1:L:113:ASP:OD2  | 1:M:311:THR:OG1  | 2.23                     | 0.49              |
| 1:N:57:SER:CB    | 1:N:163:LYS:HE2  | 2.41                     | 0.49              |
| 1:U:55:GLU:N     | 1:U:166:ALA:O    | 2.45                     | 0.49              |
| 1:a:199:TRP:CD1  | 1:a:297:PRO:HD3  | 2.48                     | 0.49              |
| 1:f:79:PHE:O     | 1:f:83:LEU:HG    | 2.12                     | 0.49              |
| 1:S:74:TYR:HD1   | 1:S:97:VAL:HG21  | 1.78                     | 0.49              |
| 1:U:61:ILE:HG12  | 1:U:161:SER:HB3  | 1.95                     | 0.49              |
| 1:a:104:GLU:OE2  | 1:b:307:ARG:NH1  | 2.40                     | 0.49              |
| 1:c:304:GLN:HG2  | 1:c:306:TYR:CE1  | 2.47                     | 0.49              |
| 1:d:169:ALA:HB3  | 1:d:170:PRO:HD3  | 1.95                     | 0.49              |
| 1:B:122:THR:CG2  | 1:B:125:TYR:H    | 2.26                     | 0.49              |
| 1:D:184:SER:HB2  | 1:D:306:TYR:CE1  | 2.47                     | 0.49              |
| 1:E:216:VAL:CG2  | 1:F:285:GLN:HA   | 2.43                     | 0.49              |
| 1:J:119:TRP:O    | 1:J:122:THR:HG22 | 2.13                     | 0.49              |
| 1:J:212:ARG:O    | 1:J:216:VAL:HG23 | 2.13                     | 0.49              |
| 1:K:301:PRO:HD2  | 1:K:302:ARG:HH11 | 1.78                     | 0.49              |
| 1:S:164:LEU:HD13 | 1:S:176:LEU:HA   | 1.95                     | 0.49              |
| 1:V:228:ILE:HD12 | 1:V:272:LEU:HD22 | 1.95                     | 0.49              |
| 1:W:83:LEU:C     | 1:W:85:VAL:H     | 2.21                     | 0.49              |
| 1:Y:128:ARG:HE   | 1:Y:167:GLU:CD   | 2.20                     | 0.49              |
| 1:b:190:HIS:CE1  | 1:c:66:THR:HG21  | 2.47                     | 0.49              |
| 1:B:55:GLU:O     | 1:B:318:ARG:HG2  | 2.13                     | 0.48              |
| 1:E:84:ASP:C     | 1:E:84:ASP:OD1   | 2.56                     | 0.48              |
| 1:H:84:ASP:OD1   | 1:H:85:VAL:HG12  | 2.13                     | 0.48              |
| 1:I:57:SER:CB    | 1:I:163:LYS:HE2  | 2.43                     | 0.48              |
| 1:V:98:MET:H     | 1:V:98:MET:HG2   | 1.46                     | 0.48              |
| 1:X:283:TYR:OH   | 1:X:287:ARG:HD3  | 2.13                     | 0.48              |
| 1:Z:77:GLN:HG2   | 1:Z:97:VAL:HG13  | 1.94                     | 0.48              |
| 1:Z:119:TRP:CE2  | 1:Z:143:MET:HB3  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:207:LYS:HG3  | 1:a:290:LEU:HD21 | 1.95                     | 0.48              |
| 1:c:227:SER:HB2  | 1:d:275:VAL:HG23 | 1.95                     | 0.48              |
| 1:A:128:ARG:HE   | 1:A:167:GLU:CD   | 2.21                     | 0.48              |
| 1:B:61:ILE:HB    | 1:B:310:ARG:CB   | 2.44                     | 0.48              |
| 1:E:211:LYS:HA   | 1:E:211:LYS:CE   | 2.29                     | 0.48              |
| 1:E:300:ASP:HA   | 1:E:302:ARG:HH11 | 1.78                     | 0.48              |
| 1:G:169:ALA:HB3  | 1:G:170:PRO:HD3  | 1.95                     | 0.48              |
| 1:H:120:LEU:HD21 | 1:H:140:LEU:HD22 | 1.95                     | 0.48              |
| 1:K:168:THR:OG1  | 1:K:171:ASP:OD2  | 2.27                     | 0.48              |
| 1:K:288:ALA:O    | 1:K:291:ASN:HB2  | 2.13                     | 0.48              |
| 1:M:209:GLN:HA   | 1:M:212:ARG:NH2  | 2.28                     | 0.48              |
| 1:P:101:ALA:HA   | 1:P:191:LEU:HD11 | 1.95                     | 0.48              |
| 1:Q:80:LEU:HD23  | 1:Q:83:LEU:HD12  | 1.95                     | 0.48              |
| 1:S:300:ASP:OD1  | 1:S:302:ARG:HD3  | 2.13                     | 0.48              |
| 1:f:81:ARG:NH1   | 1:f:95:PRO:O     | 2.41                     | 0.48              |
| 1:f:201:ALA:O    | 1:f:205:GLN:HB3  | 2.13                     | 0.48              |
| 1:I:64:ARG:NE    | 1:I:99:ASP:OD1   | 2.46                     | 0.48              |
| 1:I:224:ARG:O    | 1:I:228:ILE:HG13 | 2.14                     | 0.48              |
| 1:J:113:ASP:OD2  | 1:K:311:THR:OG1  | 2.28                     | 0.48              |
| 1:T:202:ARG:NH2  | 1:T:205:GLN:NE2  | 2.61                     | 0.48              |
| 1:A:153:ASP:N    | 1:A:158:VAL:HG12 | 2.29                     | 0.48              |
| 1:A:275:VAL:HG13 | 1:A:276:GLY:O    | 2.14                     | 0.48              |
| 1:B:202:ARG:HH21 | 1:B:205:GLN:CD   | 2.22                     | 0.48              |
| 1:G:124:TYR:CG   | 1:G:175:LEU:HD11 | 2.48                     | 0.48              |
| 1:I:124:TYR:OH   | 1:I:167:GLU:HG3  | 2.13                     | 0.48              |
| 1:L:57:SER:CB    | 1:L:163:LYS:HE3  | 2.40                     | 0.48              |
| 1:P:122:THR:CG2  | 1:P:125:TYR:H    | 2.26                     | 0.48              |
| 1:P:285:GLN:O    | 1:P:289:MET:HB2  | 2.13                     | 0.48              |
| 1:U:122:THR:O    | 1:U:126:LYS:HG3  | 2.13                     | 0.48              |
| 1:V:214:GLU:HG3  | 1:V:283:TYR:CE1  | 2.48                     | 0.48              |
| 1:d:126:LYS:HA   | 1:d:129:MET:HG3  | 1.95                     | 0.48              |
| 1:f:226:ASN:OD1  | 1:f:230:GLN:NE2  | 2.45                     | 0.48              |
| 1:B:81:ARG:HH12  | 1:B:96:SER:HA    | 1.77                     | 0.48              |
| 1:H:81:ARG:NH2   | 1:H:95:PRO:O     | 2.34                     | 0.48              |
| 1:I:104:GLU:CD   | 1:J:307:ARG:HH22 | 2.21                     | 0.48              |
| 1:I:169:ALA:HB3  | 1:I:170:PRO:HD3  | 1.95                     | 0.48              |
| 1:K:126:LYS:HA   | 1:K:129:MET:HG3  | 1.95                     | 0.48              |
| 1:N:58:SER:OG    | 1:N:313:GLU:O    | 2.28                     | 0.48              |
| 1:R:108:GLN:OE1  | 1:R:114:THR:OG1  | 2.30                     | 0.48              |
| 1:S:81:ARG:HA    | 1:S:84:ASP:OD2   | 2.14                     | 0.48              |
| 1:U:152:GLY:N    | 1:U:160:ASP:OD2  | 2.37                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:66:THR:OG1   | 1:b:69:MET:HE3   | 2.13                     | 0.48              |
| 1:D:153:ASP:H    | 1:D:158:VAL:HB   | 1.79                     | 0.48              |
| 1:N:272:LEU:HA   | 1:N:275:VAL:HG12 | 1.95                     | 0.48              |
| 1:P:199:TRP:CD1  | 1:P:297:PRO:HD3  | 2.49                     | 0.48              |
| 1:T:199:TRP:O    | 1:T:203:THR:OG1  | 2.23                     | 0.48              |
| 1:U:202:ARG:HH21 | 1:U:205:GLN:CD   | 2.22                     | 0.48              |
| 1:W:122:THR:O    | 1:W:126:LYS:HG3  | 2.13                     | 0.48              |
| 1:Z:214:GLU:HG2  | 1:Z:279:PHE:CZ   | 2.49                     | 0.48              |
| 1:d:194:GLU:CD   | 1:e:66:THR:HB    | 2.38                     | 0.48              |
| 1:f:212:ARG:O    | 1:f:216:VAL:HG23 | 2.14                     | 0.48              |
| 1:H:63:ASP:CG    | 1:H:64:ARG:H     | 2.22                     | 0.48              |
| 1:N:105:PHE:HB2  | 1:N:305:THR:HG23 | 1.95                     | 0.48              |
| 1:S:300:ASP:OD1  | 1:S:302:ARG:HB2  | 2.13                     | 0.48              |
| 1:Y:68:ASN:OD1   | 1:f:197:GLY:HA3  | 2.14                     | 0.48              |
| 1:Z:121:GLN:O    | 1:Z:121:GLN:HG2  | 2.14                     | 0.48              |
| 1:b:56:TRP:CD1   | 1:b:168:THR:HA   | 2.49                     | 0.48              |
| 1:b:61:ILE:HG21  | 1:b:61:ILE:HD13  | 1.54                     | 0.48              |
| 1:b:185:GLN:HE22 | 1:b:301:PRO:HB2  | 1.79                     | 0.48              |
| 1:c:57:SER:CB    | 1:c:163:LYS:HE2  | 2.43                     | 0.48              |
| 1:e:70:LEU:HD11  | 1:e:98:MET:HB3   | 1.96                     | 0.48              |
| 1:A:289:MET:HE2  | 1:H:212:ARG:NE   | 2.28                     | 0.48              |
| 1:C:77:GLN:HG2   | 1:C:97:VAL:CG1   | 2.43                     | 0.48              |
| 1:F:119:TRP:O    | 1:F:125:TYR:HB3  | 2.14                     | 0.48              |
| 1:F:300:ASP:OD2  | 1:F:302:ARG:NH2  | 2.47                     | 0.48              |
| 1:P:180:VAL:HG11 | 1:P:308:TYR:CE1  | 2.49                     | 0.48              |
| 1:R:109:LEU:HD23 | 1:R:149:PHE:CE1  | 2.48                     | 0.48              |
| 1:T:73:TYR:CZ    | 1:T:191:LEU:HB3  | 2.48                     | 0.48              |
| 1:T:134:LYS:NZ   | 1:U:316:VAL:HB   | 2.29                     | 0.48              |
| 1:U:194:GLU:OE2  | 1:V:67:VAL:HG23  | 2.14                     | 0.48              |
| 1:V:83:LEU:C     | 1:V:85:VAL:H     | 2.21                     | 0.48              |
| 1:V:268:ARG:HD2  | 1:V:268:ARG:HA   | 1.62                     | 0.48              |
| 1:Y:316:VAL:HG23 | 1:Y:317:LYS:HD3  | 1.96                     | 0.48              |
| 1:Z:216:VAL:HG21 | 1:a:285:GLN:HG2  | 1.94                     | 0.48              |
| 1:d:78:GLN:HE21  | 1:d:97:VAL:HG23  | 1.77                     | 0.48              |
| 1:E:153:ASP:H    | 1:E:158:VAL:HB   | 1.79                     | 0.48              |
| 1:F:63:ASP:HB2   | 1:F:309:LEU:HD11 | 1.95                     | 0.48              |
| 1:G:187:ALA:HB1  | 1:G:305:THR:HG21 | 1.96                     | 0.48              |
| 1:H:205:GLN:HG3  | 1:H:206:MET:N    | 2.29                     | 0.48              |
| 1:a:69:MET:HB3   | 1:a:304:GLN:HB3  | 1.95                     | 0.48              |
| 1:a:194:GLU:OE2  | 1:a:194:GLU:HA   | 2.14                     | 0.48              |
| 1:f:169:ALA:C    | 1:f:314:GLU:HG2  | 2.39                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:206:MET:CE   | 1:f:289:MET:HG2  | 2.44                     | 0.48              |
| 1:A:292:THR:CG2  | 1:H:212:ARG:HD3  | 2.43                     | 0.48              |
| 1:B:74:TYR:CZ    | 1:B:78:GLN:HG3   | 2.49                     | 0.48              |
| 1:B:103:LYS:O    | 1:B:107:MET:HB2  | 2.13                     | 0.48              |
| 1:B:190:HIS:O    | 1:B:193:ASP:HB2  | 2.14                     | 0.48              |
| 1:C:213:GLN:NE2  | 1:C:286:ASN:HD22 | 2.11                     | 0.48              |
| 1:L:169:ALA:HB3  | 1:L:170:PRO:HD3  | 1.96                     | 0.48              |
| 1:M:119:TRP:CE3  | 1:M:122:THR:HG21 | 2.48                     | 0.48              |
| 1:S:223:ARG:O    | 1:S:227:SER:OG   | 2.31                     | 0.48              |
| 1:a:130:VAL:HG23 | 1:a:132:ASN:H    | 1.78                     | 0.48              |
| 1:c:169:ALA:HB3  | 1:c:170:PRO:HD3  | 1.96                     | 0.48              |
| 1:e:126:LYS:HA   | 1:e:129:MET:HE2  | 1.96                     | 0.48              |
| 1:A:119:TRP:CE2  | 1:A:143:MET:HG2  | 2.49                     | 0.47              |
| 1:H:55:GLU:HG3   | 1:H:167:GLU:HA   | 1.95                     | 0.47              |
| 1:H:199:TRP:CG   | 1:H:297:PRO:HD3  | 2.48                     | 0.47              |
| 1:K:74:TYR:HD1   | 1:K:97:VAL:HG21  | 1.79                     | 0.47              |
| 1:N:120:LEU:O    | 1:N:126:LYS:HE3  | 2.14                     | 0.47              |
| 1:P:168:THR:OG1  | 1:P:171:ASP:OD2  | 2.29                     | 0.47              |
| 1:P:203:THR:CG2  | 1:P:207:LYS:HE3  | 2.42                     | 0.47              |
| 1:T:199:TRP:CE2  | 1:T:293:LEU:HD12 | 2.49                     | 0.47              |
| 1:b:275:VAL:HG13 | 1:b:276:GLY:O    | 2.14                     | 0.47              |
| 1:d:141:ASP:O    | 1:d:145:ASN:ND2  | 2.46                     | 0.47              |
| 1:d:270:GLU:HA   | 1:d:273:GLN:HB2  | 1.95                     | 0.47              |
| 1:e:168:THR:OG1  | 1:e:171:ASP:OD2  | 2.19                     | 0.47              |
| 1:e:213:GLN:HE22 | 1:e:286:ASN:HD22 | 1.62                     | 0.47              |
| 1:A:227:SER:CB   | 1:B:275:VAL:HG22 | 2.42                     | 0.47              |
| 1:C:101:ALA:HA   | 1:C:191:LEU:HD21 | 1.96                     | 0.47              |
| 1:C:210:VAL:HG13 | 1:C:283:TYR:HE1  | 1.79                     | 0.47              |
| 1:F:105:PHE:CE2  | 1:F:109:LEU:HD22 | 2.49                     | 0.47              |
| 1:R:210:VAL:HA   | 1:R:213:GLN:HE21 | 1.79                     | 0.47              |
| 1:U:119:TRP:CD2  | 1:U:143:MET:HB3  | 2.49                     | 0.47              |
| 1:U:302:ARG:HH22 | 1:a:287:ARG:NH2  | 2.11                     | 0.47              |
| 1:e:169:ALA:HB3  | 1:e:170:PRO:HD3  | 1.96                     | 0.47              |
| 1:H:61:ILE:O     | 1:H:309:LEU:N    | 2.33                     | 0.47              |
| 1:M:228:ILE:HD11 | 1:M:272:LEU:HD22 | 1.95                     | 0.47              |
| 1:O:122:THR:O    | 1:O:126:LYS:CG   | 2.63                     | 0.47              |
| 1:R:122:THR:CG2  | 1:R:124:TYR:HB3  | 2.44                     | 0.47              |
| 1:V:130:VAL:HG23 | 1:V:132:ASN:H    | 1.79                     | 0.47              |
| 1:W:77:GLN:HG2   | 1:W:97:VAL:HG13  | 1.96                     | 0.47              |
| 1:e:116:ARG:HA   | 1:e:144:ILE:HG12 | 1.96                     | 0.47              |
| 1:N:124:TYR:CD2  | 1:N:175:LEU:HD11 | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:96:SER:OG    | 1:Q:98:MET:HE2   | 2.13                     | 0.47              |
| 1:T:206:MET:HB3  | 1:T:290:LEU:HG   | 1.97                     | 0.47              |
| 1:Y:119:TRP:CD2  | 1:Y:143:MET:HB3  | 2.49                     | 0.47              |
| 1:a:169:ALA:HB3  | 1:a:170:PRO:HD3  | 1.97                     | 0.47              |
| 1:A:215:GLU:HA   | 1:A:215:GLU:OE2  | 2.14                     | 0.47              |
| 1:M:122:THR:HG22 | 1:M:125:TYR:HB3  | 1.96                     | 0.47              |
| 1:M:266:GLN:O    | 1:M:266:GLN:HG2  | 2.14                     | 0.47              |
| 1:O:118:PHE:CG   | 1:O:179:TYR:HD1  | 2.32                     | 0.47              |
| 1:P:122:THR:HG22 | 1:P:125:TYR:H    | 1.78                     | 0.47              |
| 1:Q:63:ASP:OD2   | 1:Q:64:ARG:HG2   | 2.15                     | 0.47              |
| 1:T:293:LEU:HD12 | 1:T:293:LEU:HA   | 1.70                     | 0.47              |
| 1:V:63:ASP:HB2   | 1:V:309:LEU:HD11 | 1.95                     | 0.47              |
| 1:f:65:PRO:HD2   | 1:f:102:TYR:HB2  | 1.96                     | 0.47              |
| 1:f:122:THR:HG22 | 1:f:125:TYR:H    | 1.77                     | 0.47              |
| 1:A:202:ARG:NH2  | 1:A:205:GLN:OE1  | 2.47                     | 0.47              |
| 1:F:156:ARG:HG3  | 1:F:158:VAL:HG23 | 1.95                     | 0.47              |
| 1:O:76:GLN:HE21  | 1:O:298:THR:HG23 | 1.79                     | 0.47              |
| 1:P:126:LYS:HA   | 1:P:129:MET:HG3  | 1.96                     | 0.47              |
| 1:R:57:SER:HB3   | 1:R:319:ASP:OD2  | 2.14                     | 0.47              |
| 1:S:202:ARG:NH2  | 1:S:205:GLN:OE1  | 2.44                     | 0.47              |
| 1:Y:66:THR:OG1   | 1:Y:69:MET:HG3   | 2.14                     | 0.47              |
| 1:Y:125:TYR:HD1  | 1:Y:143:MET:HE2  | 1.80                     | 0.47              |
| 1:c:194:GLU:OE2  | 1:c:194:GLU:HA   | 2.13                     | 0.47              |
| 1:C:286:ASN:O    | 1:C:290:LEU:HB2  | 2.14                     | 0.47              |
| 1:K:187:ALA:HB3  | 1:K:305:THR:HG21 | 1.96                     | 0.47              |
| 1:L:229:GLU:HG3  | 1:L:269:LEU:HD11 | 1.97                     | 0.47              |
| 1:Q:120:LEU:HD21 | 1:Q:140:LEU:HD22 | 1.95                     | 0.47              |
| 1:R:109:LEU:HD23 | 1:R:149:PHE:CD1  | 2.50                     | 0.47              |
| 1:V:61:ILE:HG22  | 1:V:309:LEU:HB2  | 1.97                     | 0.47              |
| 1:W:124:TYR:OH   | 1:W:167:GLU:HG3  | 2.14                     | 0.47              |
| 1:W:216:VAL:HG13 | 1:X:284:ASP:HB2  | 1.97                     | 0.47              |
| 1:a:147:ILE:HG12 | 1:a:164:LEU:HD12 | 1.97                     | 0.47              |
| 1:a:198:ALA:HB2  | 1:b:67:VAL:HG21  | 1.97                     | 0.47              |
| 1:b:224:ARG:HA   | 1:b:224:ARG:HD2  | 1.60                     | 0.47              |
| 1:c:77:GLN:OE1   | 1:c:195:LEU:HD13 | 2.14                     | 0.47              |
| 1:d:280:ASP:OD1  | 1:d:283:TYR:N    | 2.45                     | 0.47              |
| 1:e:98:MET:H     | 1:e:98:MET:HG2   | 1.28                     | 0.47              |
| 1:A:112:TRP:CD1  | 1:B:310:ARG:HG3  | 2.49                     | 0.47              |
| 1:F:56:TRP:HE3   | 1:F:315:PRO:HG2  | 1.79                     | 0.47              |
| 1:F:122:THR:CG2  | 1:F:125:TYR:H    | 2.25                     | 0.47              |
| 1:F:272:LEU:HA   | 1:F:275:VAL:HG12 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:292:THR:O    | 1:G:295:VAL:HG22 | 2.15                     | 0.47              |
| 1:L:96:SER:HG    | 1:L:98:MET:HG2   | 1.79                     | 0.47              |
| 1:O:124:TYR:OH   | 1:O:167:GLU:HG3  | 2.15                     | 0.47              |
| 1:P:199:TRP:CG   | 1:P:297:PRO:HD3  | 2.48                     | 0.47              |
| 1:Q:64:ARG:HE    | 1:Q:99:ASP:HA    | 1.80                     | 0.47              |
| 1:S:60:ALA:HB2   | 1:S:312:PRO:HG3  | 1.96                     | 0.47              |
| 1:S:118:PHE:CG   | 1:S:179:TYR:HD1  | 2.33                     | 0.47              |
| 1:T:295:VAL:HG11 | 1:b:300:ASP:OD2  | 2.15                     | 0.47              |
| 1:X:122:THR:CG2  | 1:X:124:TYR:HB3  | 2.44                     | 0.47              |
| 1:Y:285:GLN:HG2  | 1:f:216:VAL:HG21 | 1.97                     | 0.47              |
| 1:A:105:PHE:HB2  | 1:A:305:THR:CG2  | 2.39                     | 0.47              |
| 1:F:286:ASN:O    | 1:F:290:LEU:HB2  | 2.15                     | 0.47              |
| 1:H:122:THR:HG23 | 1:H:124:TYR:HB3  | 1.97                     | 0.47              |
| 1:L:66:THR:O     | 1:L:69:MET:HB2   | 2.14                     | 0.47              |
| 1:Q:57:SER:CB    | 1:Q:163:LYS:HE2  | 2.45                     | 0.47              |
| 1:Q:108:GLN:OE1  | 1:Q:186:ARG:NE   | 2.39                     | 0.47              |
| 1:R:137:ALA:C    | 1:S:316:VAL:HG11 | 2.40                     | 0.47              |
| 1:T:56:TRP:CE3   | 1:T:169:ALA:HB2  | 2.50                     | 0.47              |
| 1:V:61:ILE:O     | 1:V:309:LEU:N    | 2.33                     | 0.47              |
| 1:a:74:TYR:CE1   | 1:a:98:MET:HE1   | 2.50                     | 0.47              |
| 1:C:76:GLN:NE2   | 1:C:298:THR:H    | 2.13                     | 0.47              |
| 1:D:61:ILE:HG22  | 1:D:309:LEU:HB2  | 1.97                     | 0.47              |
| 1:D:69:MET:O     | 1:D:304:GLN:N    | 2.48                     | 0.47              |
| 1:M:60:ALA:HB2   | 1:M:312:PRO:HG3  | 1.97                     | 0.47              |
| 1:O:130:VAL:HG23 | 1:O:132:ASN:H    | 1.80                     | 0.47              |
| 1:R:119:TRP:NE1  | 1:R:143:MET:O    | 2.48                     | 0.47              |
| 1:X:122:THR:HG23 | 1:X:124:TYR:HB3  | 1.96                     | 0.47              |
| 1:b:141:ASP:O    | 1:b:145:ASN:ND2  | 2.48                     | 0.47              |
| 1:B:120:LEU:HD11 | 1:B:140:LEU:HD21 | 1.97                     | 0.46              |
| 1:G:124:TYR:HE1  | 1:G:143:MET:SD   | 2.38                     | 0.46              |
| 1:I:211:LYS:HA   | 1:I:211:LYS:HE3  | 1.97                     | 0.46              |
| 1:K:130:VAL:HG23 | 1:K:132:ASN:H    | 1.80                     | 0.46              |
| 1:R:60:ALA:HB2   | 1:R:312:PRO:HG3  | 1.97                     | 0.46              |
| 1:S:226:ASN:O    | 1:S:230:GLN:HG3  | 2.15                     | 0.46              |
| 1:T:100:GLU:OE1  | 1:T:103:LYS:HD3  | 2.14                     | 0.46              |
| 1:Z:168:THR:OG1  | 1:Z:171:ASP:OD2  | 2.31                     | 0.46              |
| 1:a:56:TRP:CE3   | 1:a:169:ALA:HB2  | 2.49                     | 0.46              |
| 1:f:206:MET:HG3  | 1:f:290:LEU:HG   | 1.98                     | 0.46              |
| 1:D:66:THR:OG1   | 1:D:69:MET:HG3   | 2.14                     | 0.46              |
| 1:G:81:ARG:NH1   | 1:G:95:PRO:O     | 2.42                     | 0.46              |
| 1:S:103:LYS:NZ   | 1:S:107:MET:HE1  | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:96:SER:HB3   | 1:a:99:ASP:OD2   | 2.16                     | 0.46              |
| 1:d:124:TYR:HE1  | 1:d:143:MET:SD   | 2.38                     | 0.46              |
| 1:f:58:SER:OG    | 1:f:173:ASN:HA   | 2.15                     | 0.46              |
| 1:f:164:LEU:HD13 | 1:f:175:LEU:C    | 2.40                     | 0.46              |
| 1:B:61:ILE:CG2   | 1:B:309:LEU:HB2  | 2.45                     | 0.46              |
| 1:J:206:MET:CE   | 1:J:289:MET:HG2  | 2.46                     | 0.46              |
| 1:M:114:THR:HG23 | 1:M:186:ARG:CD   | 2.43                     | 0.46              |
| 1:P:63:ASP:HB2   | 1:P:309:LEU:HD11 | 1.97                     | 0.46              |
| 1:S:120:LEU:HD21 | 1:S:140:LEU:HD22 | 1.97                     | 0.46              |
| 1:V:122:THR:CG2  | 1:V:124:TYR:HB3  | 2.46                     | 0.46              |
| 1:X:79:PHE:O     | 1:X:83:LEU:HG    | 2.16                     | 0.46              |
| 1:b:76:GLN:O     | 1:b:79:PHE:HB3   | 2.16                     | 0.46              |
| 1:B:164:LEU:HB2  | 1:B:176:LEU:HD13 | 1.98                     | 0.46              |
| 1:F:184:SER:HA   | 1:F:305:THR:CG2  | 2.46                     | 0.46              |
| 1:Q:124:TYR:OH   | 1:Q:167:GLU:HG3  | 2.16                     | 0.46              |
| 1:S:124:TYR:OH   | 1:S:167:GLU:HG3  | 2.16                     | 0.46              |
| 1:T:194:GLU:OE2  | 1:U:66:THR:HB    | 2.15                     | 0.46              |
| 1:U:132:ASN:HD21 | 1:U:134:LYS:HB3  | 1.80                     | 0.46              |
| 1:W:125:TYR:HA   | 1:W:143:MET:HE1  | 1.98                     | 0.46              |
| 1:X:121:GLN:O    | 1:X:121:GLN:HG2  | 2.15                     | 0.46              |
| 1:a:96:SER:OG    | 1:a:98:MET:HG2   | 2.14                     | 0.46              |
| 1:c:199:TRP:CE2  | 1:c:293:LEU:HD12 | 2.48                     | 0.46              |
| 1:d:210:VAL:HA   | 1:d:213:GLN:HE21 | 1.80                     | 0.46              |
| 1:f:77:GLN:OE1   | 1:f:77:GLN:HA    | 2.15                     | 0.46              |
| 1:B:64:ARG:NE    | 1:B:99:ASP:OD1   | 2.34                     | 0.46              |
| 1:B:122:THR:HG22 | 1:B:125:TYR:H    | 1.81                     | 0.46              |
| 1:E:61:ILE:HD13  | 1:E:61:ILE:HG21  | 1.67                     | 0.46              |
| 1:O:64:ARG:HA    | 1:O:102:TYR:CD1  | 2.50                     | 0.46              |
| 1:P:119:TRP:CE2  | 1:P:143:MET:HB2  | 2.50                     | 0.46              |
| 1:a:74:TYR:CE1   | 1:a:98:MET:CE    | 2.99                     | 0.46              |
| 1:c:126:LYS:O    | 1:c:129:MET:HG3  | 2.15                     | 0.46              |
| 1:d:132:ASN:HB3  | 1:d:135:ALA:HB3  | 1.96                     | 0.46              |
| 1:e:228:ILE:HD13 | 1:e:228:ILE:HG21 | 1.72                     | 0.46              |
| 1:B:74:TYR:HE1   | 1:B:98:MET:HE1   | 1.80                     | 0.46              |
| 1:K:188:ALA:HA   | 1:K:303:PHE:CZ   | 2.50                     | 0.46              |
| 1:L:210:VAL:HG13 | 1:L:283:TYR:CE1  | 2.51                     | 0.46              |
| 1:L:298:THR:OG1  | 1:L:298:THR:O    | 2.33                     | 0.46              |
| 1:M:216:VAL:HG22 | 1:N:285:GLN:HA   | 1.97                     | 0.46              |
| 1:P:149:PHE:HE1  | 1:P:160:ASP:HB3  | 1.81                     | 0.46              |
| 1:P:169:ALA:HB3  | 1:P:170:PRO:HD3  | 1.98                     | 0.46              |
| 1:W:198:ALA:HA   | 1:X:67:VAL:HG11  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:216:VAL:HG13 | 1:X:284:ASP:CB   | 2.46                     | 0.46              |
| 1:b:121:GLN:O    | 1:b:121:GLN:HG2  | 2.15                     | 0.46              |
| 1:c:214:GLU:HG3  | 1:c:283:TYR:CE1  | 2.50                     | 0.46              |
| 1:E:275:VAL:HG13 | 1:E:276:GLY:N    | 2.21                     | 0.46              |
| 1:G:199:TRP:CZ2  | 1:G:293:LEU:HA   | 2.51                     | 0.46              |
| 1:J:64:ARG:HG2   | 1:J:102:TYR:HB2  | 1.97                     | 0.46              |
| 1:L:191:LEU:O    | 1:L:194:GLU:HB2  | 2.16                     | 0.46              |
| 1:N:164:LEU:HB2  | 1:N:176:LEU:HD13 | 1.96                     | 0.46              |
| 1:P:289:MET:O    | 1:P:293:LEU:HB2  | 2.16                     | 0.46              |
| 1:U:280:ASP:OD2  | 1:U:283:TYR:N    | 2.47                     | 0.46              |
| 1:V:214:GLU:OE2  | 1:V:283:TYR:OH   | 2.17                     | 0.46              |
| 1:Y:97:VAL:O     | 1:Y:100:GLU:HB2  | 2.15                     | 0.46              |
| 1:a:112:TRP:CE2  | 1:a:144:ILE:HG21 | 2.51                     | 0.46              |
| 1:b:96:SER:HB3   | 1:b:99:ASP:OD2   | 2.16                     | 0.46              |
| 1:d:268:ARG:HD2  | 1:d:268:ARG:HA   | 1.54                     | 0.46              |
| 1:e:61:ILE:HB    | 1:e:310:ARG:HB3  | 1.98                     | 0.46              |
| 1:e:121:GLN:O    | 1:e:121:GLN:HG2  | 2.15                     | 0.46              |
| 1:C:122:THR:HG23 | 1:C:124:TYR:N    | 2.31                     | 0.46              |
| 1:F:122:THR:HG23 | 1:F:124:TYR:HB3  | 1.98                     | 0.46              |
| 1:I:202:ARG:NH2  | 1:I:205:GLN:OE1  | 2.48                     | 0.46              |
| 1:K:185:GLN:OE1  | 1:K:185:GLN:HA   | 2.16                     | 0.46              |
| 1:M:83:LEU:CD2   | 1:M:289:MET:HE2  | 2.45                     | 0.46              |
| 1:T:201:ALA:O    | 1:T:205:GLN:HB3  | 2.16                     | 0.46              |
| 1:W:266:GLN:O    | 1:W:266:GLN:HG2  | 2.16                     | 0.46              |
| 1:Z:57:SER:CB    | 1:Z:163:LYS:HE2  | 2.46                     | 0.46              |
| 1:e:101:ALA:HA   | 1:e:191:LEU:HD11 | 1.98                     | 0.46              |
| 1:A:122:THR:O    | 1:A:126:LYS:HG3  | 2.15                     | 0.46              |
| 1:I:57:SER:HB2   | 1:I:163:LYS:HE2  | 1.98                     | 0.46              |
| 1:L:101:ALA:HA   | 1:L:191:LEU:HD11 | 1.98                     | 0.46              |
| 1:M:216:VAL:CG2  | 1:N:285:GLN:HA   | 2.45                     | 0.46              |
| 1:Q:64:ARG:HA    | 1:Q:102:TYR:CG   | 2.51                     | 0.46              |
| 1:V:96:SER:OG    | 1:V:98:MET:HG2   | 2.15                     | 0.46              |
| 1:d:98:MET:H     | 1:d:98:MET:HG3   | 1.46                     | 0.46              |
| 1:e:184:SER:HB2  | 1:e:306:TYR:CE1  | 2.51                     | 0.46              |
| 1:A:130:VAL:HG23 | 1:A:132:ASN:H    | 1.81                     | 0.46              |
| 1:F:64:ARG:CZ    | 1:F:102:TYR:HD2  | 2.28                     | 0.46              |
| 1:G:96:SER:HB3   | 1:G:99:ASP:OD2   | 2.15                     | 0.46              |
| 1:G:304:GLN:OE1  | 1:G:306:TYR:CZ   | 2.68                     | 0.46              |
| 1:H:60:ALA:HA    | 1:H:310:ARG:O    | 2.15                     | 0.46              |
| 1:J:213:GLN:NE2  | 1:J:286:ASN:HD22 | 2.13                     | 0.46              |
| 1:P:63:ASP:OD1   | 1:P:64:ARG:HG2   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:209:GLN:HA   | 1:R:212:ARG:NH2  | 2.31                     | 0.46              |
| 1:T:124:TYR:CD1  | 1:T:143:MET:HE1  | 2.51                     | 0.46              |
| 1:U:57:SER:OG    | 1:U:319:ASP:OD1  | 2.32                     | 0.46              |
| 1:U:301:PRO:HD2  | 1:U:302:ARG:CD   | 2.46                     | 0.46              |
| 1:V:214:GLU:HA   | 1:V:279:PHE:HE2  | 1.81                     | 0.46              |
| 1:W:141:ASP:O    | 1:W:145:ASN:ND2  | 2.49                     | 0.46              |
| 1:Z:96:SER:HB3   | 1:Z:99:ASP:OD2   | 2.16                     | 0.46              |
| 1:Z:169:ALA:HB3  | 1:Z:170:PRO:HD3  | 1.98                     | 0.46              |
| 1:e:128:ARG:HB3  | 1:e:139:LEU:HD21 | 1.98                     | 0.46              |
| 1:L:300:ASP:O    | 1:L:303:PHE:HD2  | 1.99                     | 0.45              |
| 1:P:185:GLN:OE1  | 1:P:185:GLN:HA   | 2.16                     | 0.45              |
| 1:Q:214:GLU:HA   | 1:Q:279:PHE:HE2  | 1.81                     | 0.45              |
| 1:U:187:ALA:HB3  | 1:U:305:THR:HG21 | 1.97                     | 0.45              |
| 1:W:119:TRP:CH2  | 1:W:175:LEU:HD13 | 2.50                     | 0.45              |
| 1:Y:169:ALA:HB3  | 1:Y:170:PRO:HD3  | 1.98                     | 0.45              |
| 1:Y:286:ASN:O    | 1:Y:290:LEU:HB2  | 2.16                     | 0.45              |
| 1:d:81:ARG:NH1   | 1:d:95:PRO:O     | 2.47                     | 0.45              |
| 1:e:64:ARG:H     | 1:e:64:ARG:HG2   | 1.57                     | 0.45              |
| 1:B:66:THR:O     | 1:B:70:LEU:HG    | 2.16                     | 0.45              |
| 1:E:126:LYS:HA   | 1:E:129:MET:HE2  | 1.97                     | 0.45              |
| 1:G:109:LEU:HD23 | 1:G:149:PHE:CE1  | 2.51                     | 0.45              |
| 1:N:124:TYR:CG   | 1:N:175:LEU:HD11 | 2.50                     | 0.45              |
| 1:N:192:ASN:HB3  | 1:N:299:LEU:HD22 | 1.97                     | 0.45              |
| 1:O:58:SER:HB2   | 1:O:172:ALA:C    | 2.40                     | 0.45              |
| 1:W:177:ARG:NH2  | 1:W:312:PRO:O    | 2.49                     | 0.45              |
| 1:c:60:ALA:HB2   | 1:c:312:PRO:HG3  | 1.98                     | 0.45              |
| 1:d:212:ARG:HD3  | 1:e:292:THR:HG21 | 1.97                     | 0.45              |
| 1:A:199:TRP:CE2  | 1:A:293:LEU:HD12 | 2.51                     | 0.45              |
| 1:A:288:ALA:O    | 1:A:291:ASN:HB2  | 2.16                     | 0.45              |
| 1:B:214:GLU:OE2  | 1:B:283:TYR:OH   | 2.31                     | 0.45              |
| 1:D:67:VAL:HG22  | 1:D:98:MET:CE    | 2.46                     | 0.45              |
| 1:D:206:MET:HG3  | 1:D:290:LEU:HG   | 1.97                     | 0.45              |
| 1:J:117:GLU:OE1  | 1:J:186:ARG:NH1  | 2.38                     | 0.45              |
| 1:O:152:GLY:HA2  | 1:O:158:VAL:HG12 | 1.98                     | 0.45              |
| 1:O:301:PRO:HD2  | 1:O:302:ARG:HD2  | 1.96                     | 0.45              |
| 1:P:269:LEU:O    | 1:P:273:GLN:HB2  | 2.15                     | 0.45              |
| 1:R:109:LEU:HD21 | 1:R:162:VAL:HB   | 1.98                     | 0.45              |
| 1:T:156:ARG:HA   | 1:T:156:ARG:HD2  | 1.33                     | 0.45              |
| 1:X:120:LEU:HD23 | 1:X:125:TYR:CE2  | 2.51                     | 0.45              |
| 1:Y:148:GLN:HE21 | 1:Y:148:GLN:HB2  | 1.53                     | 0.45              |
| 1:d:122:THR:CG2  | 1:d:125:TYR:H    | 2.29                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:180:VAL:HG11 | 1:d:308:TYR:OH   | 2.16                     | 0.45              |
| 1:e:212:ARG:HH11 | 1:f:292:THR:HG21 | 1.82                     | 0.45              |
| 1:f:220:ILE:HG13 | 1:f:220:ILE:H    | 1.59                     | 0.45              |
| 1:A:304:GLN:NE2  | 1:A:306:TYR:O    | 2.50                     | 0.45              |
| 1:B:56:TRP:CD1   | 1:B:168:THR:HA   | 2.51                     | 0.45              |
| 1:B:64:ARG:HA    | 1:B:102:TYR:CD1  | 2.51                     | 0.45              |
| 1:D:199:TRP:CE2  | 1:D:297:PRO:HD3  | 2.52                     | 0.45              |
| 1:J:122:THR:O    | 1:J:126:LYS:HG3  | 2.15                     | 0.45              |
| 1:K:106:VAL:HG13 | 1:K:149:PHE:CZ   | 2.51                     | 0.45              |
| 1:K:125:TYR:HA   | 1:K:143:MET:HE1  | 1.98                     | 0.45              |
| 1:P:61:ILE:HG13  | 1:P:161:SER:HB3  | 1.97                     | 0.45              |
| 1:Q:79:PHE:O     | 1:Q:83:LEU:HG    | 2.15                     | 0.45              |
| 1:T:124:TYR:CE1  | 1:T:143:MET:HE1  | 2.51                     | 0.45              |
| 1:X:56:TRP:CE3   | 1:X:169:ALA:HB2  | 2.51                     | 0.45              |
| 1:c:125:TYR:HA   | 1:c:143:MET:HE1  | 1.98                     | 0.45              |
| 1:E:216:VAL:HG21 | 1:F:285:GLN:HG3  | 1.98                     | 0.45              |
| 1:J:106:VAL:HG13 | 1:J:149:PHE:CZ   | 2.52                     | 0.45              |
| 1:M:96:SER:HB3   | 1:M:99:ASP:OD2   | 2.17                     | 0.45              |
| 1:M:124:TYR:CD1  | 1:M:143:MET:HE1  | 2.52                     | 0.45              |
| 1:R:69:MET:HE2   | 1:R:304:GLN:NE2  | 2.32                     | 0.45              |
| 1:U:101:ALA:HA   | 1:U:191:LEU:HD11 | 1.99                     | 0.45              |
| 1:V:119:TRP:NE1  | 1:V:143:MET:O    | 2.50                     | 0.45              |
| 1:W:115:ARG:HG2  | 1:W:147:ILE:HD12 | 1.98                     | 0.45              |
| 1:W:124:TYR:CE2  | 1:W:171:ASP:HB3  | 2.51                     | 0.45              |
| 1:X:270:GLU:O    | 1:X:273:GLN:HB2  | 2.17                     | 0.45              |
| 1:Z:74:TYR:HE1   | 1:Z:98:MET:SD    | 2.38                     | 0.45              |
| 1:b:58:SER:HB2   | 1:b:176:LEU:CD2  | 2.46                     | 0.45              |
| 1:B:194:GLU:CD   | 1:C:66:THR:HB    | 2.42                     | 0.45              |
| 1:C:77:GLN:HG2   | 1:C:97:VAL:HG13  | 1.98                     | 0.45              |
| 1:D:122:THR:CG2  | 1:D:125:TYR:H    | 2.29                     | 0.45              |
| 1:F:120:LEU:HD23 | 1:F:125:TYR:CE2  | 2.51                     | 0.45              |
| 1:O:128:ARG:HE   | 1:O:167:GLU:CD   | 2.24                     | 0.45              |
| 1:T:202:ARG:HE   | 1:T:205:GLN:CG   | 2.25                     | 0.45              |
| 1:U:177:ARG:NH2  | 1:U:312:PRO:O    | 2.49                     | 0.45              |
| 1:Z:67:VAL:HG13  | 1:Z:74:TYR:CD2   | 2.52                     | 0.45              |
| 1:Z:105:PHE:HB2  | 1:Z:305:THR:CG2  | 2.39                     | 0.45              |
| 1:d:77:GLN:HG3   | 1:d:97:VAL:HG22  | 1.98                     | 0.45              |
| 1:f:122:THR:CG2  | 1:f:124:TYR:HB3  | 2.46                     | 0.45              |
| 1:D:228:ILE:HG22 | 1:D:269:LEU:HD13 | 1.98                     | 0.45              |
| 1:H:125:TYR:OH   | 1:H:140:LEU:HB2  | 2.15                     | 0.45              |
| 1:J:96:SER:CB    | 1:J:98:MET:HE2   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:109:LEU:HD23 | 1:J:149:PHE:CD1  | 2.52                     | 0.45              |
| 1:L:64:ARG:HA    | 1:L:102:TYR:HB2  | 1.98                     | 0.45              |
| 1:O:60:ALA:HB2   | 1:O:312:PRO:HG3  | 1.99                     | 0.45              |
| 1:T:196:LYS:HG3  | 1:T:299:LEU:CD2  | 2.27                     | 0.45              |
| 1:X:105:PHE:HB2  | 1:X:305:THR:CG2  | 2.46                     | 0.45              |
| 1:X:125:TYR:OH   | 1:X:136:ASP:HB3  | 2.16                     | 0.45              |
| 1:e:177:ARG:NH2  | 1:e:312:PRO:O    | 2.49                     | 0.45              |
| 1:e:216:VAL:HG13 | 1:f:284:ASP:HB3  | 1.99                     | 0.45              |
| 1:f:153:ASP:O    | 1:f:158:VAL:HG23 | 2.17                     | 0.45              |
| 1:f:169:ALA:HB3  | 1:f:170:PRO:HD3  | 1.99                     | 0.45              |
| 1:f:221:TYR:CE1  | 1:f:272:LEU:HG   | 2.51                     | 0.45              |
| 1:D:268:ARG:HA   | 1:D:271:ASN:HB3  | 1.99                     | 0.45              |
| 1:F:101:ALA:HA   | 1:F:191:LEU:HD21 | 1.99                     | 0.45              |
| 1:L:100:GLU:OE1  | 1:L:103:LYS:HD3  | 2.17                     | 0.45              |
| 1:S:77:GLN:HG2   | 1:S:97:VAL:HG12  | 1.99                     | 0.45              |
| 1:Z:122:THR:O    | 1:Z:126:LYS:HG3  | 2.16                     | 0.45              |
| 1:c:73:TYR:CZ    | 1:c:191:LEU:HB3  | 2.51                     | 0.45              |
| 1:d:120:LEU:HD23 | 1:d:120:LEU:HA   | 1.80                     | 0.45              |
| 1:f:214:GLU:OE2  | 1:f:283:TYR:OH   | 2.19                     | 0.45              |
| 1:B:300:ASP:O    | 1:B:303:PHE:HD2  | 1.99                     | 0.45              |
| 1:C:289:MET:HB2  | 1:C:289:MET:HE3  | 1.53                     | 0.45              |
| 1:E:216:VAL:HG22 | 1:F:285:GLN:HA   | 1.98                     | 0.45              |
| 1:F:123:ASP:O    | 1:F:127:GLN:HB2  | 2.17                     | 0.45              |
| 1:H:286:ASN:O    | 1:H:290:LEU:HB2  | 2.16                     | 0.45              |
| 1:N:308:TYR:CE1  | 1:N:312:PRO:HD3  | 2.51                     | 0.45              |
| 1:T:266:GLN:HE21 | 1:T:269:LEU:HD22 | 1.81                     | 0.45              |
| 1:V:64:ARG:HD3   | 1:V:99:ASP:OD1   | 2.17                     | 0.45              |
| 1:Z:66:THR:H     | 1:Z:69:MET:HB2   | 1.81                     | 0.45              |
| 1:a:182:PHE:CE2  | 1:a:186:ARG:HD2  | 2.52                     | 0.45              |
| 1:c:69:MET:O     | 1:c:303:PHE:HB2  | 2.16                     | 0.45              |
| 1:A:141:ASP:O    | 1:A:145:ASN:ND2  | 2.50                     | 0.45              |
| 1:G:199:TRP:CD2  | 1:G:297:PRO:HD3  | 2.51                     | 0.45              |
| 1:H:192:ASN:HD22 | 1:H:192:ASN:HA   | 1.64                     | 0.45              |
| 1:I:290:LEU:HD23 | 1:I:290:LEU:HA   | 1.81                     | 0.45              |
| 1:J:199:TRP:CD1  | 1:J:297:PRO:HD3  | 2.52                     | 0.45              |
| 1:P:122:THR:CG2  | 1:P:124:TYR:HB3  | 2.47                     | 0.45              |
| 1:U:126:LYS:O    | 1:U:129:MET:HB2  | 2.17                     | 0.45              |
| 1:c:132:ASN:HD22 | 1:c:135:ALA:H    | 1.65                     | 0.45              |
| 1:d:272:LEU:HA   | 1:d:275:VAL:HG12 | 1.98                     | 0.45              |
| 1:A:66:THR:HB    | 1:H:194:GLU:OE2  | 2.16                     | 0.44              |
| 1:A:116:ARG:HG3  | 1:A:140:LEU:HD21 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:215:GLU:OE1  | 1:B:218:LYS:HG2  | 2.17                     | 0.44              |
| 1:E:300:ASP:HA   | 1:E:302:ARG:NH1  | 2.32                     | 0.44              |
| 1:I:126:LYS:HA   | 1:I:129:MET:HE2  | 1.99                     | 0.44              |
| 1:Q:65:PRO:CD    | 1:Q:102:TYR:HB2  | 2.46                     | 0.44              |
| 1:Q:124:TYR:CD2  | 1:Q:175:LEU:HD11 | 2.52                     | 0.44              |
| 1:Q:169:ALA:HB3  | 1:Q:170:PRO:HD3  | 1.99                     | 0.44              |
| 1:S:103:LYS:HZ3  | 1:S:107:MET:HE1  | 1.82                     | 0.44              |
| 1:X:120:LEU:HG   | 1:X:140:LEU:HD11 | 1.99                     | 0.44              |
| 1:Y:301:PRO:HD2  | 1:Y:302:ARG:HD3  | 1.99                     | 0.44              |
| 1:a:152:GLY:HA2  | 1:a:158:VAL:HG12 | 1.99                     | 0.44              |
| 1:a:293:LEU:HD12 | 1:a:293:LEU:HA   | 1.87                     | 0.44              |
| 1:B:63:ASP:CG    | 1:B:64:ARG:H     | 2.26                     | 0.44              |
| 1:E:289:MET:HE2  | 1:E:289:MET:HB2  | 1.86                     | 0.44              |
| 1:F:119:TRP:NE1  | 1:F:143:MET:O    | 2.50                     | 0.44              |
| 1:H:156:ARG:HG3  | 1:H:158:VAL:HG23 | 1.99                     | 0.44              |
| 1:H:299:LEU:HD12 | 1:O:121:GLN:NE2  | 2.33                     | 0.44              |
| 1:K:117:GLU:OE1  | 1:K:186:ARG:NH1  | 2.40                     | 0.44              |
| 1:K:130:VAL:N    | 1:K:136:ASP:OD1  | 2.42                     | 0.44              |
| 1:N:218:LYS:O    | 1:N:218:LYS:HG3  | 2.17                     | 0.44              |
| 1:O:300:ASP:OD1  | 1:O:302:ARG:HD3  | 2.17                     | 0.44              |
| 1:S:66:THR:O     | 1:S:70:LEU:HG    | 2.16                     | 0.44              |
| 1:S:228:ILE:HD13 | 1:S:228:ILE:HG21 | 1.61                     | 0.44              |
| 1:T:291:ASN:HD22 | 1:b:298:THR:HA   | 1.82                     | 0.44              |
| 1:V:213:GLN:HE22 | 1:V:283:TYR:HA   | 1.81                     | 0.44              |
| 1:X:81:ARG:HH21  | 1:X:100:GLU:HG3  | 1.82                     | 0.44              |
| 1:X:128:ARG:HE   | 1:X:167:GLU:CD   | 2.24                     | 0.44              |
| 1:c:268:ARG:HD2  | 1:c:268:ARG:HA   | 1.84                     | 0.44              |
| 1:d:112:TRP:CD1  | 1:d:112:TRP:C    | 2.95                     | 0.44              |
| 1:f:57:SER:N     | 1:f:315:PRO:HG3  | 2.32                     | 0.44              |
| 1:K:128:ARG:HE   | 1:K:167:GLU:CD   | 2.25                     | 0.44              |
| 1:N:199:TRP:CD1  | 1:N:203:THR:HG1  | 2.35                     | 0.44              |
| 1:P:164:LEU:HB2  | 1:P:176:LEU:HD13 | 1.99                     | 0.44              |
| 1:P:206:MET:HG2  | 1:P:290:LEU:HG   | 2.00                     | 0.44              |
| 1:R:152:GLY:HA2  | 1:R:158:VAL:HG12 | 2.00                     | 0.44              |
| 1:R:169:ALA:HB3  | 1:R:170:PRO:HD3  | 1.99                     | 0.44              |
| 1:U:289:MET:O    | 1:U:293:LEU:HB2  | 2.17                     | 0.44              |
| 1:b:156:ARG:HD2  | 1:b:156:ARG:HA   | 1.78                     | 0.44              |
| 1:c:119:TRP:CE2  | 1:c:143:MET:HB3  | 2.52                     | 0.44              |
| 1:e:119:TRP:CE2  | 1:e:143:MET:HB3  | 2.51                     | 0.44              |
| 1:B:56:TRP:CE3   | 1:B:169:ALA:HB2  | 2.52                     | 0.44              |
| 1:B:116:ARG:HG3  | 1:B:144:ILE:HD11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:146:ASN:O    | 1:D:164:LEU:HA   | 2.18                     | 0.44              |
| 1:F:184:SER:HB2  | 1:F:306:TYR:CD1  | 2.52                     | 0.44              |
| 1:V:56:TRP:CE3   | 1:V:315:PRO:HG2  | 2.50                     | 0.44              |
| 1:W:305:THR:HG22 | 1:W:305:THR:O    | 2.16                     | 0.44              |
| 1:X:269:LEU:O    | 1:X:273:GLN:HG3  | 2.18                     | 0.44              |
| 1:Z:61:ILE:HB    | 1:Z:310:ARG:HB3  | 2.00                     | 0.44              |
| 1:b:290:LEU:HD23 | 1:b:290:LEU:HA   | 1.80                     | 0.44              |
| 1:f:164:LEU:HD13 | 1:f:176:LEU:N    | 2.32                     | 0.44              |
| 1:B:139:LEU:O    | 1:B:143:MET:HG3  | 2.18                     | 0.44              |
| 1:G:66:THR:O     | 1:G:69:MET:HB3   | 2.18                     | 0.44              |
| 1:K:105:PHE:HB2  | 1:K:305:THR:CG2  | 2.39                     | 0.44              |
| 1:M:118:PHE:CG   | 1:M:179:TYR:HD1  | 2.35                     | 0.44              |
| 1:Q:68:ASN:ND2   | 1:X:194:GLU:OE2  | 2.49                     | 0.44              |
| 1:a:169:ALA:C    | 1:a:314:GLU:HG2  | 2.42                     | 0.44              |
| 1:e:148:GLN:HE21 | 1:e:148:GLN:HB2  | 1.64                     | 0.44              |
| 1:H:105:PHE:CE2  | 1:H:109:LEU:HD22 | 2.52                     | 0.44              |
| 1:H:207:LYS:HG2  | 1:H:290:LEU:HD11 | 1.98                     | 0.44              |
| 1:K:139:LEU:HD11 | 1:K:143:MET:HE3  | 2.00                     | 0.44              |
| 1:P:105:PHE:HB2  | 1:P:305:THR:CG2  | 2.33                     | 0.44              |
| 1:P:202:ARG:NH2  | 1:P:205:GLN:NE2  | 2.65                     | 0.44              |
| 1:X:119:TRP:CD2  | 1:X:143:MET:HB3  | 2.52                     | 0.44              |
| 1:X:169:ALA:HB3  | 1:X:170:PRO:HD3  | 2.00                     | 0.44              |
| 1:a:268:ARG:O    | 1:a:272:LEU:HD23 | 2.18                     | 0.44              |
| 1:e:122:THR:HG23 | 1:e:124:TYR:HB3  | 2.00                     | 0.44              |
| 1:F:184:SER:HB2  | 1:F:306:TYR:HE1  | 1.82                     | 0.44              |
| 1:J:98:MET:SD    | 1:J:98:MET:N     | 2.89                     | 0.44              |
| 1:O:194:GLU:OE2  | 1:O:194:GLU:HA   | 2.18                     | 0.44              |
| 1:O:212:ARG:O    | 1:O:216:VAL:HG23 | 2.18                     | 0.44              |
| 1:O:221:TYR:HB2  | 1:O:277:PRO:HA   | 2.00                     | 0.44              |
| 1:Q:272:LEU:HA   | 1:Q:275:VAL:HG12 | 2.00                     | 0.44              |
| 1:S:169:ALA:C    | 1:S:314:GLU:HG2  | 2.43                     | 0.44              |
| 1:U:96:SER:OG    | 1:U:97:VAL:N     | 2.49                     | 0.44              |
| 1:a:206:MET:HG2  | 1:a:290:LEU:HA   | 2.00                     | 0.44              |
| 1:d:193:ASP:O    | 1:d:196:LYS:HB3  | 2.18                     | 0.44              |
| 1:d:289:MET:O    | 1:d:293:LEU:HB2  | 2.17                     | 0.44              |
| 1:A:64:ARG:HE    | 1:A:99:ASP:HA    | 1.83                     | 0.44              |
| 1:D:129:MET:HA   | 1:D:136:ASP:OD1  | 2.18                     | 0.44              |
| 1:G:105:PHE:HB2  | 1:G:305:THR:CG2  | 2.48                     | 0.44              |
| 1:H:76:GLN:O     | 1:H:79:PHE:HB3   | 2.18                     | 0.44              |
| 1:H:122:THR:HG22 | 1:H:125:TYR:H    | 1.82                     | 0.44              |
| 1:T:56:TRP:CD1   | 1:T:168:THR:HA   | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:83:LEU:HB3   | 1:U:202:ARG:NH1  | 2.29                     | 0.44              |
| 1:V:217:ALA:HB1  | 1:V:277:PRO:HB2  | 2.00                     | 0.44              |
| 1:Y:77:GLN:HB3   | 1:Y:97:VAL:HG11  | 1.99                     | 0.44              |
| 1:Y:202:ARG:NH2  | 1:Y:205:GLN:OE1  | 2.51                     | 0.44              |
| 1:Z:64:ARG:HG2   | 1:Z:102:TYR:CB   | 2.48                     | 0.44              |
| 1:c:221:TYR:CE1  | 1:c:272:LEU:HG   | 2.53                     | 0.44              |
| 1:c:275:VAL:HG13 | 1:c:276:GLY:O    | 2.18                     | 0.44              |
| 1:D:80:LEU:HD12  | 1:D:195:LEU:HD12 | 2.00                     | 0.44              |
| 1:D:212:ARG:HH11 | 1:E:292:THR:HG21 | 1.82                     | 0.44              |
| 1:K:115:ARG:HD3  | 1:K:147:ILE:CG2  | 2.47                     | 0.44              |
| 1:M:55:GLU:O     | 1:M:318:ARG:HG2  | 2.18                     | 0.44              |
| 1:P:229:GLU:HG3  | 1:P:269:LEU:HD11 | 2.00                     | 0.44              |
| 1:Q:56:TRP:CE3   | 1:Q:169:ALA:HB2  | 2.52                     | 0.44              |
| 1:U:152:GLY:HA2  | 1:U:158:VAL:HG12 | 1.99                     | 0.44              |
| 1:U:194:GLU:OE2  | 1:U:194:GLU:HA   | 2.18                     | 0.44              |
| 1:V:124:TYR:OH   | 1:V:167:GLU:N    | 2.42                     | 0.44              |
| 1:V:266:GLN:HE21 | 1:V:269:LEU:CD2  | 2.30                     | 0.44              |
| 1:Y:292:THR:HG21 | 1:f:212:ARG:HD3  | 1.99                     | 0.44              |
| 1:d:76:GLN:NE2   | 1:d:195:LEU:HD21 | 2.32                     | 0.44              |
| 1:A:107:MET:HE3  | 1:B:307:ARG:NH2  | 2.33                     | 0.43              |
| 1:B:120:LEU:HG   | 1:B:140:LEU:HD11 | 2.00                     | 0.43              |
| 1:F:72:GLY:O     | 1:F:76:GLN:HG3   | 2.17                     | 0.43              |
| 1:J:57:SER:CB    | 1:J:163:LYS:HE2  | 2.47                     | 0.43              |
| 1:K:98:MET:H     | 1:K:98:MET:HG2   | 1.11                     | 0.43              |
| 1:N:96:SER:HB3   | 1:N:99:ASP:OD2   | 2.18                     | 0.43              |
| 1:O:122:THR:HG23 | 1:O:124:TYR:HB3  | 2.00                     | 0.43              |
| 1:R:62:THR:HG1   | 1:R:102:TYR:HH   | 1.56                     | 0.43              |
| 1:V:122:THR:HG23 | 1:V:124:TYR:HB3  | 1.99                     | 0.43              |
| 1:b:58:SER:HB2   | 1:b:176:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:61:ILE:O     | 1:B:309:LEU:N    | 2.36                     | 0.43              |
| 1:D:81:ARG:O     | 1:D:85:VAL:HG12  | 2.18                     | 0.43              |
| 1:G:125:TYR:CD1  | 1:G:143:MET:CE   | 2.83                     | 0.43              |
| 1:H:210:VAL:HG22 | 1:H:286:ASN:CB   | 2.46                     | 0.43              |
| 1:K:228:ILE:HD12 | 1:K:272:LEU:CD2  | 2.48                     | 0.43              |
| 1:L:83:LEU:HB3   | 1:L:202:ARG:HD3  | 2.00                     | 0.43              |
| 1:M:304:GLN:HG2  | 1:M:306:TYR:CE1  | 2.53                     | 0.43              |
| 1:Q:300:ASP:OD1  | 1:Q:302:ARG:HB2  | 2.18                     | 0.43              |
| 1:S:67:VAL:HG13  | 1:S:74:TYR:CD2   | 2.53                     | 0.43              |
| 1:X:290:LEU:HD23 | 1:X:290:LEU:HA   | 1.79                     | 0.43              |
| 1:Y:55:GLU:O     | 1:Y:318:ARG:HG2  | 2.18                     | 0.43              |
| 1:Y:126:LYS:HA   | 1:Y:129:MET:HE2  | 1.98                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:194:GLU:OE2  | 1:a:68:ASN:OD1   | 2.36                     | 0.43              |
| 1:a:61:ILE:HG23  | 1:a:160:ASP:O    | 2.18                     | 0.43              |
| 1:f:122:THR:HG23 | 1:f:124:TYR:HB3  | 2.00                     | 0.43              |
| 1:G:103:LYS:O    | 1:G:107:MET:HB2  | 2.18                     | 0.43              |
| 1:S:198:ALA:CA   | 1:T:67:VAL:HG11  | 2.49                     | 0.43              |
| 1:S:280:ASP:O    | 1:S:283:TYR:HB3  | 2.18                     | 0.43              |
| 1:U:210:VAL:HG13 | 1:U:283:TYR:CE1  | 2.53                     | 0.43              |
| 1:Z:218:LYS:HE3  | 1:Z:218:LYS:HB2  | 1.72                     | 0.43              |
| 1:b:80:LEU:HD23  | 1:b:83:LEU:HD12  | 2.00                     | 0.43              |
| 1:b:221:TYR:CE1  | 1:b:272:LEU:HG   | 2.52                     | 0.43              |
| 1:A:290:LEU:HD23 | 1:A:290:LEU:HA   | 1.81                     | 0.43              |
| 1:B:216:VAL:O    | 1:B:220:ILE:HG13 | 2.19                     | 0.43              |
| 1:F:266:GLN:O    | 1:F:269:LEU:HB3  | 2.18                     | 0.43              |
| 1:I:300:ASP:OD1  | 1:I:302:ARG:HB2  | 2.19                     | 0.43              |
| 1:L:64:ARG:H     | 1:L:64:ARG:HG2   | 1.58                     | 0.43              |
| 1:T:64:ARG:NE    | 1:T:99:ASP:OD1   | 2.50                     | 0.43              |
| 1:T:291:ASN:ND2  | 1:b:298:THR:HA   | 2.33                     | 0.43              |
| 1:W:152:GLY:HA2  | 1:W:158:VAL:HG12 | 2.00                     | 0.43              |
| 1:X:177:ARG:NH2  | 1:X:312:PRO:O    | 2.52                     | 0.43              |
| 1:Y:293:LEU:HD12 | 1:Y:293:LEU:HA   | 1.84                     | 0.43              |
| 1:Z:214:GLU:HG3  | 1:Z:283:TYR:CE1  | 2.53                     | 0.43              |
| 1:d:64:ARG:HD3   | 1:d:99:ASP:OD1   | 2.19                     | 0.43              |
| 1:D:150:ILE:HA   | 1:D:151:PRO:HD2  | 1.91                     | 0.43              |
| 1:G:266:GLN:O    | 1:G:269:LEU:N    | 2.45                     | 0.43              |
| 1:Q:114:THR:HG22 | 1:Q:179:TYR:CE1  | 2.53                     | 0.43              |
| 1:R:227:SER:HB2  | 1:S:275:VAL:CG2  | 2.48                     | 0.43              |
| 1:S:169:ALA:HB3  | 1:S:170:PRO:HD3  | 2.00                     | 0.43              |
| 1:W:169:ALA:HB3  | 1:W:170:PRO:HD3  | 1.99                     | 0.43              |
| 1:a:223:ARG:O    | 1:a:227:SER:HB3  | 2.18                     | 0.43              |
| 1:f:105:PHE:HA   | 1:f:187:ALA:HB2  | 2.00                     | 0.43              |
| 1:B:67:VAL:HG13  | 1:B:74:TYR:CG    | 2.53                     | 0.43              |
| 1:B:84:ASP:CG    | 1:B:85:VAL:N     | 2.76                     | 0.43              |
| 1:B:203:THR:OG1  | 1:B:293:LEU:HD11 | 2.19                     | 0.43              |
| 1:G:141:ASP:HB2  | 1:H:316:VAL:HG11 | 1.99                     | 0.43              |
| 1:J:132:ASN:HB3  | 1:J:135:ALA:HB3  | 2.00                     | 0.43              |
| 1:L:293:LEU:HD12 | 1:L:293:LEU:HA   | 1.80                     | 0.43              |
| 1:R:118:PHE:CG   | 1:R:179:TYR:HD1  | 2.36                     | 0.43              |
| 1:U:212:ARG:O    | 1:U:216:VAL:HG23 | 2.18                     | 0.43              |
| 1:W:130:VAL:HG23 | 1:W:132:ASN:H    | 1.83                     | 0.43              |
| 1:X:174:ASN:HB3  | 1:X:178:GLN:NE2  | 2.33                     | 0.43              |
| 1:b:98:MET:HG2   | 1:b:98:MET:H     | 1.14                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:58:SER:HB3   | 1:B:312:PRO:HB3  | 2.00                     | 0.43              |
| 1:D:122:THR:HG23 | 1:D:124:TYR:N    | 2.34                     | 0.43              |
| 1:G:204:ILE:HB   | 1:O:302:ARG:HH21 | 1.84                     | 0.43              |
| 1:J:207:LYS:HA   | 1:J:290:LEU:HD11 | 2.00                     | 0.43              |
| 1:N:128:ARG:HB3  | 1:N:139:LEU:HD21 | 2.01                     | 0.43              |
| 1:O:169:ALA:HA   | 1:O:315:PRO:HG2  | 2.00                     | 0.43              |
| 1:P:116:ARG:HA   | 1:P:144:ILE:HG12 | 2.00                     | 0.43              |
| 1:W:61:ILE:HG21  | 1:W:61:ILE:HD13  | 1.59                     | 0.43              |
| 1:c:80:LEU:HD11  | 1:c:199:TRP:HB2  | 2.01                     | 0.43              |
| 1:c:122:THR:HG22 | 1:c:125:TYR:H    | 1.84                     | 0.43              |
| 1:c:169:ALA:HB1  | 1:c:314:GLU:HG2  | 2.00                     | 0.43              |
| 1:d:228:ILE:HD12 | 1:d:272:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:162:VAL:HG13 | 1:B:176:LEU:HD11 | 2.01                     | 0.43              |
| 1:H:269:LEU:O    | 1:H:273:GLN:HG3  | 2.18                     | 0.43              |
| 1:I:170:PRO:O    | 1:I:174:ASN:ND2  | 2.52                     | 0.43              |
| 1:L:61:ILE:HB    | 1:L:310:ARG:HB3  | 2.01                     | 0.43              |
| 1:L:141:ASP:OD2  | 1:L:145:ASN:ND2  | 2.49                     | 0.43              |
| 1:M:61:ILE:HB    | 1:M:310:ARG:HB3  | 2.00                     | 0.43              |
| 1:M:280:ASP:OD2  | 1:M:283:TYR:N    | 2.48                     | 0.43              |
| 1:T:292:THR:CG2  | 1:b:302:ARG:HH12 | 2.28                     | 0.43              |
| 1:W:81:ARG:NE    | 1:W:97:VAL:HG22  | 2.33                     | 0.43              |
| 1:W:119:TRP:CD2  | 1:W:143:MET:HB3  | 2.53                     | 0.43              |
| 1:X:115:ARG:HD3  | 1:X:147:ILE:HB   | 2.01                     | 0.43              |
| 1:f:199:TRP:CD1  | 1:f:297:PRO:HD3  | 2.53                     | 0.43              |
| 1:f:199:TRP:CZ2  | 1:f:293:LEU:HA   | 2.54                     | 0.43              |
| 1:F:61:ILE:N     | 1:F:310:ARG:HB3  | 2.34                     | 0.43              |
| 1:F:122:THR:HG23 | 1:F:124:TYR:H    | 1.84                     | 0.43              |
| 1:G:196:LYS:CE   | 1:O:298:THR:HG22 | 2.46                     | 0.43              |
| 1:K:58:SER:HB2   | 1:K:172:ALA:C    | 2.44                     | 0.43              |
| 1:M:225:MET:HE3  | 1:M:225:MET:HB2  | 1.82                     | 0.43              |
| 1:N:102:TYR:O    | 1:N:106:VAL:HG23 | 2.18                     | 0.43              |
| 1:S:104:GLU:HA   | 1:S:107:MET:HE3  | 2.00                     | 0.43              |
| 1:S:228:ILE:HD13 | 1:S:268:ARG:HG3  | 2.01                     | 0.43              |
| 1:Y:211:LYS:HA   | 1:Y:211:LYS:HE3  | 2.01                     | 0.43              |
| 1:Z:216:VAL:HG22 | 1:a:285:GLN:HA   | 2.01                     | 0.43              |
| 1:e:300:ASP:OD1  | 1:e:302:ARG:NH1  | 2.51                     | 0.43              |
| 1:B:153:ASP:H    | 1:B:158:VAL:HB   | 1.84                     | 0.43              |
| 1:E:57:SER:HA    | 1:E:164:LEU:O    | 2.18                     | 0.43              |
| 1:G:204:ILE:HB   | 1:O:302:ARG:NH2  | 2.34                     | 0.43              |
| 1:L:141:ASP:HA   | 1:L:144:ILE:HD12 | 2.00                     | 0.43              |
| 1:M:98:MET:HG2   | 1:M:98:MET:H     | 1.50                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:122:THR:O    | 1:P:126:LYS:HG3  | 2.19                     | 0.43              |
| 1:S:98:MET:SD    | 1:S:98:MET:N     | 2.79                     | 0.43              |
| 1:T:207:LYS:NZ   | 1:T:294:ASN:HD21 | 2.17                     | 0.43              |
| 1:U:73:TYR:CZ    | 1:U:191:LEU:HB3  | 2.54                     | 0.43              |
| 1:V:56:TRP:CD1   | 1:V:168:THR:HA   | 2.53                     | 0.43              |
| 1:W:122:THR:CG2  | 1:W:124:TYR:HB3  | 2.48                     | 0.43              |
| 1:Z:122:THR:CG2  | 1:Z:124:TYR:HB3  | 2.48                     | 0.43              |
| 1:A:64:ARG:HA    | 1:A:102:TYR:CG   | 2.54                     | 0.42              |
| 1:C:124:TYR:O    | 1:C:128:ARG:HD2  | 2.19                     | 0.42              |
| 1:D:64:ARG:O     | 1:D:307:ARG:HG2  | 2.19                     | 0.42              |
| 1:V:213:GLN:NE2  | 1:V:283:TYR:HA   | 2.34                     | 0.42              |
| 1:W:103:LYS:O    | 1:W:107:MET:HB2  | 2.18                     | 0.42              |
| 1:Z:73:TYR:CE1   | 1:Z:191:LEU:HB3  | 2.54                     | 0.42              |
| 1:a:214:GLU:OE2  | 1:a:283:TYR:OH   | 2.28                     | 0.42              |
| 1:c:211:LYS:HA   | 1:c:211:LYS:HE3  | 2.01                     | 0.42              |
| 1:d:275:VAL:HG13 | 1:d:276:GLY:O    | 2.19                     | 0.42              |
| 1:e:268:ARG:NH1  | 1:e:268:ARG:CG   | 2.78                     | 0.42              |
| 1:D:64:ARG:HA    | 1:D:102:TYR:HB2  | 2.01                     | 0.42              |
| 1:G:103:LYS:HZ2  | 1:G:107:MET:HE1  | 1.83                     | 0.42              |
| 1:G:153:ASP:H    | 1:G:158:VAL:HB   | 1.84                     | 0.42              |
| 1:H:58:SER:O     | 1:H:163:LYS:HG3  | 2.18                     | 0.42              |
| 1:H:153:ASP:H    | 1:H:158:VAL:HB   | 1.84                     | 0.42              |
| 1:K:294:ASN:HD22 | 1:K:294:ASN:HA   | 1.63                     | 0.42              |
| 1:O:229:GLU:HG3  | 1:O:269:LEU:CD1  | 2.48                     | 0.42              |
| 1:Q:280:ASP:O    | 1:Q:283:TYR:HB3  | 2.19                     | 0.42              |
| 1:R:105:PHE:CE2  | 1:R:109:LEU:HD22 | 2.53                     | 0.42              |
| 1:R:293:LEU:HD12 | 1:R:293:LEU:HA   | 1.81                     | 0.42              |
| 1:T:295:VAL:HG22 | 1:b:300:ASP:HB2  | 2.01                     | 0.42              |
| 1:V:105:PHE:HB2  | 1:V:305:THR:HG23 | 2.00                     | 0.42              |
| 1:Y:76:GLN:NE2   | 1:Y:297:PRO:HA   | 2.34                     | 0.42              |
| 1:Y:125:TYR:HD1  | 1:Y:143:MET:CE   | 2.32                     | 0.42              |
| 1:Z:300:ASP:OD1  | 1:Z:302:ARG:HB2  | 2.18                     | 0.42              |
| 1:f:58:SER:CB    | 1:f:173:ASN:HA   | 2.49                     | 0.42              |
| 1:f:120:LEU:HD21 | 1:f:140:LEU:HD22 | 2.01                     | 0.42              |
| 1:B:203:THR:HA   | 1:B:293:LEU:HG   | 2.01                     | 0.42              |
| 1:F:280:ASP:OD1  | 1:F:283:TYR:N    | 2.35                     | 0.42              |
| 1:H:56:TRP:O     | 1:H:165:ILE:HA   | 2.20                     | 0.42              |
| 1:M:125:TYR:HB2  | 1:M:143:MET:SD   | 2.59                     | 0.42              |
| 1:N:107:MET:HB3  | 1:N:107:MET:HE2  | 1.74                     | 0.42              |
| 1:N:210:VAL:HG13 | 1:N:283:TYR:CE1  | 2.53                     | 0.42              |
| 1:P:104:GLU:O    | 1:P:108:GLN:HG2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:107:MET:HE1  | 1:U:63:ASP:OD2   | 2.19                     | 0.42              |
| 1:V:187:ALA:HB3  | 1:V:305:THR:HG21 | 2.01                     | 0.42              |
| 1:a:112:TRP:CZ2  | 1:a:144:ILE:HG21 | 2.55                     | 0.42              |
| 1:A:301:PRO:HD2  | 1:A:302:ARG:HH11 | 1.84                     | 0.42              |
| 1:B:268:ARG:HD2  | 1:B:268:ARG:HA   | 1.76                     | 0.42              |
| 1:F:61:ILE:HG23  | 1:F:160:ASP:O    | 2.19                     | 0.42              |
| 1:F:150:ILE:HA   | 1:F:151:PRO:HD2  | 1.87                     | 0.42              |
| 1:H:96:SER:O     | 1:H:99:ASP:HB2   | 2.19                     | 0.42              |
| 1:I:118:PHE:CG   | 1:I:179:TYR:HD1  | 2.37                     | 0.42              |
| 1:M:268:ARG:HA   | 1:M:268:ARG:HD3  | 1.91                     | 0.42              |
| 1:S:57:SER:CB    | 1:S:163:LYS:HE2  | 2.49                     | 0.42              |
| 1:T:63:ASP:OD1   | 1:T:64:ARG:N     | 2.44                     | 0.42              |
| 1:T:148:GLN:HE21 | 1:T:148:GLN:HB2  | 1.61                     | 0.42              |
| 1:Z:79:PHE:CE2   | 1:Z:83:LEU:HD11  | 2.54                     | 0.42              |
| 1:a:60:ALA:HB2   | 1:a:312:PRO:HG3  | 2.00                     | 0.42              |
| 1:D:290:LEU:HD23 | 1:D:290:LEU:HA   | 1.92                     | 0.42              |
| 1:G:128:ARG:CB   | 1:G:139:LEU:HD21 | 2.50                     | 0.42              |
| 1:G:203:THR:HA   | 1:G:293:LEU:HD23 | 2.01                     | 0.42              |
| 1:G:267:ALA:O    | 1:G:271:ASN:HB2  | 2.19                     | 0.42              |
| 1:H:63:ASP:CG    | 1:H:64:ARG:N     | 2.77                     | 0.42              |
| 1:L:266:GLN:HE21 | 1:L:269:LEU:HD22 | 1.83                     | 0.42              |
| 1:N:169:ALA:HB3  | 1:N:170:PRO:HD3  | 2.01                     | 0.42              |
| 1:N:210:VAL:HG13 | 1:N:283:TYR:HE1  | 1.83                     | 0.42              |
| 1:R:62:THR:OG1   | 1:R:102:TYR:OH   | 2.27                     | 0.42              |
| 1:U:214:GLU:OE2  | 1:U:283:TYR:OH   | 2.14                     | 0.42              |
| 1:Y:177:ARG:HG3  | 1:Y:312:PRO:HB2  | 2.01                     | 0.42              |
| 1:b:56:TRP:CE3   | 1:b:169:ALA:HB2  | 2.54                     | 0.42              |
| 1:b:104:GLU:CD   | 1:c:307:ARG:HH22 | 2.27                     | 0.42              |
| 1:e:294:ASN:HD22 | 1:e:294:ASN:HA   | 1.69                     | 0.42              |
| 1:f:57:SER:O     | 1:f:315:PRO:HB3  | 2.19                     | 0.42              |
| 1:D:73:TYR:OH    | 1:D:191:LEU:HD22 | 2.20                     | 0.42              |
| 1:E:152:GLY:N    | 1:E:160:ASP:OD2  | 2.36                     | 0.42              |
| 1:F:185:GLN:HE22 | 1:F:301:PRO:HB2  | 1.83                     | 0.42              |
| 1:I:194:GLU:OE2  | 1:I:194:GLU:HA   | 2.20                     | 0.42              |
| 1:J:229:GLU:HG3  | 1:J:269:LEU:HD11 | 2.01                     | 0.42              |
| 1:L:69:MET:O     | 1:L:304:GLN:N    | 2.52                     | 0.42              |
| 1:M:202:ARG:NH2  | 1:M:205:GLN:OE1  | 2.46                     | 0.42              |
| 1:R:177:ARG:HG3  | 1:R:312:PRO:HB2  | 2.02                     | 0.42              |
| 1:b:64:ARG:H     | 1:b:64:ARG:HG2   | 1.56                     | 0.42              |
| 1:A:119:TRP:CH2  | 1:A:143:MET:HG2  | 2.55                     | 0.42              |
| 1:I:216:VAL:HG13 | 1:J:284:ASP:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:280:ASP:OD1  | 1:N:283:TYR:N    | 2.50                     | 0.42              |
| 1:O:141:ASP:O    | 1:O:145:ASN:ND2  | 2.53                     | 0.42              |
| 1:P:64:ARG:HG2   | 1:P:64:ARG:H     | 1.51                     | 0.42              |
| 1:P:268:ARG:HA   | 1:P:268:ARG:HD2  | 1.60                     | 0.42              |
| 1:Q:60:ALA:HB2   | 1:Q:312:PRO:HG3  | 2.02                     | 0.42              |
| 1:R:169:ALA:C    | 1:R:314:GLU:HG2  | 2.45                     | 0.42              |
| 1:W:60:ALA:HB2   | 1:W:312:PRO:HG3  | 2.01                     | 0.42              |
| 1:W:115:ARG:HB3  | 1:W:144:ILE:HA   | 2.01                     | 0.42              |
| 1:b:180:VAL:HG11 | 1:b:308:TYR:OH   | 2.18                     | 0.42              |
| 1:c:272:LEU:HA   | 1:c:275:VAL:HG12 | 2.01                     | 0.42              |
| 1:E:228:ILE:HG22 | 1:E:269:LEU:HD13 | 2.01                     | 0.42              |
| 1:L:300:ASP:O    | 1:L:303:PHE:CD2  | 2.73                     | 0.42              |
| 1:N:156:ARG:O    | 1:N:157:ALA:HB3  | 2.18                     | 0.42              |
| 1:P:202:ARG:CZ   | 1:P:205:GLN:HE21 | 2.33                     | 0.42              |
| 1:U:57:SER:CB    | 1:U:163:LYS:HE2  | 2.49                     | 0.42              |
| 1:U:291:ASN:O    | 1:U:294:ASN:HB2  | 2.20                     | 0.42              |
| 1:W:105:PHE:HB2  | 1:W:305:THR:CG2  | 2.43                     | 0.42              |
| 1:Y:56:TRP:CD1   | 1:Y:168:THR:HA   | 2.54                     | 0.42              |
| 1:d:130:VAL:HG23 | 1:d:132:ASN:H    | 1.84                     | 0.42              |
| 1:A:58:SER:O     | 1:A:163:LYS:HA   | 2.19                     | 0.42              |
| 1:D:275:VAL:HG13 | 1:D:276:GLY:N    | 2.34                     | 0.42              |
| 1:G:210:VAL:HA   | 1:G:213:GLN:NE2  | 2.31                     | 0.42              |
| 1:G:217:ALA:HB1  | 1:G:277:PRO:HB3  | 2.02                     | 0.42              |
| 1:H:266:GLN:HG2  | 1:H:266:GLN:O    | 2.19                     | 0.42              |
| 1:O:63:ASP:HB2   | 1:O:309:LEU:HD11 | 2.01                     | 0.42              |
| 1:S:225:MET:CE   | 1:S:273:GLN:HG3  | 2.43                     | 0.42              |
| 1:Y:65:PRO:HD2   | 1:Y:102:TYR:HB2  | 2.02                     | 0.42              |
| 1:c:102:TYR:HA   | 1:c:105:PHE:HB3  | 2.01                     | 0.42              |
| 1:c:216:VAL:HG13 | 1:d:284:ASP:CB   | 2.48                     | 0.42              |
| 1:d:96:SER:HB3   | 1:d:99:ASP:OD2   | 2.20                     | 0.42              |
| 1:C:73:TYR:CE1   | 1:C:191:LEU:HB3  | 2.55                     | 0.42              |
| 1:C:132:ASN:HB3  | 1:C:135:ALA:HB3  | 2.02                     | 0.42              |
| 1:D:224:ARG:HA   | 1:D:227:SER:OG   | 2.20                     | 0.42              |
| 1:I:152:GLY:HA2  | 1:I:158:VAL:HG12 | 2.02                     | 0.42              |
| 1:M:216:VAL:HG21 | 1:N:285:GLN:HG2  | 2.02                     | 0.42              |
| 1:N:126:LYS:O    | 1:N:129:MET:CG   | 2.67                     | 0.42              |
| 1:N:268:ARG:HD2  | 1:N:268:ARG:HA   | 1.59                     | 0.42              |
| 1:Q:109:LEU:HD23 | 1:Q:149:PHE:CE1  | 2.54                     | 0.42              |
| 1:S:66:THR:OG1   | 1:S:69:MET:SD    | 2.73                     | 0.42              |
| 1:S:153:ASP:OD2  | 1:S:156:ARG:HD2  | 2.19                     | 0.42              |
| 1:T:70:LEU:HB2   | 1:T:74:TYR:HB2   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:57:SER:HA    | 1:U:164:LEU:O    | 2.20                     | 0.42              |
| 1:U:148:GLN:HE21 | 1:U:148:GLN:HB2  | 1.61                     | 0.42              |
| 1:Y:66:THR:HB    | 1:f:194:GLU:CD   | 2.44                     | 0.42              |
| 1:b:96:SER:HG    | 1:b:98:MET:HG2   | 1.84                     | 0.42              |
| 1:b:107:MET:HE3  | 1:b:107:MET:HB3  | 1.63                     | 0.42              |
| 1:d:148:GLN:HE21 | 1:d:148:GLN:HB2  | 1.53                     | 0.42              |
| 1:d:168:THR:OG1  | 1:d:171:ASP:OD2  | 2.21                     | 0.42              |
| 1:F:67:VAL:HG12  | 1:F:98:MET:CE    | 2.50                     | 0.41              |
| 1:G:122:THR:CG2  | 1:G:124:TYR:HB3  | 2.50                     | 0.41              |
| 1:H:56:TRP:CD1   | 1:H:168:THR:HA   | 2.55                     | 0.41              |
| 1:H:74:TYR:CZ    | 1:H:78:GLN:HG3   | 2.55                     | 0.41              |
| 1:L:209:GLN:HA   | 1:L:212:ARG:NH2  | 2.35                     | 0.41              |
| 1:L:294:ASN:HD22 | 1:L:294:ASN:HA   | 1.66                     | 0.41              |
| 1:N:226:ASN:OD1  | 1:N:230:GLN:NE2  | 2.48                     | 0.41              |
| 1:P:184:SER:HB2  | 1:P:306:TYR:CD1  | 2.55                     | 0.41              |
| 1:P:207:LYS:O    | 1:P:211:LYS:HB2  | 2.20                     | 0.41              |
| 1:Q:293:LEU:HD12 | 1:Q:293:LEU:HA   | 1.91                     | 0.41              |
| 1:S:188:ALA:HA   | 1:S:303:PHE:CZ   | 2.55                     | 0.41              |
| 1:S:198:ALA:HA   | 1:T:67:VAL:HG11  | 2.01                     | 0.41              |
| 1:X:112:TRP:CD2  | 1:X:144:ILE:HG21 | 2.55                     | 0.41              |
| 1:a:74:TYR:HA    | 1:a:97:VAL:HG11  | 2.02                     | 0.41              |
| 1:b:67:VAL:HG13  | 1:b:74:TYR:CG    | 2.54                     | 0.41              |
| 1:d:280:ASP:O    | 1:d:283:TYR:HB3  | 2.19                     | 0.41              |
| 1:e:77:GLN:OE1   | 1:e:77:GLN:HA    | 2.20                     | 0.41              |
| 1:D:55:GLU:O     | 1:D:319:ASP:N    | 2.39                     | 0.41              |
| 1:D:68:ASN:ND2   | 1:D:68:ASN:H     | 2.18                     | 0.41              |
| 1:D:223:ARG:NH1  | 1:E:284:ASP:OD2  | 2.53                     | 0.41              |
| 1:J:130:VAL:HG23 | 1:J:132:ASN:H    | 1.86                     | 0.41              |
| 1:K:182:PHE:CE2  | 1:K:186:ARG:HD2  | 2.55                     | 0.41              |
| 1:L:156:ARG:HE   | 1:L:156:ARG:HA   | 1.85                     | 0.41              |
| 1:M:211:LYS:HE3  | 1:M:211:LYS:HA   | 2.01                     | 0.41              |
| 1:N:98:MET:H     | 1:N:98:MET:HG2   | 1.00                     | 0.41              |
| 1:Q:101:ALA:HA   | 1:Q:191:LEU:HD11 | 2.02                     | 0.41              |
| 1:S:63:ASP:OD1   | 1:S:64:ARG:N     | 2.48                     | 0.41              |
| 1:S:268:ARG:HD2  | 1:S:268:ARG:HA   | 1.76                     | 0.41              |
| 1:V:121:GLN:HG2  | 1:V:121:GLN:O    | 2.19                     | 0.41              |
| 1:X:119:TRP:NE1  | 1:X:143:MET:O    | 2.53                     | 0.41              |
| 1:Y:63:ASP:OD2   | 1:Y:64:ARG:N     | 2.44                     | 0.41              |
| 1:Y:69:MET:CE    | 1:Y:304:GLN:HB3  | 2.50                     | 0.41              |
| 1:b:224:ARG:HB3  | 1:b:272:LEU:CD2  | 2.46                     | 0.41              |
| 1:A:77:GLN:HA    | 1:A:77:GLN:OE1   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:60:ALA:HB2   | 1:D:312:PRO:HG3  | 2.02                     | 0.41              |
| 1:D:293:LEU:HD12 | 1:D:293:LEU:HA   | 1.78                     | 0.41              |
| 1:I:293:LEU:HD12 | 1:I:293:LEU:HA   | 1.88                     | 0.41              |
| 1:L:63:ASP:OD1   | 1:L:64:ARG:HG2   | 2.20                     | 0.41              |
| 1:L:97:VAL:HB    | 1:L:98:MET:HE2   | 2.02                     | 0.41              |
| 1:N:58:SER:HB2   | 1:N:172:ALA:C    | 2.45                     | 0.41              |
| 1:N:173:ASN:HB2  | 1:N:314:GLU:HA   | 2.01                     | 0.41              |
| 1:Q:194:GLU:HA   | 1:Q:194:GLU:OE2  | 2.21                     | 0.41              |
| 1:U:281:LEU:O    | 1:U:285:GLN:HG3  | 2.20                     | 0.41              |
| 1:W:57:SER:OG    | 1:W:163:LYS:HE2  | 2.20                     | 0.41              |
| 1:X:101:ALA:HA   | 1:X:191:LEU:HD11 | 2.01                     | 0.41              |
| 1:f:162:VAL:HG13 | 1:f:176:LEU:HD11 | 2.01                     | 0.41              |
| 1:f:184:SER:HB2  | 1:f:306:TYR:CE1  | 2.55                     | 0.41              |
| 1:f:206:MET:HE1  | 1:f:289:MET:HG2  | 2.01                     | 0.41              |
| 1:f:223:ARG:O    | 1:f:227:SER:HB3  | 2.20                     | 0.41              |
| 1:B:61:ILE:HD13  | 1:B:61:ILE:HG21  | 1.65                     | 0.41              |
| 1:E:304:GLN:HG2  | 1:E:306:TYR:O    | 2.20                     | 0.41              |
| 1:M:56:TRP:CD1   | 1:M:168:THR:HA   | 2.56                     | 0.41              |
| 1:M:156:ARG:O    | 1:M:157:ALA:HB3  | 2.20                     | 0.41              |
| 1:N:203:THR:O    | 1:N:207:LYS:HB2  | 2.20                     | 0.41              |
| 1:O:194:GLU:OE2  | 1:P:66:THR:HB    | 2.20                     | 0.41              |
| 1:P:143:MET:HE2  | 1:P:143:MET:HB3  | 1.77                     | 0.41              |
| 1:P:179:TYR:O    | 1:P:182:PHE:HB3  | 2.20                     | 0.41              |
| 1:R:56:TRP:CE3   | 1:R:315:PRO:HG2  | 2.53                     | 0.41              |
| 1:U:73:TYR:OH    | 1:U:191:LEU:HB3  | 2.20                     | 0.41              |
| 1:W:199:TRP:O    | 1:W:203:THR:OG1  | 2.32                     | 0.41              |
| 1:X:74:TYR:OH    | 1:X:78:GLN:NE2   | 2.46                     | 0.41              |
| 1:Z:61:ILE:HG22  | 1:Z:309:LEU:HB2  | 2.03                     | 0.41              |
| 1:b:199:TRP:CG   | 1:b:297:PRO:HD3  | 2.54                     | 0.41              |
| 1:d:81:ARG:NH2   | 1:d:95:PRO:O     | 2.49                     | 0.41              |
| 1:A:125:TYR:OH   | 1:A:136:ASP:HB3  | 2.20                     | 0.41              |
| 1:C:56:TRP:CE3   | 1:C:169:ALA:HB2  | 2.55                     | 0.41              |
| 1:C:291:ASN:O    | 1:C:295:VAL:HG23 | 2.21                     | 0.41              |
| 1:J:188:ALA:HB1  | 1:J:303:PHE:CE2  | 2.55                     | 0.41              |
| 1:J:225:MET:CE   | 1:J:273:GLN:HG2  | 2.50                     | 0.41              |
| 1:K:115:ARG:HG3  | 1:K:179:TYR:OH   | 2.20                     | 0.41              |
| 1:K:177:ARG:NH2  | 1:K:312:PRO:O    | 2.54                     | 0.41              |
| 1:M:57:SER:HA    | 1:M:164:LEU:O    | 2.20                     | 0.41              |
| 1:N:225:MET:HE1  | 1:N:273:GLN:HE21 | 1.86                     | 0.41              |
| 1:O:149:PHE:C    | 1:O:150:ILE:HG13 | 2.45                     | 0.41              |
| 1:T:292:THR:HG22 | 1:b:302:ARG:CZ   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:301:PRO:HD2  | 1:U:302:ARG:HD3  | 2.02                     | 0.41              |
| 1:W:63:ASP:OD1   | 1:W:64:ARG:HG2   | 2.20                     | 0.41              |
| 1:a:180:VAL:HG11 | 1:a:308:TYR:OH   | 2.20                     | 0.41              |
| 1:c:187:ALA:CB   | 1:c:305:THR:HG21 | 2.42                     | 0.41              |
| 1:d:125:TYR:HA   | 1:d:143:MET:HE1  | 2.02                     | 0.41              |
| 1:f:203:THR:O    | 1:f:207:LYS:HG2  | 2.20                     | 0.41              |
| 1:f:289:MET:O    | 1:f:293:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:122:THR:HG22 | 1:A:125:TYR:H    | 1.85                     | 0.41              |
| 1:B:55:GLU:HG2   | 1:B:167:GLU:HA   | 2.02                     | 0.41              |
| 1:C:74:TYR:CE2   | 1:C:78:GLN:HG3   | 2.55                     | 0.41              |
| 1:D:80:LEU:HA    | 1:D:83:LEU:HD12  | 2.01                     | 0.41              |
| 1:D:180:VAL:HG23 | 1:D:181:ALA:N    | 2.36                     | 0.41              |
| 1:F:64:ARG:HA    | 1:F:102:TYR:CG   | 2.56                     | 0.41              |
| 1:F:73:TYR:OH    | 1:F:191:LEU:HD22 | 2.21                     | 0.41              |
| 1:G:65:PRO:HB2   | 1:G:69:MET:HG2   | 2.02                     | 0.41              |
| 1:H:122:THR:O    | 1:H:126:LYS:HE3  | 2.21                     | 0.41              |
| 1:K:225:MET:CB   | 1:K:272:LEU:HD11 | 2.44                     | 0.41              |
| 1:M:124:TYR:HE1  | 1:M:143:MET:HE2  | 1.84                     | 0.41              |
| 1:N:64:ARG:NE    | 1:N:99:ASP:OD1   | 2.53                     | 0.41              |
| 1:O:119:TRP:HE3  | 1:O:122:THR:HG21 | 1.80                     | 0.41              |
| 1:R:124:TYR:OH   | 1:R:167:GLU:HG3  | 2.20                     | 0.41              |
| 1:T:184:SER:HB2  | 1:T:306:TYR:CD1  | 2.56                     | 0.41              |
| 1:V:294:ASN:HD22 | 1:V:294:ASN:HA   | 1.64                     | 0.41              |
| 1:Y:56:TRP:O     | 1:Y:165:ILE:HA   | 2.20                     | 0.41              |
| 1:Y:223:ARG:HH12 | 1:Z:284:ASP:CG   | 2.29                     | 0.41              |
| 1:a:198:ALA:HA   | 1:b:67:VAL:HG11  | 2.01                     | 0.41              |
| 1:b:223:ARG:NH2  | 1:c:284:ASP:OD1  | 2.50                     | 0.41              |
| 1:b:300:ASP:OD1  | 1:b:302:ARG:HB2  | 2.20                     | 0.41              |
| 1:B:68:ASN:H     | 1:B:68:ASN:ND2   | 2.18                     | 0.41              |
| 1:D:147:ILE:HA   | 1:D:163:LYS:O    | 2.20                     | 0.41              |
| 1:D:182:PHE:CE2  | 1:D:186:ARG:HD2  | 2.56                     | 0.41              |
| 1:E:74:TYR:HE1   | 1:E:98:MET:CE    | 2.33                     | 0.41              |
| 1:F:96:SER:OG    | 1:F:98:MET:SD    | 2.68                     | 0.41              |
| 1:J:182:PHE:CE2  | 1:J:186:ARG:HD2  | 2.55                     | 0.41              |
| 1:J:206:MET:O    | 1:J:206:MET:HG3  | 2.21                     | 0.41              |
| 1:M:104:GLU:CD   | 1:N:307:ARG:HH22 | 2.29                     | 0.41              |
| 1:O:176:LEU:HD12 | 1:O:176:LEU:HA   | 1.85                     | 0.41              |
| 1:P:202:ARG:HH21 | 1:P:205:GLN:HE21 | 1.68                     | 0.41              |
| 1:R:127:GLN:HE21 | 1:R:127:GLN:HB2  | 1.77                     | 0.41              |
| 1:S:74:TYR:CE1   | 1:S:98:MET:HE1   | 2.55                     | 0.41              |
| 1:W:194:GLU:OE2  | 1:W:194:GLU:HA   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:198:ALA:CA   | 1:X:67:VAL:HG11  | 2.51                     | 0.41              |
| 1:W:221:TYR:HB2  | 1:W:277:PRO:HB3  | 2.03                     | 0.41              |
| 1:X:177:ARG:HG3  | 1:X:312:PRO:HB2  | 2.03                     | 0.41              |
| 1:Y:194:GLU:OE2  | 1:Y:194:GLU:HA   | 2.20                     | 0.41              |
| 1:A:69:MET:CE    | 1:A:307:ARG:HB3  | 2.42                     | 0.41              |
| 1:B:81:ARG:C     | 1:B:83:LEU:H     | 2.29                     | 0.41              |
| 1:D:266:GLN:NE2  | 1:D:269:LEU:HD23 | 2.36                     | 0.41              |
| 1:E:291:ASN:O    | 1:E:294:ASN:HB2  | 2.21                     | 0.41              |
| 1:E:293:LEU:HA   | 1:E:293:LEU:HD12 | 1.73                     | 0.41              |
| 1:I:63:ASP:OD2   | 1:I:159:ASN:ND2  | 2.54                     | 0.41              |
| 1:J:202:ARG:CZ   | 1:J:205:GLN:HG2  | 2.51                     | 0.41              |
| 1:L:76:GLN:CB    | 1:L:195:LEU:HD11 | 2.51                     | 0.41              |
| 1:P:180:VAL:HG11 | 1:P:308:TYR:CZ   | 2.56                     | 0.41              |
| 1:P:288:ALA:O    | 1:P:291:ASN:HB2  | 2.21                     | 0.41              |
| 1:U:194:GLU:OE2  | 1:V:66:THR:HB    | 2.21                     | 0.41              |
| 1:U:290:LEU:HD23 | 1:U:290:LEU:HA   | 1.84                     | 0.41              |
| 1:X:171:ASP:O    | 1:X:175:LEU:HB2  | 2.20                     | 0.41              |
| 1:X:272:LEU:HA   | 1:X:275:VAL:HG12 | 2.02                     | 0.41              |
| 1:Y:216:VAL:HG13 | 1:Z:284:ASP:HB3  | 2.03                     | 0.41              |
| 1:Y:290:LEU:HD23 | 1:Y:290:LEU:HA   | 1.92                     | 0.41              |
| 1:Z:280:ASP:O    | 1:Z:283:TYR:HB3  | 2.20                     | 0.41              |
| 1:a:104:GLU:OE1  | 1:b:307:ARG:NH2  | 2.40                     | 0.41              |
| 1:c:169:ALA:C    | 1:c:314:GLU:HG2  | 2.45                     | 0.41              |
| 1:e:64:ARG:HA    | 1:e:102:TYR:CG   | 2.55                     | 0.41              |
| 1:A:137:ALA:O    | 1:A:140:LEU:HB3  | 2.21                     | 0.41              |
| 1:B:57:SER:HA    | 1:B:164:LEU:O    | 2.21                     | 0.41              |
| 1:C:283:TYR:OH   | 1:C:287:ARG:HD3  | 2.20                     | 0.41              |
| 1:D:122:THR:HG23 | 1:D:124:TYR:H    | 1.84                     | 0.41              |
| 1:D:300:ASP:OD1  | 1:D:302:ARG:NH1  | 2.54                     | 0.41              |
| 1:E:275:VAL:CG1  | 1:E:276:GLY:H    | 2.24                     | 0.41              |
| 1:G:268:ARG:HA   | 1:G:268:ARG:HD2  | 1.72                     | 0.41              |
| 1:H:73:TYR:CD1   | 1:H:195:LEU:HD22 | 2.56                     | 0.41              |
| 1:I:67:VAL:O     | 1:I:70:LEU:HB2   | 2.21                     | 0.41              |
| 1:I:169:ALA:C    | 1:I:314:GLU:HG2  | 2.45                     | 0.41              |
| 1:J:61:ILE:HB    | 1:J:310:ARG:HB3  | 2.03                     | 0.41              |
| 1:J:69:MET:HG2   | 1:J:304:GLN:HB3  | 2.03                     | 0.41              |
| 1:J:294:ASN:HD22 | 1:J:294:ASN:HA   | 1.66                     | 0.41              |
| 1:K:120:LEU:O    | 1:K:126:LYS:HE3  | 2.21                     | 0.41              |
| 1:K:206:MET:HG2  | 1:K:290:LEU:HG   | 2.03                     | 0.41              |
| 1:N:77:GLN:HA    | 1:N:77:GLN:OE1   | 2.21                     | 0.41              |
| 1:O:209:GLN:HA   | 1:O:212:ARG:NH2  | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:272:LEU:HA   | 1:O:275:VAL:HG12 | 2.02                     | 0.41              |
| 1:Q:146:ASN:HD22 | 1:Q:146:ASN:HA   | 1.68                     | 0.41              |
| 1:R:213:GLN:NE2  | 1:R:286:ASN:HD22 | 2.18                     | 0.41              |
| 1:S:61:ILE:HG22  | 1:S:309:LEU:HD12 | 2.01                     | 0.41              |
| 1:S:74:TYR:CD1   | 1:S:97:VAL:HG22  | 2.56                     | 0.41              |
| 1:T:70:LEU:HA    | 1:T:303:PHE:HD1  | 1.86                     | 0.41              |
| 1:T:122:THR:CG2  | 1:T:125:TYR:H    | 2.34                     | 0.41              |
| 1:W:128:ARG:HE   | 1:W:167:GLU:CD   | 2.29                     | 0.41              |
| 1:X:141:ASP:HA   | 1:X:144:ILE:HD12 | 2.03                     | 0.41              |
| 1:Y:122:THR:CG2  | 1:Y:124:TYR:HB3  | 2.51                     | 0.41              |
| 1:Y:305:THR:HG23 | 1:Y:305:THR:O    | 2.21                     | 0.41              |
| 1:Z:225:MET:HE3  | 1:Z:225:MET:HB2  | 1.88                     | 0.41              |
| 1:c:300:ASP:OD1  | 1:c:302:ARG:HD3  | 2.21                     | 0.41              |
| 1:B:67:VAL:HG13  | 1:B:74:TYR:CD1   | 2.56                     | 0.41              |
| 1:G:125:TYR:HA   | 1:G:143:MET:HE1  | 2.03                     | 0.41              |
| 1:H:118:PHE:HE1  | 1:H:178:GLN:HB3  | 1.86                     | 0.41              |
| 1:I:300:ASP:OD1  | 1:I:302:ARG:HD3  | 2.21                     | 0.41              |
| 1:K:280:ASP:OD1  | 1:K:282:ASP:HB2  | 2.21                     | 0.41              |
| 1:P:280:ASP:O    | 1:P:283:TYR:HB3  | 2.21                     | 0.41              |
| 1:Q:61:ILE:O     | 1:Q:309:LEU:N    | 2.33                     | 0.41              |
| 1:U:60:ALA:HB2   | 1:U:312:PRO:HG3  | 2.03                     | 0.41              |
| 1:V:124:TYR:OH   | 1:V:167:GLU:HG3  | 2.21                     | 0.41              |
| 1:b:69:MET:HG3   | 1:b:304:GLN:HB3  | 2.01                     | 0.41              |
| 1:c:147:ILE:HG12 | 1:c:164:LEU:HD12 | 2.03                     | 0.41              |
| 1:d:305:THR:HG23 | 1:d:305:THR:O    | 2.21                     | 0.41              |
| 1:e:119:TRP:CG   | 1:e:143:MET:HB3  | 2.55                     | 0.41              |
| 1:f:207:LYS:NZ   | 1:f:294:ASN:HD21 | 2.18                     | 0.41              |
| 1:B:74:TYR:OH    | 1:B:78:GLN:NE2   | 2.53                     | 0.40              |
| 1:C:70:LEU:HA    | 1:C:303:PHE:HD1  | 1.86                     | 0.40              |
| 1:D:177:ARG:NH2  | 1:D:312:PRO:O    | 2.54                     | 0.40              |
| 1:G:76:GLN:HE21  | 1:G:298:THR:H    | 1.68                     | 0.40              |
| 1:G:80:LEU:HD23  | 1:G:80:LEU:HA    | 1.80                     | 0.40              |
| 1:H:119:TRP:CE2  | 1:H:143:MET:HB3  | 2.56                     | 0.40              |
| 1:J:141:ASP:O    | 1:J:145:ASN:ND2  | 2.54                     | 0.40              |
| 1:M:104:GLU:OE1  | 1:N:307:ARG:NH2  | 2.46                     | 0.40              |
| 1:P:228:ILE:HG22 | 1:P:269:LEU:HD12 | 2.03                     | 0.40              |
| 1:S:198:ALA:N    | 1:T:67:VAL:HG11  | 2.36                     | 0.40              |
| 1:Z:74:TYR:CD1   | 1:Z:97:VAL:HB    | 2.56                     | 0.40              |
| 1:f:59:THR:O     | 1:f:312:PRO:HA   | 2.20                     | 0.40              |
| 1:f:268:ARG:HA   | 1:f:268:ARG:HD2  | 1.76                     | 0.40              |
| 1:A:122:THR:CG2  | 1:A:125:TYR:H    | 2.34                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:122:THR:HG23 | 1:F:124:TYR:N    | 2.37                     | 0.40              |
| 1:F:125:TYR:HB2  | 1:F:143:MET:SD   | 2.61                     | 0.40              |
| 1:Q:105:PHE:HA   | 1:Q:187:ALA:HB2  | 2.03                     | 0.40              |
| 1:U:203:THR:HA   | 1:U:293:LEU:HG   | 2.04                     | 0.40              |
| 1:U:209:GLN:O    | 1:U:213:GLN:HG3  | 2.21                     | 0.40              |
| 1:W:76:GLN:NE2   | 1:W:297:PRO:HA   | 2.36                     | 0.40              |
| 1:W:119:TRP:NE1  | 1:W:143:MET:O    | 2.54                     | 0.40              |
| 1:Y:162:VAL:HG13 | 1:Y:176:LEU:HD11 | 2.02                     | 0.40              |
| 1:a:227:SER:HB2  | 1:b:275:VAL:HG23 | 2.03                     | 0.40              |
| 1:c:122:THR:O    | 1:c:126:LYS:HG3  | 2.21                     | 0.40              |
| 1:c:124:TYR:CD2  | 1:c:175:LEU:HD11 | 2.57                     | 0.40              |
| 1:e:188:ALA:HB1  | 1:e:303:PHE:CE2  | 2.56                     | 0.40              |
| 1:f:119:TRP:CE2  | 1:f:143:MET:HB3  | 2.56                     | 0.40              |
| 1:f:221:TYR:HE1  | 1:f:272:LEU:O    | 2.04                     | 0.40              |
| 1:C:150:ILE:HA   | 1:C:151:PRO:HD2  | 1.91                     | 0.40              |
| 1:D:199:TRP:CG   | 1:D:297:PRO:HD3  | 2.56                     | 0.40              |
| 1:E:80:LEU:HD23  | 1:E:80:LEU:HA    | 1.90                     | 0.40              |
| 1:G:125:TYR:OH   | 1:G:140:LEU:HB2  | 2.22                     | 0.40              |
| 1:G:128:ARG:HB3  | 1:G:139:LEU:HD21 | 2.04                     | 0.40              |
| 1:L:216:VAL:O    | 1:L:220:ILE:HG13 | 2.22                     | 0.40              |
| 1:R:210:VAL:O    | 1:R:213:GLN:HB2  | 2.21                     | 0.40              |
| 1:S:212:ARG:HG2  | 1:T:288:ALA:CB   | 2.48                     | 0.40              |
| 1:V:286:ASN:O    | 1:V:290:LEU:HB2  | 2.21                     | 0.40              |
| 1:W:294:ASN:HD22 | 1:W:294:ASN:HA   | 1.60                     | 0.40              |
| 1:X:137:ALA:O    | 1:X:140:LEU:HB3  | 2.21                     | 0.40              |
| 1:X:146:ASN:HB3  | 1:X:165:ILE:HB   | 2.04                     | 0.40              |
| 1:a:104:GLU:HA   | 1:a:107:MET:HE2  | 2.03                     | 0.40              |
| 1:d:147:ILE:HG12 | 1:d:164:LEU:HD12 | 2.02                     | 0.40              |
| 1:f:64:ARG:HA    | 1:f:102:TYR:CG   | 2.56                     | 0.40              |
| 1:f:188:ALA:HB1  | 1:f:303:PHE:CE2  | 2.57                     | 0.40              |
| 1:F:56:TRP:CE3   | 1:F:169:ALA:HB2  | 2.56                     | 0.40              |
| 1:G:121:GLN:C    | 1:G:121:GLN:CD   | 2.90                     | 0.40              |
| 1:G:123:ASP:O    | 1:G:127:GLN:HG3  | 2.22                     | 0.40              |
| 1:I:61:ILE:HG22  | 1:I:309:LEU:HB2  | 2.02                     | 0.40              |
| 1:N:57:SER:O     | 1:N:315:PRO:HB3  | 2.22                     | 0.40              |
| 1:O:77:GLN:OE1   | 1:O:77:GLN:HA    | 2.21                     | 0.40              |
| 1:O:180:VAL:HG11 | 1:O:308:TYR:CE1  | 2.57                     | 0.40              |
| 1:P:122:THR:HG23 | 1:P:124:TYR:HB3  | 2.02                     | 0.40              |
| 1:R:148:GLN:HE21 | 1:R:148:GLN:HB2  | 1.55                     | 0.40              |
| 1:R:225:MET:HE2  | 1:R:225:MET:HB2  | 1.88                     | 0.40              |
| 1:U:132:ASN:ND2  | 1:U:134:LYS:HB3  | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:122:THR:CG2  | 1:V:125:TYR:H    | 2.34                     | 0.40              |
| 1:V:210:VAL:HA   | 1:V:213:GLN:HE21 | 1.86                     | 0.40              |
| 1:V:213:GLN:NE2  | 1:V:286:ASN:HD22 | 2.19                     | 0.40              |
| 1:W:124:TYR:OH   | 1:W:167:GLU:N    | 2.42                     | 0.40              |
| 1:a:59:THR:HA    | 1:a:162:VAL:O    | 2.21                     | 0.40              |
| 1:a:98:MET:HG2   | 1:a:98:MET:H     | 1.63                     | 0.40              |
| 1:b:126:LYS:HA   | 1:b:129:MET:SD   | 2.61                     | 0.40              |
| 1:c:169:ALA:CB   | 1:c:314:GLU:HG2  | 2.52                     | 0.40              |
| 1:c:199:TRP:NE1  | 1:c:293:LEU:O    | 2.43                     | 0.40              |
| 1:d:191:LEU:O    | 1:d:194:GLU:HB2  | 2.22                     | 0.40              |
| 1:A:148:GLN:HE21 | 1:A:148:GLN:HB2  | 1.57                     | 0.40              |
| 1:C:187:ALA:CB   | 1:C:305:THR:HG21 | 2.48                     | 0.40              |
| 1:E:77:GLN:OE1   | 1:E:195:LEU:HD13 | 2.21                     | 0.40              |
| 1:F:70:LEU:HD11  | 1:F:98:MET:HA    | 2.04                     | 0.40              |
| 1:F:169:ALA:HB3  | 1:F:170:PRO:HD3  | 2.03                     | 0.40              |
| 1:M:119:TRP:HE3  | 1:M:122:THR:HG21 | 1.85                     | 0.40              |
| 1:P:79:PHE:O     | 1:P:83:LEU:HG    | 2.21                     | 0.40              |
| 1:S:308:TYR:CE2  | 1:S:311:THR:HG23 | 2.57                     | 0.40              |
| 1:W:109:LEU:HD12 | 1:W:109:LEU:HA   | 1.96                     | 0.40              |
| 1:Z:64:ARG:O     | 1:Z:307:ARG:HG2  | 2.21                     | 0.40              |
| 1:a:81:ARG:O     | 1:a:85:VAL:HG22  | 2.21                     | 0.40              |
| 1:d:61:ILE:HG13  | 1:d:161:SER:HB3  | 2.04                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------------|--------------------------|-------------------|
| 1:D:196:LYS:NZ | 1:L:296:GLY:O[2_546] | 1.93                     | 0.27              |

## 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     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | B     | 215/356 (60%) | 212 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | C     | 215/356 (60%) | 213 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | D     | 215/356 (60%) | 211 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | E     | 215/356 (60%) | 212 (99%) | 2 (1%)  | 1 (0%)   | 24          | 63  |
| 1   | F     | 215/356 (60%) | 210 (98%) | 4 (2%)  | 1 (0%)   | 24          | 63  |
| 1   | G     | 215/356 (60%) | 211 (98%) | 3 (1%)  | 1 (0%)   | 24          | 63  |
| 1   | H     | 215/356 (60%) | 211 (98%) | 3 (1%)  | 1 (0%)   | 24          | 63  |
| 1   | I     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | J     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | K     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | L     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | M     | 215/356 (60%) | 207 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | N     | 215/356 (60%) | 208 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | O     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | P     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Q     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | R     | 215/356 (60%) | 211 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | S     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | T     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | U     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | V     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | W     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | X     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Y     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | Z     | 215/356 (60%) | 211 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | a     | 215/356 (60%) | 208 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | b     | 215/356 (60%) | 211 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | c     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | d     | 215/356 (60%) | 210 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | e     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | f     | 215/356 (60%) | 209 (97%) | 6 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |
|-----|-------|------------------|------------|----------|----------|-------------|
| All | All   | 6880/11392 (60%) | 6715 (98%) | 161 (2%) | 4 (0%)   | 48 83       |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 275 | VAL  |
| 1   | H     | 303 | PHE  |
| 1   | F     | 318 | ARG  |
| 1   | G     | 269 | 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     | 190/296 (64%) | 159 (84%) | 31 (16%) | 2 11        |
| 1   | B     | 190/296 (64%) | 170 (90%) | 20 (10%) | 6 21        |
| 1   | C     | 190/296 (64%) | 165 (87%) | 25 (13%) | 4 15        |
| 1   | D     | 190/296 (64%) | 171 (90%) | 19 (10%) | 7 24        |
| 1   | E     | 190/296 (64%) | 163 (86%) | 27 (14%) | 3 13        |
| 1   | F     | 190/296 (64%) | 172 (90%) | 18 (10%) | 8 25        |
| 1   | G     | 190/296 (64%) | 170 (90%) | 20 (10%) | 6 21        |
| 1   | H     | 190/296 (64%) | 169 (89%) | 21 (11%) | 6 20        |
| 1   | I     | 190/296 (64%) | 163 (86%) | 27 (14%) | 3 13        |
| 1   | J     | 190/296 (64%) | 166 (87%) | 24 (13%) | 4 16        |
| 1   | K     | 190/296 (64%) | 166 (87%) | 24 (13%) | 4 16        |
| 1   | L     | 190/296 (64%) | 163 (86%) | 27 (14%) | 3 13        |
| 1   | M     | 190/296 (64%) | 158 (83%) | 32 (17%) | 2 10        |
| 1   | N     | 190/296 (64%) | 168 (88%) | 22 (12%) | 5 18        |
| 1   | O     | 190/296 (64%) | 168 (88%) | 22 (12%) | 5 18        |
| 1   | P     | 190/296 (64%) | 167 (88%) | 23 (12%) | 5 17        |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | Q     | 190/296 (64%)   | 166 (87%)  | 24 (13%)  | 4           | 16 |
| 1   | R     | 190/296 (64%)   | 164 (86%)  | 26 (14%)  | 3           | 14 |
| 1   | S     | 190/296 (64%)   | 166 (87%)  | 24 (13%)  | 4           | 16 |
| 1   | T     | 190/296 (64%)   | 166 (87%)  | 24 (13%)  | 4           | 16 |
| 1   | U     | 190/296 (64%)   | 166 (87%)  | 24 (13%)  | 4           | 16 |
| 1   | V     | 190/296 (64%)   | 169 (89%)  | 21 (11%)  | 6           | 20 |
| 1   | W     | 190/296 (64%)   | 171 (90%)  | 19 (10%)  | 7           | 24 |
| 1   | X     | 190/296 (64%)   | 169 (89%)  | 21 (11%)  | 6           | 20 |
| 1   | Y     | 190/296 (64%)   | 157 (83%)  | 33 (17%)  | 2           | 9  |
| 1   | Z     | 190/296 (64%)   | 163 (86%)  | 27 (14%)  | 3           | 13 |
| 1   | a     | 190/296 (64%)   | 165 (87%)  | 25 (13%)  | 4           | 15 |
| 1   | b     | 190/296 (64%)   | 165 (87%)  | 25 (13%)  | 4           | 15 |
| 1   | c     | 190/296 (64%)   | 167 (88%)  | 23 (12%)  | 5           | 17 |
| 1   | d     | 190/296 (64%)   | 169 (89%)  | 21 (11%)  | 6           | 20 |
| 1   | e     | 190/296 (64%)   | 159 (84%)  | 31 (16%)  | 2           | 11 |
| 1   | f     | 190/296 (64%)   | 168 (88%)  | 22 (12%)  | 5           | 18 |
| All | All   | 6080/9472 (64%) | 5308 (87%) | 772 (13%) | 4           | 16 |

All (772) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 55  | GLU  |
| 1   | A     | 61  | ILE  |
| 1   | A     | 67  | VAL  |
| 1   | A     | 68  | ASN  |
| 1   | A     | 85  | VAL  |
| 1   | A     | 96  | SER  |
| 1   | A     | 98  | MET  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 107 | MET  |
| 1   | A     | 121 | GLN  |
| 1   | A     | 122 | THR  |
| 1   | A     | 134 | LYS  |
| 1   | A     | 147 | ILE  |
| 1   | A     | 148 | GLN  |
| 1   | A     | 150 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 155 | THR  |
| 1   | A     | 158 | VAL  |
| 1   | A     | 205 | GLN  |
| 1   | A     | 206 | MET  |
| 1   | A     | 211 | LYS  |
| 1   | A     | 216 | VAL  |
| 1   | A     | 227 | SER  |
| 1   | A     | 282 | ASP  |
| 1   | A     | 289 | MET  |
| 1   | A     | 290 | LEU  |
| 1   | A     | 292 | THR  |
| 1   | A     | 293 | LEU  |
| 1   | A     | 299 | LEU  |
| 1   | A     | 302 | ARG  |
| 1   | A     | 305 | THR  |
| 1   | A     | 317 | LYS  |
| 1   | B     | 61  | ILE  |
| 1   | B     | 62  | THR  |
| 1   | B     | 67  | VAL  |
| 1   | B     | 84  | ASP  |
| 1   | B     | 85  | VAL  |
| 1   | B     | 98  | MET  |
| 1   | B     | 106 | VAL  |
| 1   | B     | 107 | MET  |
| 1   | B     | 121 | GLN  |
| 1   | B     | 142 | GLU  |
| 1   | B     | 148 | GLN  |
| 1   | B     | 153 | ASP  |
| 1   | B     | 189 | SER  |
| 1   | B     | 211 | LYS  |
| 1   | B     | 218 | LYS  |
| 1   | B     | 268 | ARG  |
| 1   | B     | 287 | ARG  |
| 1   | B     | 293 | LEU  |
| 1   | B     | 305 | THR  |
| 1   | B     | 316 | VAL  |
| 1   | C     | 55  | GLU  |
| 1   | C     | 67  | VAL  |
| 1   | C     | 68  | ASN  |
| 1   | C     | 97  | VAL  |
| 1   | C     | 98  | MET  |
| 1   | C     | 107 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 114 | THR  |
| 1   | C     | 121 | GLN  |
| 1   | C     | 122 | THR  |
| 1   | C     | 133 | SER  |
| 1   | C     | 134 | LYS  |
| 1   | C     | 155 | THR  |
| 1   | C     | 163 | LYS  |
| 1   | C     | 206 | MET  |
| 1   | C     | 210 | VAL  |
| 1   | C     | 225 | MET  |
| 1   | C     | 272 | LEU  |
| 1   | C     | 282 | ASP  |
| 1   | C     | 290 | LEU  |
| 1   | C     | 292 | THR  |
| 1   | C     | 293 | LEU  |
| 1   | C     | 305 | THR  |
| 1   | C     | 307 | ARG  |
| 1   | C     | 316 | VAL  |
| 1   | C     | 318 | ARG  |
| 1   | D     | 58  | SER  |
| 1   | D     | 64  | ARG  |
| 1   | D     | 85  | VAL  |
| 1   | D     | 98  | MET  |
| 1   | D     | 122 | THR  |
| 1   | D     | 130 | VAL  |
| 1   | D     | 134 | LYS  |
| 1   | D     | 148 | GLN  |
| 1   | D     | 158 | VAL  |
| 1   | D     | 204 | ILE  |
| 1   | D     | 205 | GLN  |
| 1   | D     | 268 | ARG  |
| 1   | D     | 273 | GLN  |
| 1   | D     | 287 | ARG  |
| 1   | D     | 290 | LEU  |
| 1   | D     | 291 | ASN  |
| 1   | D     | 293 | LEU  |
| 1   | D     | 302 | ARG  |
| 1   | D     | 305 | THR  |
| 1   | E     | 61  | ILE  |
| 1   | E     | 67  | VAL  |
| 1   | E     | 68  | ASN  |
| 1   | E     | 84  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 98  | MET  |
| 1   | E     | 111 | SER  |
| 1   | E     | 121 | GLN  |
| 1   | E     | 122 | THR  |
| 1   | E     | 148 | GLN  |
| 1   | E     | 156 | ARG  |
| 1   | E     | 185 | GLN  |
| 1   | E     | 202 | ARG  |
| 1   | E     | 205 | GLN  |
| 1   | E     | 211 | LYS  |
| 1   | E     | 215 | GLU  |
| 1   | E     | 224 | ARG  |
| 1   | E     | 266 | GLN  |
| 1   | E     | 268 | ARG  |
| 1   | E     | 271 | ASN  |
| 1   | E     | 282 | ASP  |
| 1   | E     | 289 | MET  |
| 1   | E     | 290 | LEU  |
| 1   | E     | 293 | LEU  |
| 1   | E     | 295 | VAL  |
| 1   | E     | 299 | LEU  |
| 1   | E     | 302 | ARG  |
| 1   | E     | 305 | THR  |
| 1   | F     | 55  | GLU  |
| 1   | F     | 59  | THR  |
| 1   | F     | 84  | ASP  |
| 1   | F     | 85  | VAL  |
| 1   | F     | 98  | MET  |
| 1   | F     | 122 | THR  |
| 1   | F     | 134 | LYS  |
| 1   | F     | 144 | ILE  |
| 1   | F     | 163 | LYS  |
| 1   | F     | 204 | ILE  |
| 1   | F     | 207 | LYS  |
| 1   | F     | 216 | VAL  |
| 1   | F     | 228 | ILE  |
| 1   | F     | 290 | LEU  |
| 1   | F     | 298 | THR  |
| 1   | F     | 302 | ARG  |
| 1   | F     | 316 | VAL  |
| 1   | F     | 318 | ARG  |
| 1   | G     | 58  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 64  | ARG  |
| 1   | G     | 69  | MET  |
| 1   | G     | 84  | ASP  |
| 1   | G     | 85  | VAL  |
| 1   | G     | 98  | MET  |
| 1   | G     | 121 | GLN  |
| 1   | G     | 122 | THR  |
| 1   | G     | 134 | LYS  |
| 1   | G     | 155 | THR  |
| 1   | G     | 211 | LYS  |
| 1   | G     | 220 | ILE  |
| 1   | G     | 268 | ARG  |
| 1   | G     | 282 | ASP  |
| 1   | G     | 287 | ARG  |
| 1   | G     | 293 | LEU  |
| 1   | G     | 299 | LEU  |
| 1   | G     | 304 | GLN  |
| 1   | G     | 305 | THR  |
| 1   | G     | 307 | ARG  |
| 1   | H     | 55  | GLU  |
| 1   | H     | 59  | THR  |
| 1   | H     | 64  | ARG  |
| 1   | H     | 85  | VAL  |
| 1   | H     | 98  | MET  |
| 1   | H     | 103 | LYS  |
| 1   | H     | 122 | THR  |
| 1   | H     | 130 | VAL  |
| 1   | H     | 134 | LYS  |
| 1   | H     | 153 | ASP  |
| 1   | H     | 158 | VAL  |
| 1   | H     | 205 | GLN  |
| 1   | H     | 206 | MET  |
| 1   | H     | 210 | VAL  |
| 1   | H     | 227 | SER  |
| 1   | H     | 271 | ASN  |
| 1   | H     | 287 | ARG  |
| 1   | H     | 290 | LEU  |
| 1   | H     | 292 | THR  |
| 1   | H     | 293 | LEU  |
| 1   | H     | 305 | THR  |
| 1   | I     | 55  | GLU  |
| 1   | I     | 58  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 59  | THR  |
| 1   | I     | 66  | THR  |
| 1   | I     | 68  | ASN  |
| 1   | I     | 85  | VAL  |
| 1   | I     | 96  | SER  |
| 1   | I     | 98  | MET  |
| 1   | I     | 106 | VAL  |
| 1   | I     | 122 | THR  |
| 1   | I     | 134 | LYS  |
| 1   | I     | 147 | ILE  |
| 1   | I     | 148 | GLN  |
| 1   | I     | 155 | THR  |
| 1   | I     | 158 | VAL  |
| 1   | I     | 202 | ARG  |
| 1   | I     | 211 | LYS  |
| 1   | I     | 282 | ASP  |
| 1   | I     | 289 | MET  |
| 1   | I     | 290 | LEU  |
| 1   | I     | 292 | THR  |
| 1   | I     | 293 | LEU  |
| 1   | I     | 298 | THR  |
| 1   | I     | 302 | ARG  |
| 1   | I     | 305 | THR  |
| 1   | I     | 311 | THR  |
| 1   | I     | 317 | LYS  |
| 1   | J     | 66  | THR  |
| 1   | J     | 68  | ASN  |
| 1   | J     | 96  | SER  |
| 1   | J     | 98  | MET  |
| 1   | J     | 121 | GLN  |
| 1   | J     | 134 | LYS  |
| 1   | J     | 147 | ILE  |
| 1   | J     | 148 | GLN  |
| 1   | J     | 155 | THR  |
| 1   | J     | 158 | VAL  |
| 1   | J     | 202 | ARG  |
| 1   | J     | 203 | THR  |
| 1   | J     | 205 | GLN  |
| 1   | J     | 210 | VAL  |
| 1   | J     | 211 | LYS  |
| 1   | J     | 227 | SER  |
| 1   | J     | 275 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 290 | LEU  |
| 1   | J     | 293 | LEU  |
| 1   | J     | 299 | LEU  |
| 1   | J     | 302 | ARG  |
| 1   | J     | 305 | THR  |
| 1   | J     | 307 | ARG  |
| 1   | J     | 316 | VAL  |
| 1   | K     | 55  | GLU  |
| 1   | K     | 68  | ASN  |
| 1   | K     | 78  | GLN  |
| 1   | K     | 85  | VAL  |
| 1   | K     | 96  | SER  |
| 1   | K     | 98  | MET  |
| 1   | K     | 107 | MET  |
| 1   | K     | 121 | GLN  |
| 1   | K     | 122 | THR  |
| 1   | K     | 134 | LYS  |
| 1   | K     | 158 | VAL  |
| 1   | K     | 202 | ARG  |
| 1   | K     | 211 | LYS  |
| 1   | K     | 225 | MET  |
| 1   | K     | 272 | LEU  |
| 1   | K     | 282 | ASP  |
| 1   | K     | 290 | LEU  |
| 1   | K     | 293 | LEU  |
| 1   | K     | 295 | VAL  |
| 1   | K     | 299 | LEU  |
| 1   | K     | 302 | ARG  |
| 1   | K     | 305 | THR  |
| 1   | K     | 316 | VAL  |
| 1   | K     | 317 | LYS  |
| 1   | L     | 58  | SER  |
| 1   | L     | 59  | THR  |
| 1   | L     | 66  | THR  |
| 1   | L     | 68  | ASN  |
| 1   | L     | 69  | MET  |
| 1   | L     | 96  | SER  |
| 1   | L     | 98  | MET  |
| 1   | L     | 121 | GLN  |
| 1   | L     | 130 | VAL  |
| 1   | L     | 134 | LYS  |
| 1   | L     | 148 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 156 | ARG  |
| 1   | L     | 158 | VAL  |
| 1   | L     | 202 | ARG  |
| 1   | L     | 205 | GLN  |
| 1   | L     | 211 | LYS  |
| 1   | L     | 215 | GLU  |
| 1   | L     | 220 | ILE  |
| 1   | L     | 225 | MET  |
| 1   | L     | 227 | SER  |
| 1   | L     | 271 | ASN  |
| 1   | L     | 275 | VAL  |
| 1   | L     | 290 | LEU  |
| 1   | L     | 293 | LEU  |
| 1   | L     | 295 | VAL  |
| 1   | L     | 302 | ARG  |
| 1   | L     | 305 | THR  |
| 1   | M     | 58  | SER  |
| 1   | M     | 66  | THR  |
| 1   | M     | 85  | VAL  |
| 1   | M     | 96  | SER  |
| 1   | M     | 97  | VAL  |
| 1   | M     | 98  | MET  |
| 1   | M     | 107 | MET  |
| 1   | M     | 114 | THR  |
| 1   | M     | 121 | GLN  |
| 1   | M     | 122 | THR  |
| 1   | M     | 130 | VAL  |
| 1   | M     | 143 | MET  |
| 1   | M     | 144 | ILE  |
| 1   | M     | 148 | GLN  |
| 1   | M     | 155 | THR  |
| 1   | M     | 156 | ARG  |
| 1   | M     | 158 | VAL  |
| 1   | M     | 202 | ARG  |
| 1   | M     | 206 | MET  |
| 1   | M     | 211 | LYS  |
| 1   | M     | 215 | GLU  |
| 1   | M     | 220 | ILE  |
| 1   | M     | 227 | SER  |
| 1   | M     | 228 | ILE  |
| 1   | M     | 230 | GLN  |
| 1   | M     | 282 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 289 | MET  |
| 1   | M     | 290 | LEU  |
| 1   | M     | 293 | LEU  |
| 1   | M     | 299 | LEU  |
| 1   | M     | 302 | ARG  |
| 1   | M     | 305 | THR  |
| 1   | N     | 67  | VAL  |
| 1   | N     | 68  | ASN  |
| 1   | N     | 85  | VAL  |
| 1   | N     | 96  | SER  |
| 1   | N     | 98  | MET  |
| 1   | N     | 117 | GLU  |
| 1   | N     | 121 | GLN  |
| 1   | N     | 122 | THR  |
| 1   | N     | 130 | VAL  |
| 1   | N     | 134 | LYS  |
| 1   | N     | 147 | ILE  |
| 1   | N     | 148 | GLN  |
| 1   | N     | 156 | ARG  |
| 1   | N     | 158 | VAL  |
| 1   | N     | 196 | LYS  |
| 1   | N     | 216 | VAL  |
| 1   | N     | 290 | LEU  |
| 1   | N     | 293 | LEU  |
| 1   | N     | 299 | LEU  |
| 1   | N     | 305 | THR  |
| 1   | N     | 307 | ARG  |
| 1   | N     | 317 | LYS  |
| 1   | O     | 55  | GLU  |
| 1   | O     | 67  | VAL  |
| 1   | O     | 96  | SER  |
| 1   | O     | 98  | MET  |
| 1   | O     | 106 | VAL  |
| 1   | O     | 107 | MET  |
| 1   | O     | 122 | THR  |
| 1   | O     | 126 | LYS  |
| 1   | O     | 134 | LYS  |
| 1   | O     | 144 | ILE  |
| 1   | O     | 148 | GLN  |
| 1   | O     | 155 | THR  |
| 1   | O     | 158 | VAL  |
| 1   | O     | 165 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 202 | ARG  |
| 1   | O     | 227 | SER  |
| 1   | O     | 282 | ASP  |
| 1   | O     | 289 | MET  |
| 1   | O     | 290 | LEU  |
| 1   | O     | 293 | LEU  |
| 1   | O     | 302 | ARG  |
| 1   | O     | 307 | ARG  |
| 1   | P     | 59  | THR  |
| 1   | P     | 61  | ILE  |
| 1   | P     | 68  | ASN  |
| 1   | P     | 85  | VAL  |
| 1   | P     | 96  | SER  |
| 1   | P     | 98  | MET  |
| 1   | P     | 121 | GLN  |
| 1   | P     | 122 | THR  |
| 1   | P     | 130 | VAL  |
| 1   | P     | 134 | LYS  |
| 1   | P     | 158 | VAL  |
| 1   | P     | 165 | ILE  |
| 1   | P     | 202 | ARG  |
| 1   | P     | 205 | GLN  |
| 1   | P     | 211 | LYS  |
| 1   | P     | 220 | ILE  |
| 1   | P     | 227 | SER  |
| 1   | P     | 275 | VAL  |
| 1   | P     | 289 | MET  |
| 1   | P     | 290 | LEU  |
| 1   | P     | 293 | LEU  |
| 1   | P     | 299 | LEU  |
| 1   | P     | 305 | THR  |
| 1   | Q     | 55  | GLU  |
| 1   | Q     | 68  | ASN  |
| 1   | Q     | 85  | VAL  |
| 1   | Q     | 96  | SER  |
| 1   | Q     | 97  | VAL  |
| 1   | Q     | 98  | MET  |
| 1   | Q     | 121 | GLN  |
| 1   | Q     | 134 | LYS  |
| 1   | Q     | 148 | GLN  |
| 1   | Q     | 155 | THR  |
| 1   | Q     | 158 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 202 | ARG  |
| 1   | Q     | 204 | ILE  |
| 1   | Q     | 211 | LYS  |
| 1   | Q     | 220 | ILE  |
| 1   | Q     | 282 | ASP  |
| 1   | Q     | 290 | LEU  |
| 1   | Q     | 292 | THR  |
| 1   | Q     | 293 | LEU  |
| 1   | Q     | 298 | THR  |
| 1   | Q     | 299 | LEU  |
| 1   | Q     | 302 | ARG  |
| 1   | Q     | 305 | THR  |
| 1   | Q     | 317 | LYS  |
| 1   | R     | 64  | ARG  |
| 1   | R     | 68  | ASN  |
| 1   | R     | 96  | SER  |
| 1   | R     | 97  | VAL  |
| 1   | R     | 98  | MET  |
| 1   | R     | 107 | MET  |
| 1   | R     | 121 | GLN  |
| 1   | R     | 122 | THR  |
| 1   | R     | 130 | VAL  |
| 1   | R     | 134 | LYS  |
| 1   | R     | 148 | GLN  |
| 1   | R     | 158 | VAL  |
| 1   | R     | 202 | ARG  |
| 1   | R     | 210 | VAL  |
| 1   | R     | 211 | LYS  |
| 1   | R     | 216 | VAL  |
| 1   | R     | 225 | MET  |
| 1   | R     | 227 | SER  |
| 1   | R     | 228 | ILE  |
| 1   | R     | 268 | ARG  |
| 1   | R     | 290 | LEU  |
| 1   | R     | 293 | LEU  |
| 1   | R     | 302 | ARG  |
| 1   | R     | 305 | THR  |
| 1   | R     | 307 | ARG  |
| 1   | R     | 317 | LYS  |
| 1   | S     | 55  | GLU  |
| 1   | S     | 68  | ASN  |
| 1   | S     | 69  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 85  | VAL  |
| 1   | S     | 96  | SER  |
| 1   | S     | 98  | MET  |
| 1   | S     | 121 | GLN  |
| 1   | S     | 122 | THR  |
| 1   | S     | 134 | LYS  |
| 1   | S     | 155 | THR  |
| 1   | S     | 158 | VAL  |
| 1   | S     | 202 | ARG  |
| 1   | S     | 224 | ARG  |
| 1   | S     | 225 | MET  |
| 1   | S     | 227 | SER  |
| 1   | S     | 228 | ILE  |
| 1   | S     | 272 | LEU  |
| 1   | S     | 282 | ASP  |
| 1   | S     | 290 | LEU  |
| 1   | S     | 293 | LEU  |
| 1   | S     | 302 | ARG  |
| 1   | S     | 305 | THR  |
| 1   | S     | 311 | THR  |
| 1   | S     | 316 | VAL  |
| 1   | T     | 55  | GLU  |
| 1   | T     | 68  | ASN  |
| 1   | T     | 85  | VAL  |
| 1   | T     | 96  | SER  |
| 1   | T     | 98  | MET  |
| 1   | T     | 117 | GLU  |
| 1   | T     | 134 | LYS  |
| 1   | T     | 148 | GLN  |
| 1   | T     | 158 | VAL  |
| 1   | T     | 196 | LYS  |
| 1   | T     | 202 | ARG  |
| 1   | T     | 203 | THR  |
| 1   | T     | 205 | GLN  |
| 1   | T     | 215 | GLU  |
| 1   | T     | 216 | VAL  |
| 1   | T     | 224 | ARG  |
| 1   | T     | 227 | SER  |
| 1   | T     | 275 | VAL  |
| 1   | T     | 290 | LEU  |
| 1   | T     | 292 | THR  |
| 1   | T     | 293 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 305 | THR  |
| 1   | T     | 316 | VAL  |
| 1   | T     | 317 | LYS  |
| 1   | U     | 62  | THR  |
| 1   | U     | 68  | ASN  |
| 1   | U     | 96  | SER  |
| 1   | U     | 97  | VAL  |
| 1   | U     | 98  | MET  |
| 1   | U     | 122 | THR  |
| 1   | U     | 134 | LYS  |
| 1   | U     | 148 | GLN  |
| 1   | U     | 155 | THR  |
| 1   | U     | 158 | VAL  |
| 1   | U     | 165 | ILE  |
| 1   | U     | 168 | THR  |
| 1   | U     | 180 | VAL  |
| 1   | U     | 202 | ARG  |
| 1   | U     | 211 | LYS  |
| 1   | U     | 215 | GLU  |
| 1   | U     | 227 | SER  |
| 1   | U     | 230 | GLN  |
| 1   | U     | 282 | ASP  |
| 1   | U     | 290 | LEU  |
| 1   | U     | 293 | LEU  |
| 1   | U     | 299 | LEU  |
| 1   | U     | 302 | ARG  |
| 1   | U     | 317 | LYS  |
| 1   | V     | 68  | ASN  |
| 1   | V     | 96  | SER  |
| 1   | V     | 98  | MET  |
| 1   | V     | 106 | VAL  |
| 1   | V     | 121 | GLN  |
| 1   | V     | 122 | THR  |
| 1   | V     | 127 | GLN  |
| 1   | V     | 134 | LYS  |
| 1   | V     | 148 | GLN  |
| 1   | V     | 158 | VAL  |
| 1   | V     | 168 | THR  |
| 1   | V     | 220 | ILE  |
| 1   | V     | 225 | MET  |
| 1   | V     | 227 | SER  |
| 1   | V     | 230 | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 290 | LEU  |
| 1   | V     | 293 | LEU  |
| 1   | V     | 299 | LEU  |
| 1   | V     | 302 | ARG  |
| 1   | V     | 305 | THR  |
| 1   | V     | 317 | LYS  |
| 1   | W     | 61  | ILE  |
| 1   | W     | 67  | VAL  |
| 1   | W     | 85  | VAL  |
| 1   | W     | 98  | MET  |
| 1   | W     | 107 | MET  |
| 1   | W     | 121 | GLN  |
| 1   | W     | 134 | LYS  |
| 1   | W     | 148 | GLN  |
| 1   | W     | 158 | VAL  |
| 1   | W     | 202 | ARG  |
| 1   | W     | 227 | SER  |
| 1   | W     | 275 | VAL  |
| 1   | W     | 282 | ASP  |
| 1   | W     | 289 | MET  |
| 1   | W     | 290 | LEU  |
| 1   | W     | 293 | LEU  |
| 1   | W     | 302 | ARG  |
| 1   | W     | 317 | LYS  |
| 1   | W     | 318 | ARG  |
| 1   | X     | 58  | SER  |
| 1   | X     | 62  | THR  |
| 1   | X     | 68  | ASN  |
| 1   | X     | 85  | VAL  |
| 1   | X     | 106 | VAL  |
| 1   | X     | 121 | GLN  |
| 1   | X     | 122 | THR  |
| 1   | X     | 134 | LYS  |
| 1   | X     | 155 | THR  |
| 1   | X     | 158 | VAL  |
| 1   | X     | 205 | GLN  |
| 1   | X     | 211 | LYS  |
| 1   | X     | 227 | SER  |
| 1   | X     | 289 | MET  |
| 1   | X     | 290 | LEU  |
| 1   | X     | 292 | THR  |
| 1   | X     | 293 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 295 | VAL  |
| 1   | X     | 299 | LEU  |
| 1   | X     | 305 | THR  |
| 1   | X     | 317 | LYS  |
| 1   | Y     | 55  | GLU  |
| 1   | Y     | 58  | SER  |
| 1   | Y     | 61  | ILE  |
| 1   | Y     | 67  | VAL  |
| 1   | Y     | 68  | ASN  |
| 1   | Y     | 69  | MET  |
| 1   | Y     | 85  | VAL  |
| 1   | Y     | 96  | SER  |
| 1   | Y     | 98  | MET  |
| 1   | Y     | 103 | LYS  |
| 1   | Y     | 106 | VAL  |
| 1   | Y     | 107 | MET  |
| 1   | Y     | 122 | THR  |
| 1   | Y     | 134 | LYS  |
| 1   | Y     | 148 | GLN  |
| 1   | Y     | 155 | THR  |
| 1   | Y     | 158 | VAL  |
| 1   | Y     | 202 | ARG  |
| 1   | Y     | 210 | VAL  |
| 1   | Y     | 211 | LYS  |
| 1   | Y     | 225 | MET  |
| 1   | Y     | 275 | VAL  |
| 1   | Y     | 282 | ASP  |
| 1   | Y     | 289 | MET  |
| 1   | Y     | 290 | LEU  |
| 1   | Y     | 292 | THR  |
| 1   | Y     | 293 | LEU  |
| 1   | Y     | 295 | VAL  |
| 1   | Y     | 299 | LEU  |
| 1   | Y     | 302 | ARG  |
| 1   | Y     | 305 | THR  |
| 1   | Y     | 307 | ARG  |
| 1   | Y     | 317 | LYS  |
| 1   | Z     | 58  | SER  |
| 1   | Z     | 68  | ASN  |
| 1   | Z     | 76  | GLN  |
| 1   | Z     | 96  | SER  |
| 1   | Z     | 98  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z     | 107 | MET  |
| 1   | Z     | 121 | GLN  |
| 1   | Z     | 122 | THR  |
| 1   | Z     | 129 | MET  |
| 1   | Z     | 134 | LYS  |
| 1   | Z     | 143 | MET  |
| 1   | Z     | 148 | GLN  |
| 1   | Z     | 150 | ILE  |
| 1   | Z     | 153 | ASP  |
| 1   | Z     | 158 | VAL  |
| 1   | Z     | 202 | ARG  |
| 1   | Z     | 203 | THR  |
| 1   | Z     | 211 | LYS  |
| 1   | Z     | 216 | VAL  |
| 1   | Z     | 227 | SER  |
| 1   | Z     | 275 | VAL  |
| 1   | Z     | 282 | ASP  |
| 1   | Z     | 290 | LEU  |
| 1   | Z     | 293 | LEU  |
| 1   | Z     | 302 | ARG  |
| 1   | Z     | 305 | THR  |
| 1   | Z     | 317 | LYS  |
| 1   | a     | 58  | SER  |
| 1   | a     | 61  | ILE  |
| 1   | a     | 66  | THR  |
| 1   | a     | 85  | VAL  |
| 1   | a     | 96  | SER  |
| 1   | a     | 98  | MET  |
| 1   | a     | 107 | MET  |
| 1   | a     | 121 | GLN  |
| 1   | a     | 122 | THR  |
| 1   | a     | 134 | LYS  |
| 1   | a     | 148 | GLN  |
| 1   | a     | 155 | THR  |
| 1   | a     | 158 | VAL  |
| 1   | a     | 202 | ARG  |
| 1   | a     | 206 | MET  |
| 1   | a     | 210 | VAL  |
| 1   | a     | 227 | SER  |
| 1   | a     | 272 | LEU  |
| 1   | a     | 282 | ASP  |
| 1   | a     | 290 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 293 | LEU  |
| 1   | a     | 299 | LEU  |
| 1   | a     | 302 | ARG  |
| 1   | a     | 305 | THR  |
| 1   | a     | 316 | VAL  |
| 1   | b     | 61  | ILE  |
| 1   | b     | 68  | ASN  |
| 1   | b     | 69  | MET  |
| 1   | b     | 96  | SER  |
| 1   | b     | 98  | MET  |
| 1   | b     | 107 | MET  |
| 1   | b     | 117 | GLU  |
| 1   | b     | 121 | GLN  |
| 1   | b     | 122 | THR  |
| 1   | b     | 133 | SER  |
| 1   | b     | 134 | LYS  |
| 1   | b     | 144 | ILE  |
| 1   | b     | 148 | GLN  |
| 1   | b     | 155 | THR  |
| 1   | b     | 205 | GLN  |
| 1   | b     | 215 | GLU  |
| 1   | b     | 224 | ARG  |
| 1   | b     | 227 | SER  |
| 1   | b     | 282 | ASP  |
| 1   | b     | 290 | LEU  |
| 1   | b     | 293 | LEU  |
| 1   | b     | 299 | LEU  |
| 1   | b     | 302 | ARG  |
| 1   | b     | 305 | THR  |
| 1   | b     | 311 | THR  |
| 1   | c     | 55  | GLU  |
| 1   | c     | 59  | THR  |
| 1   | c     | 96  | SER  |
| 1   | c     | 98  | MET  |
| 1   | c     | 121 | GLN  |
| 1   | c     | 122 | THR  |
| 1   | c     | 148 | GLN  |
| 1   | c     | 155 | THR  |
| 1   | c     | 156 | ARG  |
| 1   | c     | 158 | VAL  |
| 1   | c     | 165 | ILE  |
| 1   | c     | 202 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | c     | 205 | GLN  |
| 1   | c     | 211 | LYS  |
| 1   | c     | 225 | MET  |
| 1   | c     | 227 | SER  |
| 1   | c     | 282 | ASP  |
| 1   | c     | 290 | LEU  |
| 1   | c     | 293 | LEU  |
| 1   | c     | 299 | LEU  |
| 1   | c     | 302 | ARG  |
| 1   | c     | 305 | THR  |
| 1   | c     | 317 | LYS  |
| 1   | d     | 59  | THR  |
| 1   | d     | 61  | ILE  |
| 1   | d     | 66  | THR  |
| 1   | d     | 68  | ASN  |
| 1   | d     | 76  | GLN  |
| 1   | d     | 85  | VAL  |
| 1   | d     | 96  | SER  |
| 1   | d     | 121 | GLN  |
| 1   | d     | 134 | LYS  |
| 1   | d     | 148 | GLN  |
| 1   | d     | 158 | VAL  |
| 1   | d     | 196 | LYS  |
| 1   | d     | 215 | GLU  |
| 1   | d     | 216 | VAL  |
| 1   | d     | 218 | LYS  |
| 1   | d     | 227 | SER  |
| 1   | d     | 230 | GLN  |
| 1   | d     | 266 | GLN  |
| 1   | d     | 290 | LEU  |
| 1   | d     | 293 | LEU  |
| 1   | d     | 305 | THR  |
| 1   | e     | 55  | GLU  |
| 1   | e     | 59  | THR  |
| 1   | e     | 67  | VAL  |
| 1   | e     | 85  | VAL  |
| 1   | e     | 96  | SER  |
| 1   | e     | 97  | VAL  |
| 1   | e     | 98  | MET  |
| 1   | e     | 121 | GLN  |
| 1   | e     | 122 | THR  |
| 1   | e     | 130 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 144 | ILE  |
| 1   | e     | 148 | GLN  |
| 1   | e     | 150 | ILE  |
| 1   | e     | 155 | THR  |
| 1   | e     | 158 | VAL  |
| 1   | e     | 202 | ARG  |
| 1   | e     | 211 | LYS  |
| 1   | e     | 216 | VAL  |
| 1   | e     | 220 | ILE  |
| 1   | e     | 227 | SER  |
| 1   | e     | 228 | ILE  |
| 1   | e     | 268 | ARG  |
| 1   | e     | 275 | VAL  |
| 1   | e     | 282 | ASP  |
| 1   | e     | 290 | LEU  |
| 1   | e     | 293 | LEU  |
| 1   | e     | 295 | VAL  |
| 1   | e     | 298 | THR  |
| 1   | e     | 299 | LEU  |
| 1   | e     | 302 | ARG  |
| 1   | e     | 307 | ARG  |
| 1   | f     | 62  | THR  |
| 1   | f     | 68  | ASN  |
| 1   | f     | 85  | VAL  |
| 1   | f     | 96  | SER  |
| 1   | f     | 98  | MET  |
| 1   | f     | 106 | VAL  |
| 1   | f     | 121 | GLN  |
| 1   | f     | 122 | THR  |
| 1   | f     | 130 | VAL  |
| 1   | f     | 134 | LYS  |
| 1   | f     | 144 | ILE  |
| 1   | f     | 148 | GLN  |
| 1   | f     | 155 | THR  |
| 1   | f     | 158 | VAL  |
| 1   | f     | 202 | ARG  |
| 1   | f     | 205 | GLN  |
| 1   | f     | 220 | ILE  |
| 1   | f     | 225 | MET  |
| 1   | f     | 227 | SER  |
| 1   | f     | 290 | LEU  |
| 1   | f     | 293 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | f     | 299 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (318) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 76  | GLN  |
| 1   | A     | 78  | GLN  |
| 1   | A     | 82  | ASN  |
| 1   | A     | 148 | GLN  |
| 1   | A     | 185 | GLN  |
| 1   | A     | 190 | HIS  |
| 1   | A     | 192 | ASN  |
| 1   | A     | 266 | GLN  |
| 1   | A     | 291 | ASN  |
| 1   | A     | 294 | ASN  |
| 1   | B     | 68  | ASN  |
| 1   | B     | 121 | GLN  |
| 1   | B     | 146 | ASN  |
| 1   | B     | 174 | ASN  |
| 1   | B     | 178 | GLN  |
| 1   | B     | 192 | ASN  |
| 1   | B     | 205 | GLN  |
| 1   | B     | 213 | GLN  |
| 1   | B     | 286 | ASN  |
| 1   | B     | 291 | ASN  |
| 1   | B     | 294 | ASN  |
| 1   | C     | 68  | ASN  |
| 1   | C     | 76  | GLN  |
| 1   | C     | 82  | ASN  |
| 1   | C     | 132 | ASN  |
| 1   | C     | 145 | ASN  |
| 1   | C     | 146 | ASN  |
| 1   | C     | 148 | GLN  |
| 1   | C     | 192 | ASN  |
| 1   | C     | 273 | GLN  |
| 1   | C     | 286 | ASN  |
| 1   | C     | 294 | ASN  |
| 1   | D     | 68  | ASN  |
| 1   | D     | 82  | ASN  |
| 1   | D     | 146 | ASN  |
| 1   | D     | 174 | ASN  |
| 1   | D     | 192 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 205 | GLN  |
| 1   | D     | 213 | GLN  |
| 1   | D     | 226 | ASN  |
| 1   | D     | 271 | ASN  |
| 1   | D     | 294 | ASN  |
| 1   | D     | 304 | GLN  |
| 1   | E     | 76  | GLN  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 127 | GLN  |
| 1   | E     | 132 | ASN  |
| 1   | E     | 146 | ASN  |
| 1   | E     | 185 | GLN  |
| 1   | E     | 192 | ASN  |
| 1   | E     | 213 | GLN  |
| 1   | E     | 291 | ASN  |
| 1   | E     | 294 | ASN  |
| 1   | F     | 78  | GLN  |
| 1   | F     | 146 | ASN  |
| 1   | F     | 174 | ASN  |
| 1   | F     | 185 | GLN  |
| 1   | F     | 192 | ASN  |
| 1   | F     | 213 | GLN  |
| 1   | F     | 266 | GLN  |
| 1   | F     | 291 | ASN  |
| 1   | G     | 82  | ASN  |
| 1   | G     | 121 | GLN  |
| 1   | G     | 127 | GLN  |
| 1   | G     | 145 | ASN  |
| 1   | G     | 146 | ASN  |
| 1   | G     | 148 | GLN  |
| 1   | G     | 174 | ASN  |
| 1   | G     | 192 | ASN  |
| 1   | G     | 209 | GLN  |
| 1   | G     | 213 | GLN  |
| 1   | G     | 273 | GLN  |
| 1   | H     | 82  | ASN  |
| 1   | H     | 146 | ASN  |
| 1   | H     | 148 | GLN  |
| 1   | H     | 190 | HIS  |
| 1   | H     | 192 | ASN  |
| 1   | H     | 213 | GLN  |
| 1   | H     | 273 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 291 | ASN  |
| 1   | H     | 294 | ASN  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 146 | ASN  |
| 1   | I     | 148 | GLN  |
| 1   | I     | 159 | ASN  |
| 1   | I     | 174 | ASN  |
| 1   | I     | 185 | GLN  |
| 1   | I     | 192 | ASN  |
| 1   | I     | 213 | GLN  |
| 1   | I     | 291 | ASN  |
| 1   | I     | 294 | ASN  |
| 1   | J     | 68  | ASN  |
| 1   | J     | 76  | GLN  |
| 1   | J     | 78  | GLN  |
| 1   | J     | 127 | GLN  |
| 1   | J     | 146 | ASN  |
| 1   | J     | 148 | GLN  |
| 1   | J     | 213 | GLN  |
| 1   | J     | 291 | ASN  |
| 1   | J     | 294 | ASN  |
| 1   | K     | 82  | ASN  |
| 1   | K     | 127 | GLN  |
| 1   | K     | 132 | ASN  |
| 1   | K     | 145 | ASN  |
| 1   | K     | 146 | ASN  |
| 1   | K     | 148 | GLN  |
| 1   | K     | 192 | ASN  |
| 1   | K     | 213 | GLN  |
| 1   | K     | 266 | GLN  |
| 1   | K     | 271 | ASN  |
| 1   | K     | 294 | ASN  |
| 1   | L     | 82  | ASN  |
| 1   | L     | 127 | GLN  |
| 1   | L     | 146 | ASN  |
| 1   | L     | 148 | GLN  |
| 1   | L     | 192 | ASN  |
| 1   | L     | 213 | GLN  |
| 1   | L     | 266 | GLN  |
| 1   | L     | 291 | ASN  |
| 1   | L     | 294 | ASN  |
| 1   | L     | 304 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 76  | GLN  |
| 1   | M     | 82  | ASN  |
| 1   | M     | 127 | GLN  |
| 1   | M     | 132 | ASN  |
| 1   | M     | 146 | ASN  |
| 1   | M     | 148 | GLN  |
| 1   | M     | 159 | ASN  |
| 1   | M     | 192 | ASN  |
| 1   | M     | 291 | ASN  |
| 1   | M     | 294 | ASN  |
| 1   | N     | 82  | ASN  |
| 1   | N     | 127 | GLN  |
| 1   | N     | 146 | ASN  |
| 1   | N     | 148 | GLN  |
| 1   | N     | 178 | GLN  |
| 1   | N     | 192 | ASN  |
| 1   | N     | 213 | GLN  |
| 1   | N     | 273 | GLN  |
| 1   | N     | 291 | ASN  |
| 1   | N     | 294 | ASN  |
| 1   | O     | 76  | GLN  |
| 1   | O     | 82  | ASN  |
| 1   | O     | 121 | GLN  |
| 1   | O     | 127 | GLN  |
| 1   | O     | 146 | ASN  |
| 1   | O     | 148 | GLN  |
| 1   | O     | 192 | ASN  |
| 1   | O     | 291 | ASN  |
| 1   | O     | 294 | ASN  |
| 1   | P     | 82  | ASN  |
| 1   | P     | 145 | ASN  |
| 1   | P     | 146 | ASN  |
| 1   | P     | 192 | ASN  |
| 1   | P     | 205 | GLN  |
| 1   | P     | 213 | GLN  |
| 1   | P     | 273 | GLN  |
| 1   | P     | 291 | ASN  |
| 1   | P     | 294 | ASN  |
| 1   | Q     | 82  | ASN  |
| 1   | Q     | 146 | ASN  |
| 1   | Q     | 148 | GLN  |
| 1   | Q     | 185 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 192 | ASN  |
| 1   | Q     | 213 | GLN  |
| 1   | Q     | 273 | GLN  |
| 1   | Q     | 291 | ASN  |
| 1   | Q     | 294 | ASN  |
| 1   | R     | 82  | ASN  |
| 1   | R     | 127 | GLN  |
| 1   | R     | 145 | ASN  |
| 1   | R     | 146 | ASN  |
| 1   | R     | 148 | GLN  |
| 1   | R     | 178 | GLN  |
| 1   | R     | 192 | ASN  |
| 1   | R     | 205 | GLN  |
| 1   | R     | 213 | GLN  |
| 1   | R     | 226 | ASN  |
| 1   | R     | 294 | ASN  |
| 1   | R     | 304 | GLN  |
| 1   | S     | 68  | ASN  |
| 1   | S     | 78  | GLN  |
| 1   | S     | 82  | ASN  |
| 1   | S     | 146 | ASN  |
| 1   | S     | 148 | GLN  |
| 1   | S     | 174 | ASN  |
| 1   | S     | 178 | GLN  |
| 1   | S     | 192 | ASN  |
| 1   | S     | 286 | ASN  |
| 1   | S     | 294 | ASN  |
| 1   | T     | 82  | ASN  |
| 1   | T     | 127 | GLN  |
| 1   | T     | 146 | ASN  |
| 1   | T     | 148 | GLN  |
| 1   | T     | 205 | GLN  |
| 1   | T     | 266 | GLN  |
| 1   | T     | 271 | ASN  |
| 1   | T     | 291 | ASN  |
| 1   | T     | 294 | ASN  |
| 1   | U     | 76  | GLN  |
| 1   | U     | 82  | ASN  |
| 1   | U     | 127 | GLN  |
| 1   | U     | 132 | ASN  |
| 1   | U     | 145 | ASN  |
| 1   | U     | 146 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 148 | GLN  |
| 1   | U     | 192 | ASN  |
| 1   | U     | 213 | GLN  |
| 1   | U     | 286 | ASN  |
| 1   | U     | 291 | ASN  |
| 1   | U     | 294 | ASN  |
| 1   | V     | 78  | GLN  |
| 1   | V     | 82  | ASN  |
| 1   | V     | 146 | ASN  |
| 1   | V     | 174 | ASN  |
| 1   | V     | 190 | HIS  |
| 1   | V     | 192 | ASN  |
| 1   | V     | 213 | GLN  |
| 1   | V     | 266 | GLN  |
| 1   | V     | 271 | ASN  |
| 1   | V     | 286 | ASN  |
| 1   | V     | 291 | ASN  |
| 1   | V     | 294 | ASN  |
| 1   | W     | 76  | GLN  |
| 1   | W     | 82  | ASN  |
| 1   | W     | 127 | GLN  |
| 1   | W     | 145 | ASN  |
| 1   | W     | 146 | ASN  |
| 1   | W     | 148 | GLN  |
| 1   | W     | 192 | ASN  |
| 1   | W     | 271 | ASN  |
| 1   | W     | 294 | ASN  |
| 1   | X     | 145 | ASN  |
| 1   | X     | 146 | ASN  |
| 1   | X     | 148 | GLN  |
| 1   | X     | 178 | GLN  |
| 1   | X     | 192 | ASN  |
| 1   | X     | 205 | GLN  |
| 1   | X     | 213 | GLN  |
| 1   | X     | 273 | GLN  |
| 1   | X     | 291 | ASN  |
| 1   | X     | 294 | ASN  |
| 1   | Y     | 76  | GLN  |
| 1   | Y     | 82  | ASN  |
| 1   | Y     | 127 | GLN  |
| 1   | Y     | 146 | ASN  |
| 1   | Y     | 148 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 178 | GLN  |
| 1   | Y     | 185 | GLN  |
| 1   | Y     | 192 | ASN  |
| 1   | Y     | 266 | GLN  |
| 1   | Y     | 294 | ASN  |
| 1   | Z     | 82  | ASN  |
| 1   | Z     | 146 | ASN  |
| 1   | Z     | 178 | GLN  |
| 1   | Z     | 192 | ASN  |
| 1   | Z     | 205 | GLN  |
| 1   | Z     | 271 | ASN  |
| 1   | Z     | 286 | ASN  |
| 1   | Z     | 291 | ASN  |
| 1   | Z     | 294 | ASN  |
| 1   | a     | 76  | GLN  |
| 1   | a     | 82  | ASN  |
| 1   | a     | 121 | GLN  |
| 1   | a     | 132 | ASN  |
| 1   | a     | 145 | ASN  |
| 1   | a     | 146 | ASN  |
| 1   | a     | 148 | GLN  |
| 1   | a     | 192 | ASN  |
| 1   | a     | 213 | GLN  |
| 1   | a     | 266 | GLN  |
| 1   | a     | 294 | ASN  |
| 1   | b     | 82  | ASN  |
| 1   | b     | 121 | GLN  |
| 1   | b     | 127 | GLN  |
| 1   | b     | 145 | ASN  |
| 1   | b     | 146 | ASN  |
| 1   | b     | 148 | GLN  |
| 1   | b     | 185 | GLN  |
| 1   | b     | 192 | ASN  |
| 1   | b     | 230 | GLN  |
| 1   | b     | 294 | ASN  |
| 1   | c     | 76  | GLN  |
| 1   | c     | 82  | ASN  |
| 1   | c     | 108 | GLN  |
| 1   | c     | 127 | GLN  |
| 1   | c     | 132 | ASN  |
| 1   | c     | 146 | ASN  |
| 1   | c     | 148 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | c     | 174 | ASN  |
| 1   | c     | 192 | ASN  |
| 1   | c     | 291 | ASN  |
| 1   | c     | 294 | ASN  |
| 1   | d     | 78  | GLN  |
| 1   | d     | 145 | ASN  |
| 1   | d     | 146 | ASN  |
| 1   | d     | 148 | GLN  |
| 1   | d     | 159 | ASN  |
| 1   | d     | 190 | HIS  |
| 1   | d     | 213 | GLN  |
| 1   | d     | 291 | ASN  |
| 1   | d     | 294 | ASN  |
| 1   | e     | 82  | ASN  |
| 1   | e     | 146 | ASN  |
| 1   | e     | 286 | ASN  |
| 1   | e     | 291 | ASN  |
| 1   | e     | 294 | ASN  |
| 1   | f     | 82  | ASN  |
| 1   | f     | 127 | GLN  |
| 1   | f     | 146 | ASN  |
| 1   | f     | 148 | GLN  |
| 1   | f     | 205 | GLN  |
| 1   | f     | 213 | GLN  |
| 1   | f     | 226 | ASN  |
| 1   | f     | 230 | GLN  |
| 1   | f     | 271 | ASN  |
| 1   | f     | 291 | ASN  |
| 1   | f     | 294 | ASN  |

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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     | 221/356 (62%) | -0.80  | 0 100 100    | 232, 286, 334, 403    | 0     |
| 1   | B     | 221/356 (62%) | -0.65  | 1 (0%) 87 77 | 200, 271, 345, 382    | 0     |
| 1   | C     | 221/356 (62%) | -0.66  | 0 100 100    | 248, 300, 381, 438    | 0     |
| 1   | D     | 221/356 (62%) | -0.75  | 0 100 100    | 223, 281, 331, 361    | 0     |
| 1   | E     | 221/356 (62%) | -0.28  | 2 (0%) 81 70 | 255, 337, 447, 534    | 0     |
| 1   | F     | 221/356 (62%) | -0.57  | 1 (0%) 87 77 | 208, 275, 322, 362    | 0     |
| 1   | G     | 221/356 (62%) | -0.52  | 4 (1%) 67 57 | 229, 279, 337, 357    | 0     |
| 1   | H     | 221/356 (62%) | -0.71  | 1 (0%) 87 77 | 228, 263, 309, 327    | 0     |
| 1   | I     | 221/356 (62%) | -0.53  | 1 (0%) 87 77 | 245, 316, 404, 442    | 0     |
| 1   | J     | 221/356 (62%) | -0.67  | 2 (0%) 81 70 | 244, 286, 351, 372    | 0     |
| 1   | K     | 221/356 (62%) | -0.73  | 3 (1%) 73 62 | 249, 287, 346, 389    | 0     |
| 1   | L     | 221/356 (62%) | -0.64  | 0 100 100    | 223, 284, 405, 432    | 0     |
| 1   | M     | 221/356 (62%) | -0.68  | 1 (0%) 87 77 | 205, 265, 333, 351    | 0     |
| 1   | N     | 221/356 (62%) | -0.50  | 5 (2%) 61 52 | 206, 290, 338, 361    | 0     |
| 1   | O     | 221/356 (62%) | -0.62  | 0 100 100    | 214, 267, 337, 376    | 0     |
| 1   | P     | 221/356 (62%) | -0.66  | 0 100 100    | 245, 283, 320, 341    | 0     |
| 1   | Q     | 221/356 (62%) | -0.63  | 1 (0%) 87 77 | 204, 276, 333, 350    | 0     |
| 1   | R     | 221/356 (62%) | -0.43  | 5 (2%) 61 52 | 229, 322, 389, 429    | 0     |
| 1   | S     | 221/356 (62%) | -0.67  | 2 (0%) 81 70 | 236, 300, 344, 456    | 0     |
| 1   | T     | 221/356 (62%) | -0.38  | 2 (0%) 81 70 | 205, 313, 404, 456    | 0     |
| 1   | U     | 221/356 (62%) | -0.65  | 2 (0%) 81 70 | 199, 286, 401, 509    | 0     |
| 1   | V     | 221/356 (62%) | -0.73  | 0 100 100    | 237, 309, 351, 378    | 0     |
| 1   | W     | 221/356 (62%) | -0.65  | 0 100 100    | 211, 301, 375, 398    | 0     |
| 1   | X     | 221/356 (62%) | -0.54  | 3 (1%) 73 62 | 240, 303, 398, 414    | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | Y     | 221/356 (62%)    | -0.50  | 1 (0%) 87 77  | 236, 326, 449, 465    | 0     |
| 1   | Z     | 221/356 (62%)    | -0.69  | 0 100 100     | 228, 310, 395, 408    | 0     |
| 1   | a     | 221/356 (62%)    | -0.58  | 0 100 100     | 231, 299, 363, 391    | 0     |
| 1   | b     | 221/356 (62%)    | -0.41  | 0 100 100     | 256, 348, 475, 550    | 0     |
| 1   | c     | 221/356 (62%)    | -0.56  | 2 (0%) 81 70  | 256, 314, 369, 399    | 0     |
| 1   | d     | 221/356 (62%)    | -0.72  | 1 (0%) 87 77  | 235, 284, 331, 372    | 0     |
| 1   | e     | 221/356 (62%)    | -0.65  | 0 100 100     | 237, 321, 358, 384    | 0     |
| 1   | f     | 221/356 (62%)    | -0.64  | 0 100 100     | 214, 289, 334, 393    | 0     |
| All | All   | 7072/11392 (62%) | -0.61  | 40 (0%) 85 75 | 199, 295, 383, 550    | 0     |

All (40) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | c     | 266 | GLN  | 4.5  |
| 1   | E     | 270 | GLU  | 4.3  |
| 1   | K     | 275 | VAL  | 3.5  |
| 1   | F     | 229 | GLU  | 3.1  |
| 1   | d     | 229 | GLU  | 3.0  |
| 1   | J     | 226 | ASN  | 3.0  |
| 1   | R     | 267 | ALA  | 2.8  |
| 1   | c     | 267 | ALA  | 2.8  |
| 1   | Y     | 277 | PRO  | 2.8  |
| 1   | R     | 298 | THR  | 2.8  |
| 1   | G     | 291 | ASN  | 2.7  |
| 1   | M     | 317 | LYS  | 2.7  |
| 1   | U     | 268 | ARG  | 2.7  |
| 1   | R     | 302 | ARG  | 2.6  |
| 1   | K     | 274 | ALA  | 2.6  |
| 1   | U     | 271 | ASN  | 2.6  |
| 1   | S     | 296 | GLY  | 2.6  |
| 1   | N     | 270 | GLU  | 2.6  |
| 1   | Q     | 298 | THR  | 2.6  |
| 1   | E     | 314 | GLU  | 2.6  |
| 1   | T     | 267 | ALA  | 2.5  |
| 1   | X     | 306 | TYR  | 2.5  |
| 1   | X     | 305 | THR  | 2.5  |
| 1   | N     | 267 | ALA  | 2.5  |
| 1   | B     | 223 | ARG  | 2.4  |
| 1   | T     | 302 | ARG  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | S     | 292 | THR  | 2.2  |
| 1   | X     | 84  | ASP  | 2.2  |
| 1   | R     | 269 | LEU  | 2.1  |
| 1   | I     | 270 | GLU  | 2.1  |
| 1   | G     | 162 | VAL  | 2.1  |
| 1   | N     | 196 | LYS  | 2.1  |
| 1   | N     | 295 | VAL  | 2.1  |
| 1   | G     | 155 | THR  | 2.1  |
| 1   | G     | 294 | ASN  | 2.1  |
| 1   | H     | 295 | VAL  | 2.1  |
| 1   | N     | 299 | LEU  | 2.0  |
| 1   | R     | 301 | PRO  | 2.0  |
| 1   | J     | 72  | GLY  | 2.0  |
| 1   | K     | 276 | GLY  | 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.