



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:32 am GMT

PDB ID : 2CB6  
Title : CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF THE MOSQUITOCIDAL TOXIN FROM BACILLUS SPHAERICUS, MUTANT E195Q  
Authors : Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.  
Deposited on : 2005-12-29  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.9-1692   |
| EDS                            | : | trunk28620   |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac                         | : | 5.8.0135   |
| CCP4                           | : | 6.5.0  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | recalc28949  |

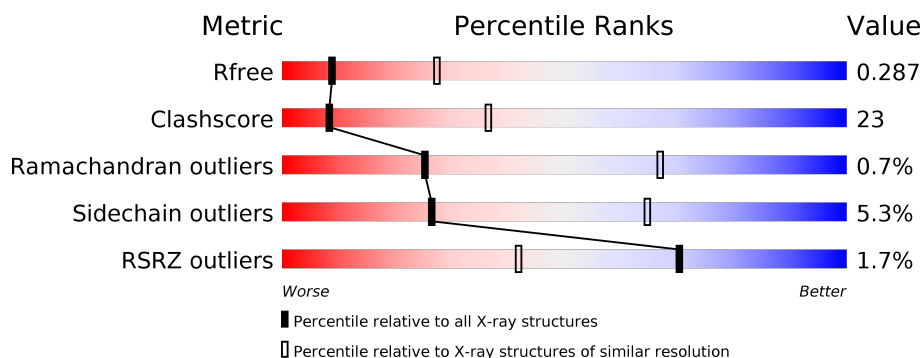
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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






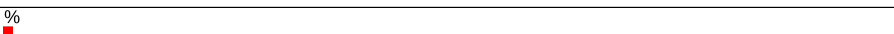
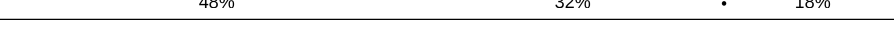




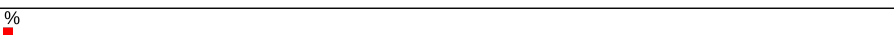
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1692 (3.00-3.00)                                      |
| Clashscore            | 112137                      | 2037 (3.00-3.00)                                      |
| Ramachandran outliers | 110173                      | 1973 (3.00-3.00)                                      |
| Sidechain outliers    | 110143                      | 1976 (3.00-3.00)                                      |
| RSRZ outliers         | 101464                      | 1716 (3.00-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 291    | <div> <div>%</div> <div> <div></div> <div>51%</div> <div>28%</div> <div>•</div> <div>18%</div> </div> </div>  |
| 1   | B     | 291    | <div> <div>3%</div> <div> <div></div> <div>46%</div> <div>33%</div> <div>•</div> <div>18%</div> </div> </div> |
| 1   | C     | 291    | <div> <div>%</div> <div> <div></div> <div>51%</div> <div>29%</div> <div>•</div> <div>16%</div> </div> </div>  |
| 1   | D     | 291    | <div> <div>%</div> <div> <div></div> <div>50%</div> <div>31%</div> <div>•</div> <div>16%</div> </div> </div>  |
| 1   | E     | 291    | <div> <div>%</div> <div> <div></div> <div>49%</div> <div>30%</div> <div>•</div> <div>18%</div> </div> </div>  |
| 1   | F     | 291    | <div> <div>3%</div> <div> <div></div> <div>46%</div> <div>32%</div> <div>•</div> <div>18%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 291    |  |
| 1   | H     | 291    |  |
| 1   | I     | 291    |  |
| 1   | J     | 291    |  |
| 1   | K     | 291    |  |
| 1   | L     | 291    |  |
| 1   | M     | 291    |  |
| 1   | N     | 291    |  |
| 1   | O     | 291    |  |
| 1   | P     | 291    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31202 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.

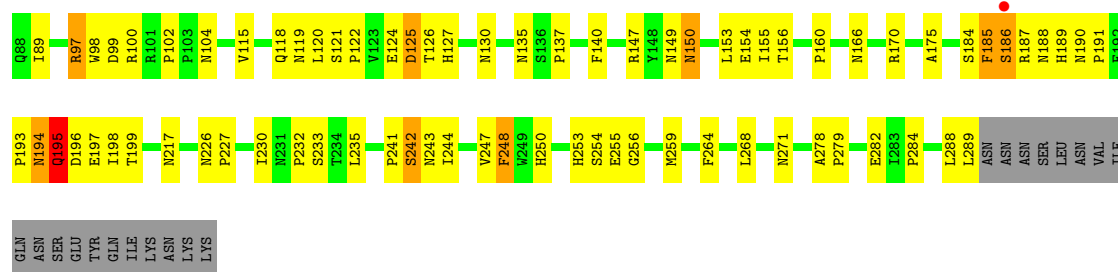
- Molecule 1 is a protein called MOSQUITOCIDAL TOXIN.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | B     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | C     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1986  | 1252 | 353 | 378 | 3 |         |         |       |
| 1   | D     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1986  | 1252 | 353 | 378 | 3 |         |         |       |
| 1   | E     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | F     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | G     | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1918  | 1210 | 338 | 367 | 3 |         |         |       |
| 1   | H     | 245      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1992  | 1255 | 354 | 380 | 3 |         |         |       |
| 1   | I     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | J     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | K     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1986  | 1252 | 353 | 378 | 3 |         |         |       |
| 1   | L     | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1918  | 1210 | 338 | 367 | 3 |         |         |       |
| 1   | M     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | N     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1223 | 346 | 367 | 3 |         |         |       |
| 1   | O     | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1918  | 1210 | 338 | 367 | 3 |         |         |       |
| 1   | P     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1986  | 1252 | 353 | 378 | 3 |         |         |       |

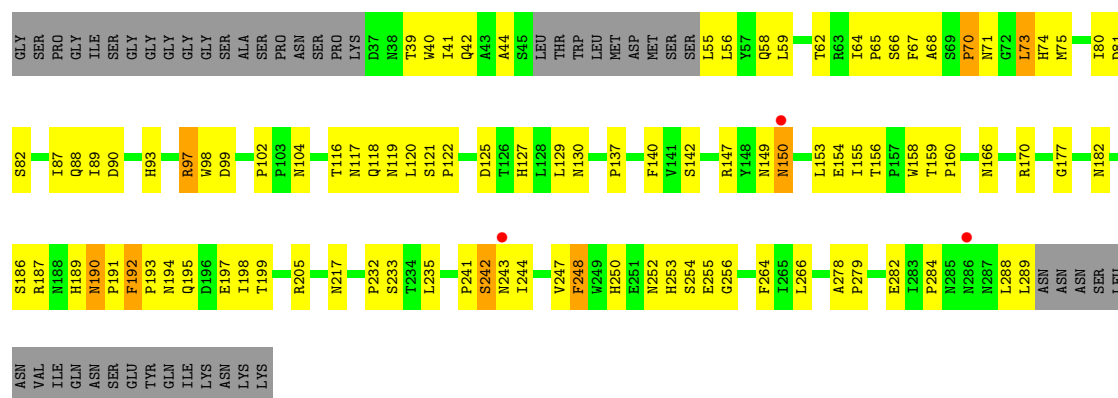
There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| B     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| C     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| D     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| E     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| F     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| G     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| H     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| I     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| J     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| K     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| L     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| M     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| N     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| O     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |
| P     | 195     | GLN      | GLU    | ENGINEERED MUTATION | UNP Q03988 |

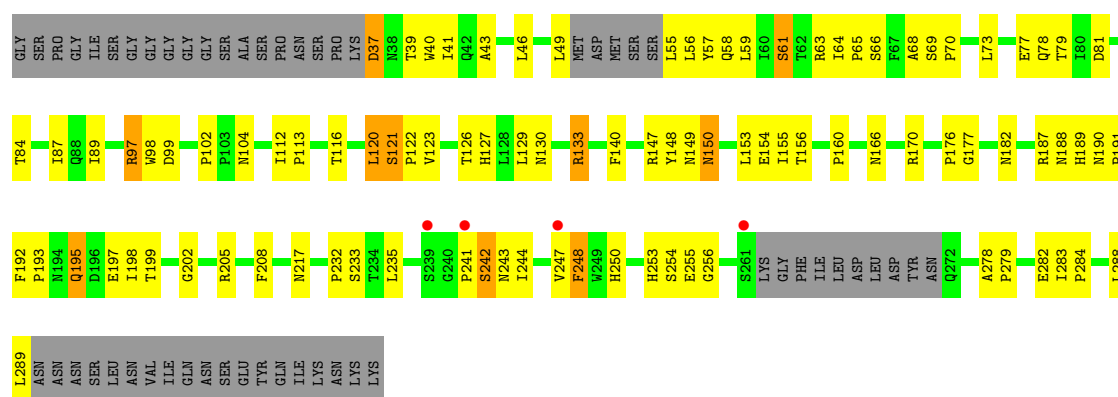




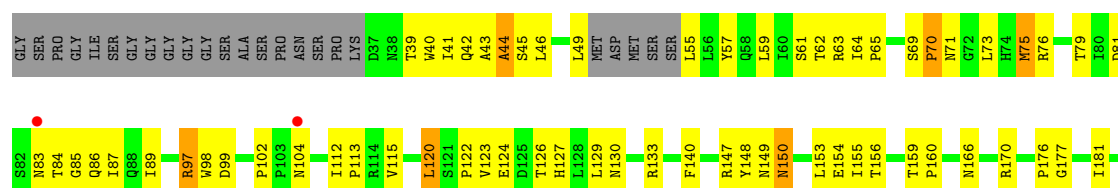
• Molecule 1: MOSQUITOCIDAL TOXIN

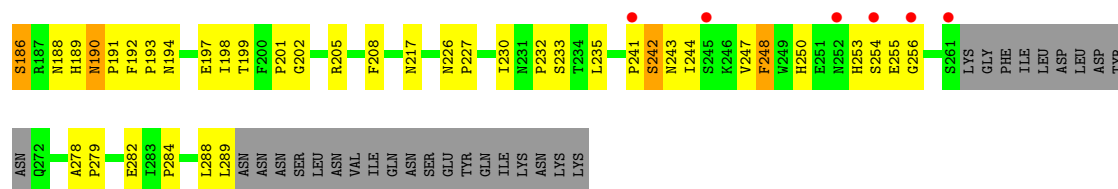


• Molecule 1: MOSQUITOCIDAL TOXIN

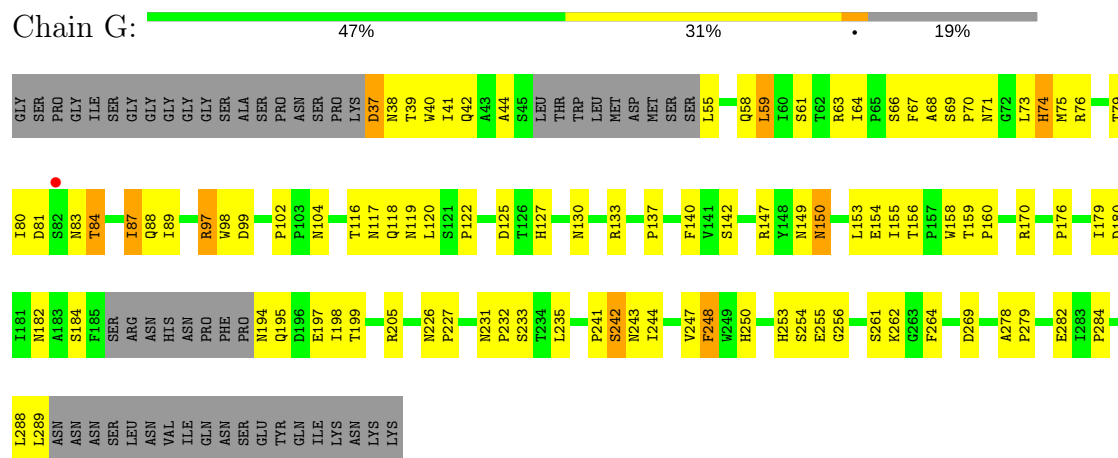


• Molecule 1: MOSQUITOCIDAL TOXIN

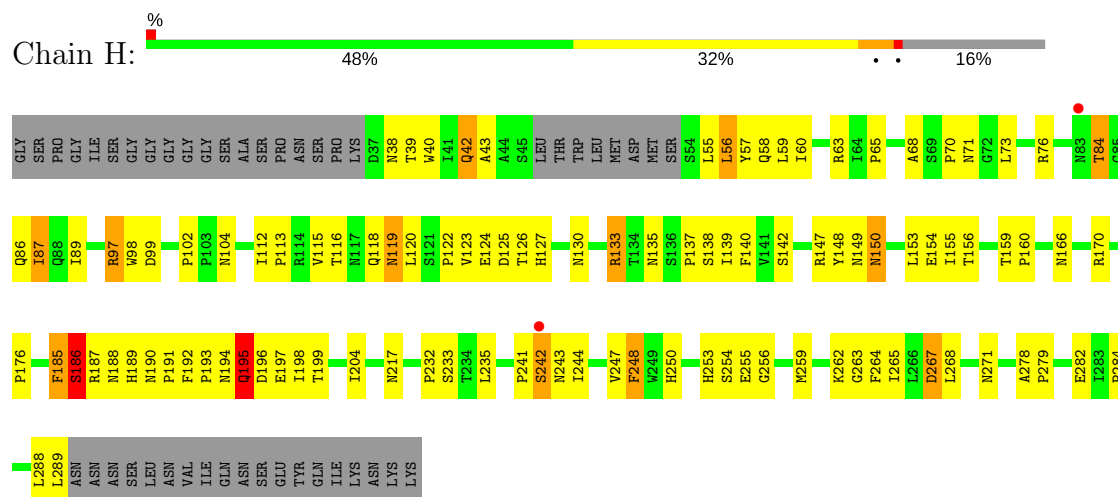




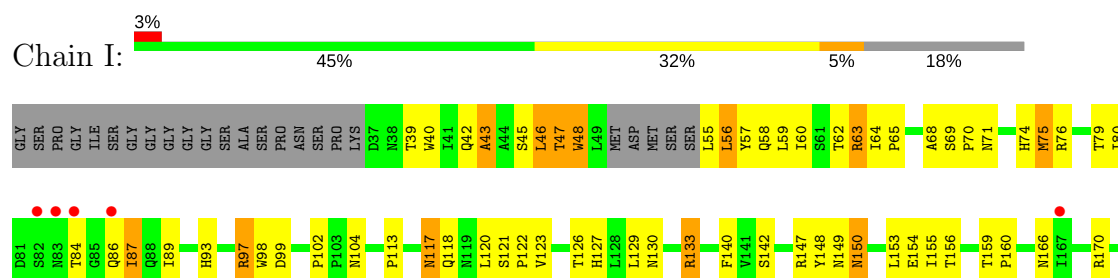
### • Molecule 1: MOSQUITOCIDAL TOXIN

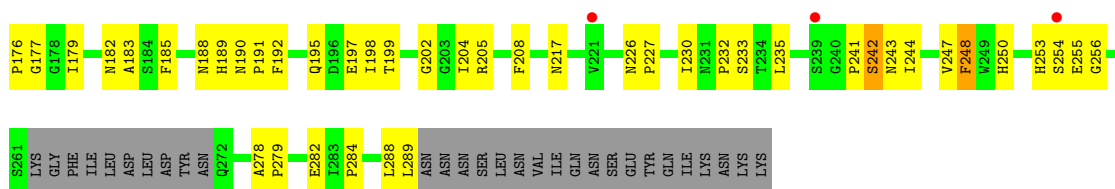


### • Molecule 1: MOSQUITOCIDAL TOXIN

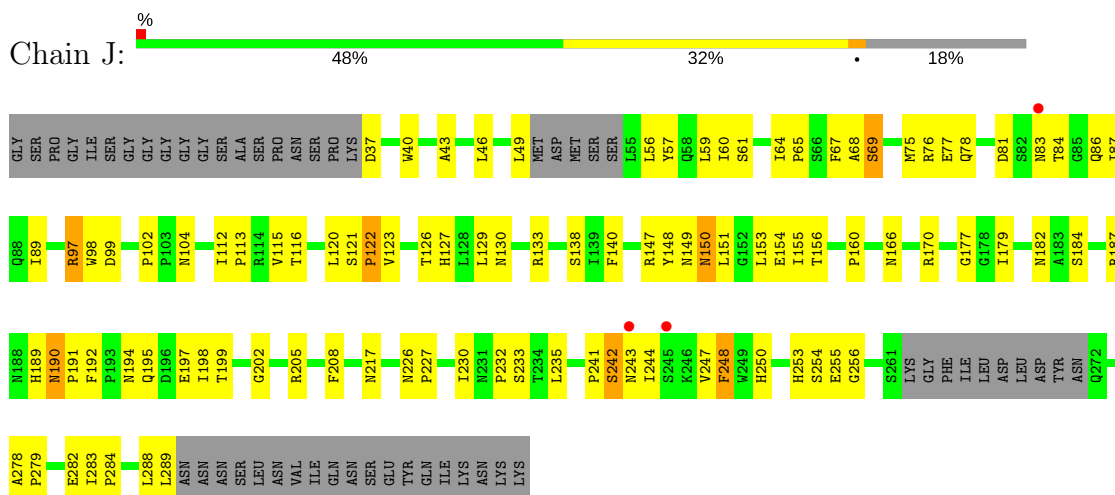


### • Molecule 1: MOSQUITOCIDAL TOXIN

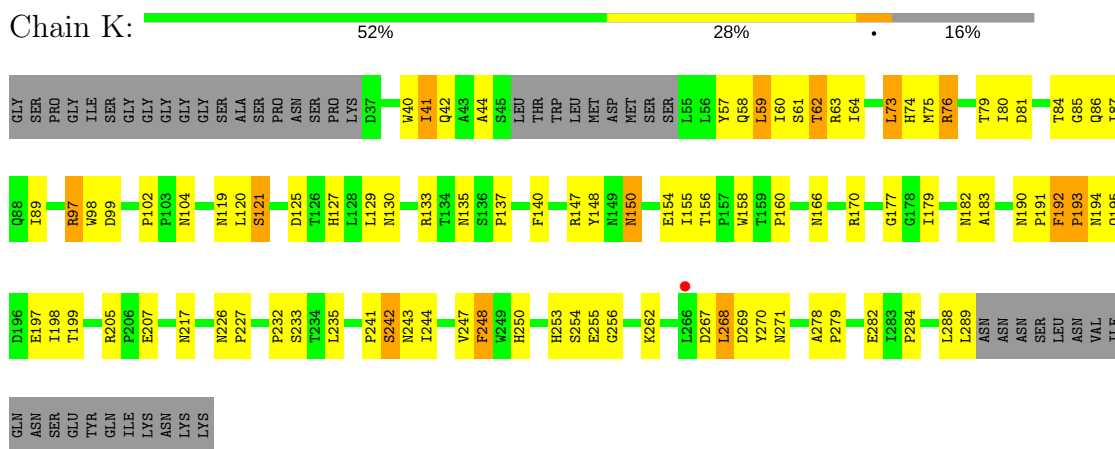




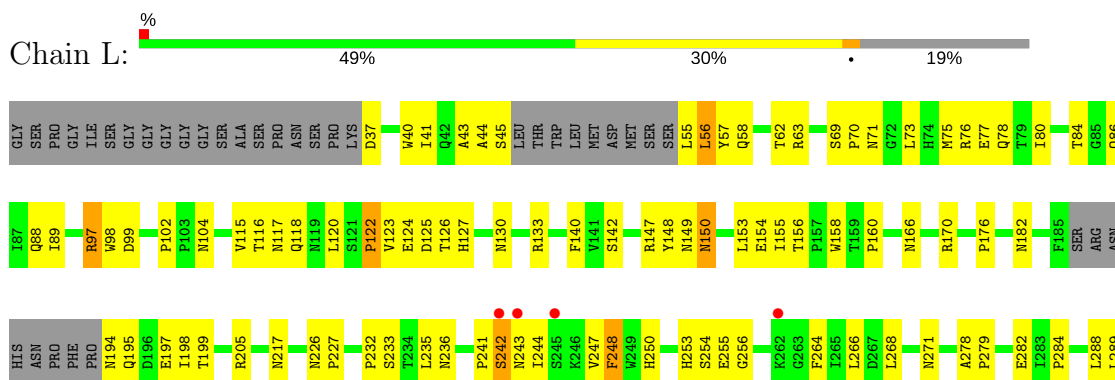
### • Molecule 1: MOSQUITOCIDAL TOXIN



### • Molecule 1: MOSQUITOCIDAL TOXIN

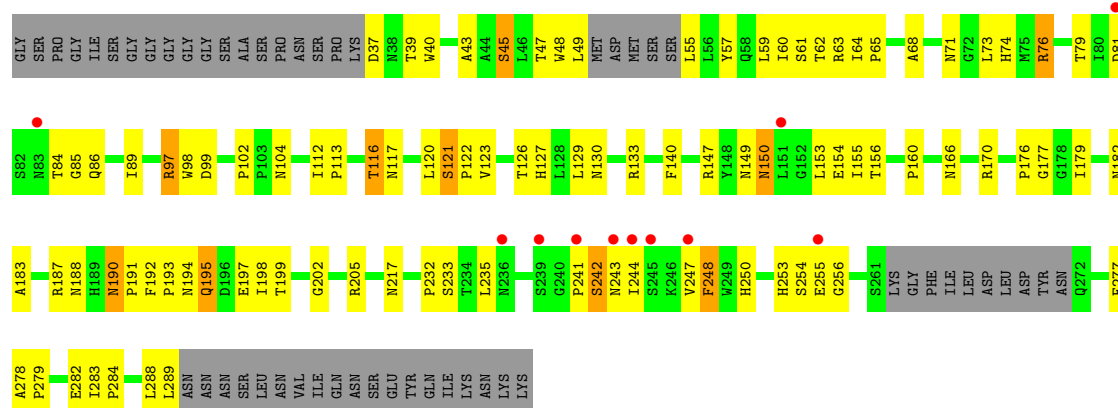


### • Molecule 1: MOSQUITOCIDAL TOXIN

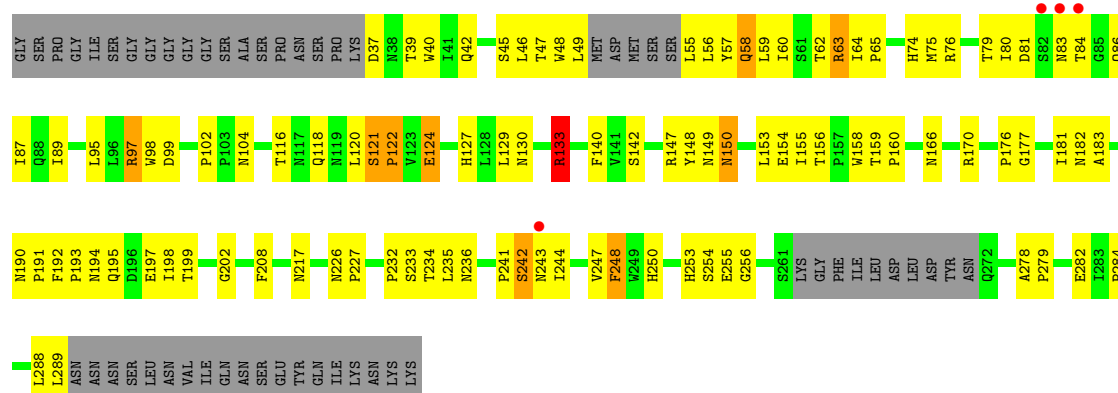


ASN  
ASN  
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SER  
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LEU  
ASN  
VAL  
ILE  
GLN  
ASN  
SER  
SER  
GLU  
TYR  
GLN  
ILE  
LYS  
ASN  
LYS  
LYS

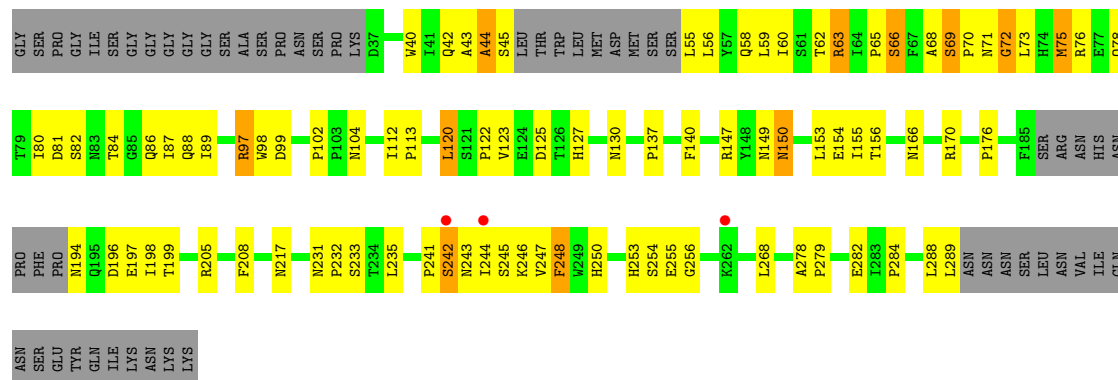
• Molecule 1: MOSQUITOCIDAL TOXIN



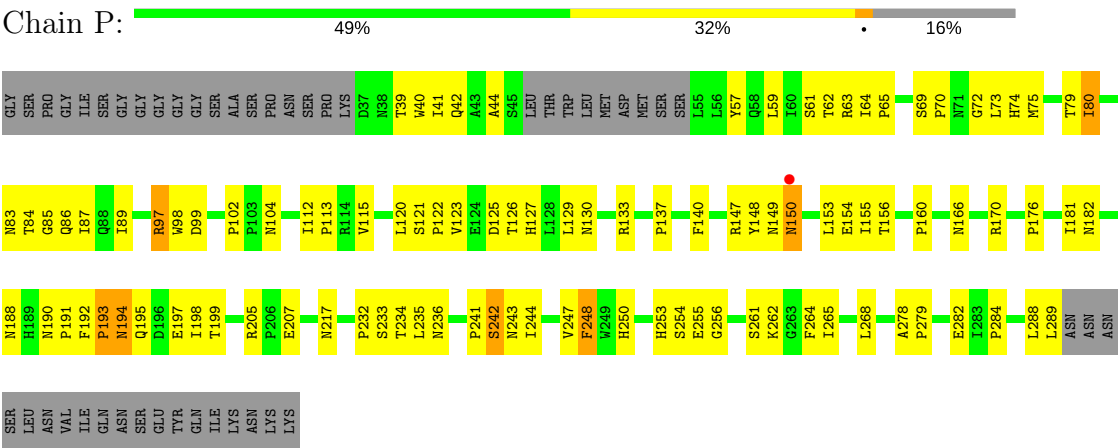
• Molecule 1: MOSQUITOCIDAL TOXIN



• Molecule 1: MOSQUITOCIDAL TOXIN



● Molecule 1: MOSQUITOCIDAL TOXIN



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 106.30Å 175.80Å 335.50Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 50.00 – 3.00<br>49.07 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (50.00-3.00)<br>99.6 (49.07-3.00)           | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.22 (at 3.01Å)   | Xtriage          |
| Refinement program  | TNT 5.6.1   | Depositor        |
| R, $R_{free}$   | 0.227 , 0.246<br>0.266 , 0.287                              | Depositor<br>DCC |
| $R_{free}$ test set   | 6300 reflections (5.00%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.0  | Xtriage          |
| Anisotropy  | 0.207   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 52.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.85  | EDS              |
| Total number of atoms   | 31202   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 39.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5553e-03.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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     | 0.48         | 0/1995  | 0.77        | 2/2726 (0.1%)   |
| 1   | B     | 0.46         | 0/1995  | 0.73        | 1/2726 (0.0%)   |
| 1   | C     | 0.49         | 0/2043  | 0.80        | 5/2790 (0.2%)   |
| 1   | D     | 0.49         | 0/2043  | 0.80        | 3/2790 (0.1%)   |
| 1   | E     | 0.47         | 0/1995  | 0.75        | 1/2726 (0.0%)   |
| 1   | F     | 0.45         | 0/1995  | 0.72        | 0/2726          |
| 1   | G     | 0.45         | 0/1970  | 0.73        | 0/2688          |
| 1   | H     | 0.48         | 0/2049  | 0.82        | 7/2798 (0.3%)   |
| 1   | I     | 0.46         | 0/1995  | 0.75        | 2/2726 (0.1%)   |
| 1   | J     | 0.46         | 0/1995  | 0.76        | 2/2726 (0.1%)   |
| 1   | K     | 0.46         | 0/2043  | 0.73        | 1/2790 (0.0%)   |
| 1   | L     | 0.48         | 0/1970  | 0.77        | 1/2688 (0.0%)   |
| 1   | M     | 0.44         | 0/1995  | 0.75        | 2/2726 (0.1%)   |
| 1   | N     | 0.48         | 0/1995  | 0.76        | 1/2726 (0.0%)   |
| 1   | O     | 0.49         | 0/1970  | 0.85        | 6/2688 (0.2%)   |
| 1   | P     | 0.48         | 0/2043  | 0.74        | 1/2790 (0.0%)   |
| All | All   | 0.47         | 0/32091 | 0.76        | 35/43830 (0.1%) |

There are no bond length outliers.

All (35) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | O     | 69  | SER  | C-N-CD  | -15.90 | 85.62       | 120.60   |
| 1   | H     | 195 | GLN  | CB-CA-C | -8.77  | 92.87       | 110.40   |
| 1   | D     | 190 | ASN  | C-N-CD  | -8.13  | 102.72      | 120.60   |
| 1   | H     | 186 | SER  | N-CA-CB | 7.42   | 121.63      | 110.50   |
| 1   | B     | 121 | SER  | C-N-CD  | -7.13  | 104.91      | 120.60   |
| 1   | J     | 121 | SER  | C-N-CD  | -6.95  | 105.31      | 120.60   |
| 1   | P     | 194 | ASN  | N-CA-C  | -6.72  | 92.86       | 111.00   |
| 1   | M     | 121 | SER  | C-N-CD  | -6.71  | 105.84      | 120.60   |
| 1   | C     | 195 | GLN  | CB-CA-C | -6.69  | 97.02       | 110.40   |
| 1   | C     | 69  | SER  | C-N-CD  | -6.59  | 106.10      | 120.60   |
| 1   | C     | 185 | PHE  | O-C-N   | -6.52  | 112.27      | 122.70   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 73  | LEU  | CB-CG-CD2 | -6.32 | 100.25      | 111.00   |
| 1   | C     | 185 | PHE  | C-N-CA    | -6.27 | 106.02      | 121.70   |
| 1   | E     | 121 | SER  | C-N-CD    | -5.99 | 107.41      | 120.60   |
| 1   | O     | 72  | GLY  | N-CA-C    | 5.97  | 128.03      | 113.10   |
| 1   | H     | 187 | ARG  | N-CA-C    | -5.89 | 95.09       | 111.00   |
| 1   | I     | 46  | LEU  | CA-CB-CG  | 5.83  | 128.72      | 115.30   |
| 1   | H     | 185 | PHE  | O-C-N     | -5.82 | 113.39      | 122.70   |
| 1   | A     | 121 | SER  | N-CA-C    | -5.80 | 95.34       | 111.00   |
| 1   | O     | 71  | ASN  | CA-C-N    | -5.78 | 104.64      | 116.20   |
| 1   | H     | 185 | PHE  | C-N-CA    | -5.76 | 107.30      | 121.70   |
| 1   | M     | 85  | GLY  | N-CA-C    | -5.75 | 98.73       | 113.10   |
| 1   | C     | 194 | ASN  | N-CA-C    | -5.63 | 95.81       | 111.00   |
| 1   | N     | 133 | ARG  | NE-CZ-NH2 | 5.60  | 123.10      | 120.30   |
| 1   | A     | 187 | ARG  | N-CA-C    | 5.56  | 126.00      | 111.00   |
| 1   | O     | 69  | SER  | N-CA-C    | -5.53 | 96.06       | 111.00   |
| 1   | J     | 187 | ARG  | N-CA-C    | 5.47  | 125.76      | 111.00   |
| 1   | O     | 71  | ASN  | C-N-CA    | 5.43  | 133.70      | 122.30   |
| 1   | O     | 73  | LEU  | N-CA-C    | -5.41 | 96.40       | 111.00   |
| 1   | D     | 55  | LEU  | CA-CB-CG  | 5.15  | 127.14      | 115.30   |
| 1   | K     | 121 | SER  | N-CA-C    | -5.12 | 97.19       | 111.00   |
| 1   | I     | 87  | ILE  | N-CA-C    | 5.08  | 124.72      | 111.00   |
| 1   | H     | 186 | SER  | CB-CA-C   | 5.08  | 119.75      | 110.10   |
| 1   | H     | 56  | LEU  | CA-CB-CG  | -5.07 | 103.63      | 115.30   |
| 1   | L     | 271 | ASN  | N-CA-C    | -5.04 | 97.38       | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1939  | 0        | 1829     | 100     | 0            |
| 1   | B     | 1939  | 0        | 1829     | 108     | 0            |
| 1   | C     | 1986  | 0        | 1872     | 95      | 0            |
| 1   | D     | 1986  | 0        | 1872     | 88      | 1            |
| 1   | E     | 1939  | 0        | 1829     | 116     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | F     | 1939  | 0        | 1829     | 106     | 0            |
| 1   | G     | 1918  | 0        | 1811     | 93      | 0            |
| 1   | H     | 1992  | 0        | 1877     | 101     | 1            |
| 1   | I     | 1939  | 0        | 1829     | 107     | 0            |
| 1   | J     | 1939  | 0        | 1829     | 86      | 0            |
| 1   | K     | 1986  | 0        | 1872     | 101     | 0            |
| 1   | L     | 1918  | 0        | 1811     | 85      | 0            |
| 1   | M     | 1939  | 0        | 1829     | 85      | 0            |
| 1   | N     | 1939  | 0        | 1829     | 94      | 0            |
| 1   | O     | 1918  | 0        | 1811     | 83      | 0            |
| 1   | P     | 1986  | 0        | 1872     | 88      | 0            |
| All | All   | 31202 | 0        | 29430    | 1406    | 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 23.

All (1406) 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:J:87:ILE:HD12  | 1:J:230:ILE:HG21 | 1.22                     | 1.15              |
| 1:I:64:ILE:HG23  | 1:I:129:LEU:HD11 | 1.25                     | 1.11              |
| 1:A:84:THR:HB    | 1:A:86:GLN:HG2   | 1.11                     | 1.10              |
| 1:A:64:ILE:HG23  | 1:A:129:LEU:HD11 | 1.17                     | 1.08              |
| 1:D:254:SER:HB3  | 1:O:244:ILE:O    | 1.53                     | 1.07              |
| 1:G:116:THR:HG22 | 1:G:118:GLN:H    | 1.18                     | 1.07              |
| 1:E:133:ARG:HD3  | 1:E:190:ASN:HD21 | 1.20                     | 1.06              |
| 1:K:133:ARG:HG3  | 1:K:191:PRO:HB3  | 1.37                     | 1.06              |
| 1:D:254:SER:CB   | 1:O:244:ILE:O    | 2.03                     | 1.06              |
| 1:I:63:ARG:HD2   | 1:L:123:VAL:HG21 | 1.28                     | 1.06              |
| 1:A:63:ARG:HG2   | 1:A:63:ARG:HH11  | 1.17                     | 1.05              |
| 1:E:46:LEU:HD12  | 1:E:202:GLY:HA2  | 1.37                     | 1.04              |
| 1:E:133:ARG:HH11 | 1:E:190:ASN:ND2  | 1.54                     | 1.03              |
| 1:D:116:THR:HG22 | 1:D:118:GLN:H    | 1.23                     | 1.03              |
| 1:C:185:PHE:HB2  | 1:C:189:HIS:HD2  | 1.24                     | 1.01              |
| 1:C:87:ILE:HD12  | 1:C:230:ILE:HG21 | 1.44                     | 0.99              |
| 1:K:190:ASN:HA   | 1:K:192:PHE:HD2  | 1.27                     | 0.99              |
| 1:C:40:TRP:CE2   | 1:C:41:ILE:HD13  | 2.00                     | 0.97              |
| 1:E:129:LEU:HD23 | 1:E:191:PRO:HD3  | 1.48                     | 0.96              |
| 1:M:84:THR:HG21  | 1:M:86:GLN:HB2   | 1.47                     | 0.96              |
| 1:M:123:VAL:HG22 | 1:P:123:VAL:HG22 | 1.48                     | 0.96              |
| 1:P:190:ASN:HB2  | 1:P:191:PRO:HA   | 1.45                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:80:ILE:HG22  | 1:G:87:ILE:HD13  | 1.46                     | 0.95              |
| 1:I:43:ALA:HB2   | 1:I:176:PRO:HD2  | 1.45                     | 0.95              |
| 1:F:64:ILE:HG23  | 1:F:129:LEU:HD11 | 1.46                     | 0.95              |
| 1:F:87:ILE:HD12  | 1:F:230:ILE:HG12 | 1.48                     | 0.94              |
| 1:I:46:LEU:HD12  | 1:I:202:GLY:HA2  | 1.48                     | 0.93              |
| 1:G:254:SER:OG   | 1:L:243:ASN:N    | 2.01                     | 0.93              |
| 1:P:133:ARG:HG3  | 1:P:191:PRO:HB3  | 1.50                     | 0.93              |
| 1:G:254:SER:CB   | 1:L:243:ASN:H    | 1.83                     | 0.92              |
| 1:H:120:LEU:HG   | 1:H:122:PRO:HD3  | 1.52                     | 0.91              |
| 1:C:87:ILE:CD1   | 1:C:230:ILE:HG21 | 2.01                     | 0.91              |
| 1:B:129:LEU:HD23 | 1:B:191:PRO:CG   | 2.00                     | 0.91              |
| 1:I:87:ILE:HD12  | 1:I:230:ILE:HG21 | 1.53                     | 0.91              |
| 1:J:190:ASN:HB2  | 1:J:191:PRO:HA   | 1.54                     | 0.90              |
| 1:E:283:ILE:CG2  | 1:H:268:LEU:HD21 | 2.02                     | 0.90              |
| 1:K:190:ASN:HB2  | 1:K:191:PRO:HA   | 1.54                     | 0.89              |
| 1:J:129:LEU:HD23 | 1:J:191:PRO:HD3  | 1.54                     | 0.89              |
| 1:G:254:SER:CB   | 1:L:243:ASN:N    | 2.36                     | 0.89              |
| 1:O:69:SER:HB2   | 1:O:72:GLY:HA2   | 1.52                     | 0.89              |
| 1:L:127:HIS:ND1  | 1:L:130:ASN:HB2  | 1.88                     | 0.88              |
| 1:J:127:HIS:ND1  | 1:J:130:ASN:HB2  | 1.89                     | 0.88              |
| 1:K:127:HIS:ND1  | 1:K:130:ASN:HB2  | 1.89                     | 0.88              |
| 1:O:127:HIS:ND1  | 1:O:130:ASN:HB2  | 1.88                     | 0.88              |
| 1:I:64:ILE:HG23  | 1:I:129:LEU:CD1  | 2.03                     | 0.88              |
| 1:N:127:HIS:ND1  | 1:N:130:ASN:HB2  | 1.88                     | 0.88              |
| 1:I:127:HIS:ND1  | 1:I:130:ASN:HB2  | 1.89                     | 0.88              |
| 1:A:127:HIS:ND1  | 1:A:130:ASN:HB2  | 1.89                     | 0.88              |
| 1:P:127:HIS:ND1  | 1:P:130:ASN:HB2  | 1.88                     | 0.88              |
| 1:B:127:HIS:ND1  | 1:B:130:ASN:HB2  | 1.89                     | 0.88              |
| 1:A:133:ARG:HD3  | 1:A:190:ASN:HD22 | 1.38                     | 0.88              |
| 1:E:127:HIS:ND1  | 1:E:130:ASN:HB2  | 1.89                     | 0.88              |
| 1:M:127:HIS:ND1  | 1:M:130:ASN:HB2  | 1.89                     | 0.87              |
| 1:H:127:HIS:ND1  | 1:H:130:ASN:HB2  | 1.88                     | 0.87              |
| 1:C:127:HIS:ND1  | 1:C:130:ASN:HB2  | 1.88                     | 0.87              |
| 1:E:64:ILE:HG23  | 1:E:129:LEU:HD11 | 1.55                     | 0.87              |
| 1:F:127:HIS:ND1  | 1:F:130:ASN:HB2  | 1.89                     | 0.87              |
| 1:N:133:ARG:HE   | 1:N:190:ASN:HD21 | 1.23                     | 0.87              |
| 1:G:127:HIS:ND1  | 1:G:130:ASN:HB2  | 1.88                     | 0.87              |
| 1:K:133:ARG:CG   | 1:K:191:PRO:HB3  | 2.03                     | 0.87              |
| 1:K:190:ASN:HA   | 1:K:192:PHE:CD2  | 2.08                     | 0.86              |
| 1:A:190:ASN:HA   | 1:A:192:PHE:H    | 1.38                     | 0.86              |
| 1:D:127:HIS:ND1  | 1:D:130:ASN:HB2  | 1.88                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:63:ARG:HD2   | 1:L:123:VAL:CG2  | 2.06                     | 0.86              |
| 1:A:129:LEU:HD23 | 1:A:191:PRO:HD3  | 1.58                     | 0.86              |
| 1:A:84:THR:CB    | 1:A:86:GLN:HG2   | 2.02                     | 0.86              |
| 1:I:133:ARG:HH11 | 1:I:190:ASN:ND2  | 1.73                     | 0.85              |
| 1:O:241:PRO:HB2  | 1:O:244:ILE:HD12 | 1.59                     | 0.85              |
| 1:L:241:PRO:HB2  | 1:L:244:ILE:HD12 | 1.59                     | 0.85              |
| 1:M:241:PRO:HB2  | 1:M:244:ILE:HD12 | 1.59                     | 0.85              |
| 1:M:283:ILE:HB   | 1:O:268:LEU:HD22 | 1.57                     | 0.85              |
| 1:D:241:PRO:HB2  | 1:D:244:ILE:HD12 | 1.59                     | 0.84              |
| 1:G:254:SER:HB3  | 1:L:244:ILE:H    | 1.42                     | 0.84              |
| 1:E:241:PRO:HB2  | 1:E:244:ILE:HD12 | 1.59                     | 0.84              |
| 1:P:64:ILE:HD13  | 1:P:73:LEU:HD13  | 1.59                     | 0.84              |
| 1:H:241:PRO:HB2  | 1:H:244:ILE:HD12 | 1.59                     | 0.84              |
| 1:B:133:ARG:HG2  | 1:B:191:PRO:HB3  | 1.57                     | 0.84              |
| 1:F:241:PRO:HB2  | 1:F:244:ILE:HD12 | 1.59                     | 0.84              |
| 1:A:241:PRO:HB2  | 1:A:244:ILE:HD12 | 1.59                     | 0.84              |
| 1:A:64:ILE:HG23  | 1:A:129:LEU:CD1  | 2.06                     | 0.83              |
| 1:C:135:ASN:HD22 | 1:C:271:ASN:HD21 | 1.26                     | 0.83              |
| 1:N:87:ILE:HD11  | 1:N:208:PHE:CE1  | 2.13                     | 0.83              |
| 1:G:241:PRO:HB2  | 1:G:244:ILE:HD12 | 1.59                     | 0.83              |
| 1:C:241:PRO:HB2  | 1:C:244:ILE:CD1  | 2.09                     | 0.83              |
| 1:I:241:PRO:HB2  | 1:I:244:ILE:CD1  | 2.09                     | 0.83              |
| 1:J:241:PRO:HB2  | 1:J:244:ILE:HD12 | 1.59                     | 0.83              |
| 1:N:241:PRO:HB2  | 1:N:244:ILE:HD12 | 1.59                     | 0.83              |
| 1:I:79:THR:HG21  | 1:I:177:GLY:H    | 1.43                     | 0.83              |
| 1:E:241:PRO:HB2  | 1:E:244:ILE:CD1  | 2.09                     | 0.83              |
| 1:G:241:PRO:HB2  | 1:G:244:ILE:CD1  | 2.09                     | 0.83              |
| 1:F:241:PRO:HB2  | 1:F:244:ILE:CD1  | 2.09                     | 0.83              |
| 1:A:241:PRO:HB2  | 1:A:244:ILE:CD1  | 2.09                     | 0.83              |
| 1:F:87:ILE:HD12  | 1:F:230:ILE:HG21 | 1.61                     | 0.83              |
| 1:L:78:GLN:O     | 1:L:88:GLN:HG3   | 1.78                     | 0.82              |
| 1:N:241:PRO:HB2  | 1:N:244:ILE:CD1  | 2.09                     | 0.82              |
| 1:P:241:PRO:HB2  | 1:P:244:ILE:CD1  | 2.09                     | 0.82              |
| 1:C:185:PHE:HB2  | 1:C:189:HIS:CD2  | 2.13                     | 0.82              |
| 1:O:241:PRO:HB2  | 1:O:244:ILE:CD1  | 2.09                     | 0.82              |
| 1:N:48:TRP:CH2   | 1:N:120:LEU:HD23 | 2.13                     | 0.82              |
| 1:B:241:PRO:HB2  | 1:B:244:ILE:CD1  | 2.09                     | 0.82              |
| 1:K:194:ASN:HB3  | 1:K:197:GLU:HB2  | 1.61                     | 0.82              |
| 1:K:241:PRO:HB2  | 1:K:244:ILE:CD1  | 2.09                     | 0.82              |
| 1:P:241:PRO:HB2  | 1:P:244:ILE:HD12 | 1.59                     | 0.82              |
| 1:C:40:TRP:CD2   | 1:C:41:ILE:HG23  | 2.15                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:241:PRO:HB2  | 1:H:244:ILE:CD1  | 2.09                     | 0.82              |
| 1:K:241:PRO:HB2  | 1:K:244:ILE:HD12 | 1.59                     | 0.82              |
| 1:B:241:PRO:HB2  | 1:B:244:ILE:HD12 | 1.59                     | 0.82              |
| 1:D:241:PRO:HB2  | 1:D:244:ILE:CD1  | 2.09                     | 0.81              |
| 1:C:241:PRO:HB2  | 1:C:244:ILE:HD12 | 1.59                     | 0.81              |
| 1:I:241:PRO:HB2  | 1:I:244:ILE:HD12 | 1.59                     | 0.81              |
| 1:G:254:SER:HB3  | 1:L:244:ILE:N    | 1.95                     | 0.81              |
| 1:M:133:ARG:HH11 | 1:M:190:ASN:HB2  | 1.46                     | 0.81              |
| 1:M:241:PRO:HB2  | 1:M:244:ILE:CD1  | 2.09                     | 0.81              |
| 1:C:154:GLU:HG2  | 1:C:289:LEU:HD22 | 1.63                     | 0.81              |
| 1:J:241:PRO:HB2  | 1:J:244:ILE:CD1  | 2.09                     | 0.81              |
| 1:I:154:GLU:HG2  | 1:I:289:LEU:HD22 | 1.63                     | 0.81              |
| 1:L:154:GLU:HG2  | 1:L:289:LEU:HD22 | 1.63                     | 0.81              |
| 1:L:241:PRO:HB2  | 1:L:244:ILE:CD1  | 2.09                     | 0.80              |
| 1:B:129:LEU:HD23 | 1:B:191:PRO:HG3  | 1.60                     | 0.80              |
| 1:H:63:ARG:HH11  | 1:H:63:ARG:HG3   | 1.46                     | 0.80              |
| 1:P:133:ARG:CG   | 1:P:191:PRO:HB3  | 2.10                     | 0.80              |
| 1:D:186:SER:HB2  | 1:D:189:HIS:HB2  | 1.62                     | 0.80              |
| 1:O:154:GLU:HG2  | 1:O:289:LEU:HD22 | 1.63                     | 0.80              |
| 1:K:154:GLU:HG2  | 1:K:289:LEU:HD22 | 1.63                     | 0.80              |
| 1:E:129:LEU:CD2  | 1:E:191:PRO:HD3  | 2.12                     | 0.80              |
| 1:D:154:GLU:HG2  | 1:D:289:LEU:HD22 | 1.63                     | 0.80              |
| 1:E:133:ARG:HH11 | 1:E:190:ASN:HD21 | 1.30                     | 0.80              |
| 1:G:154:GLU:HG2  | 1:G:289:LEU:HD22 | 1.63                     | 0.80              |
| 1:P:57:TYR:HE1   | 1:P:73:LEU:HD23  | 1.45                     | 0.80              |
| 1:A:154:GLU:HG2  | 1:A:289:LEU:HD22 | 1.63                     | 0.79              |
| 1:F:87:ILE:CD1   | 1:F:230:ILE:HG21 | 2.12                     | 0.79              |
| 1:E:129:LEU:HD23 | 1:E:191:PRO:CD   | 2.13                     | 0.79              |
| 1:N:154:GLU:HG2  | 1:N:289:LEU:HD22 | 1.63                     | 0.79              |
| 1:J:154:GLU:HG2  | 1:J:289:LEU:HD22 | 1.63                     | 0.79              |
| 1:D:255:GLU:OE2  | 1:O:242:SER:HB3  | 1.83                     | 0.79              |
| 1:P:154:GLU:HG2  | 1:P:289:LEU:HD22 | 1.63                     | 0.79              |
| 1:H:154:GLU:HG2  | 1:H:289:LEU:HD22 | 1.63                     | 0.79              |
| 1:G:254:SER:HG   | 1:L:243:ASN:H    | 1.28                     | 0.79              |
| 1:B:154:GLU:HG2  | 1:B:289:LEU:HD22 | 1.63                     | 0.78              |
| 1:F:79:THR:HG21  | 1:F:177:GLY:H    | 1.48                     | 0.78              |
| 1:M:84:THR:CG2   | 1:M:86:GLN:HB2   | 2.12                     | 0.78              |
| 1:E:154:GLU:HG2  | 1:E:289:LEU:HD22 | 1.63                     | 0.78              |
| 1:M:154:GLU:HG2  | 1:M:289:LEU:HD22 | 1.63                     | 0.78              |
| 1:D:254:SER:HB3  | 1:O:244:ILE:C    | 2.03                     | 0.78              |
| 1:F:154:GLU:HG2  | 1:F:289:LEU:HD22 | 1.63                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:133:ARG:HE   | 1:B:190:ASN:HD22 | 1.29                     | 0.78              |
| 1:B:43:ALA:HB2   | 1:B:176:PRO:HD2  | 1.66                     | 0.78              |
| 1:H:185:PHE:HB2  | 1:H:189:HIS:HD2  | 1.47                     | 0.78              |
| 1:I:46:LEU:HD11  | 1:I:113:PRO:HG2  | 1.66                     | 0.78              |
| 1:E:87:ILE:CD1   | 1:E:176:PRO:HD3  | 2.14                     | 0.78              |
| 1:J:84:THR:HB    | 1:J:86:GLN:HG3   | 1.66                     | 0.77              |
| 1:E:133:ARG:HD3  | 1:E:190:ASN:ND2  | 1.98                     | 0.77              |
| 1:D:40:TRP:CD2   | 1:D:41:ILE:HG23  | 2.19                     | 0.77              |
| 1:J:46:LEU:HD12  | 1:J:202:GLY:HA2  | 1.66                     | 0.77              |
| 1:C:84:THR:OG1   | 1:C:86:GLN:HB2   | 1.85                     | 0.77              |
| 1:H:115:VAL:HG11 | 1:H:125:ASP:HB3  | 1.66                     | 0.77              |
| 1:J:87:ILE:CD1   | 1:J:230:ILE:HG21 | 2.12                     | 0.77              |
| 1:A:49:LEU:HD21  | 1:A:56:LEU:HD21  | 1.65                     | 0.76              |
| 1:F:87:ILE:CD1   | 1:F:230:ILE:HG12 | 2.15                     | 0.76              |
| 1:G:39:THR:HA    | 1:G:42:GLN:HG3   | 1.67                     | 0.76              |
| 1:B:122:PRO:HD3  | 1:D:62:THR:HG21  | 1.65                     | 0.76              |
| 1:M:283:ILE:HB   | 1:O:268:LEU:CD2  | 2.14                     | 0.76              |
| 1:D:252:ASN:O    | 1:O:245:SER:HA   | 1.85                     | 0.76              |
| 1:N:182:ASN:HB2  | 1:N:195:GLN:O    | 1.85                     | 0.76              |
| 1:G:87:ILE:HD11  | 1:G:176:PRO:HB3  | 1.67                     | 0.76              |
| 1:A:63:ARG:HG2   | 1:A:63:ARG:NH1   | 1.97                     | 0.76              |
| 1:I:129:LEU:HD23 | 1:I:191:PRO:HD3  | 1.67                     | 0.76              |
| 1:G:254:SER:HB3  | 1:L:243:ASN:N    | 1.99                     | 0.76              |
| 1:J:87:ILE:HD11  | 1:J:208:PHE:CE1  | 2.20                     | 0.76              |
| 1:E:150:ASN:ND2  | 1:P:207:GLU:OE1  | 2.18                     | 0.76              |
| 1:P:129:LEU:HD23 | 1:P:191:PRO:HD3  | 1.65                     | 0.76              |
| 1:N:59:LEU:HA    | 1:O:122:PRO:HG2  | 1.67                     | 0.76              |
| 1:C:40:TRP:NE1   | 1:C:41:ILE:HD13  | 2.01                     | 0.75              |
| 1:D:254:SER:O    | 1:O:246:LYS:HE3  | 1.86                     | 0.75              |
| 1:A:129:LEU:HD23 | 1:A:191:PRO:CD   | 2.17                     | 0.75              |
| 1:D:58:GLN:O     | 1:D:62:THR:HG23  | 1.87                     | 0.75              |
| 1:E:288:LEU:HD13 | 1:P:86:GLN:NE2   | 2.02                     | 0.75              |
| 1:L:84:THR:OG1   | 1:L:86:GLN:HG2   | 1.85                     | 0.74              |
| 1:F:76:ARG:HD2   | 1:F:198:ILE:HG21 | 1.69                     | 0.74              |
| 1:L:56:LEU:HD12  | 1:L:56:LEU:O     | 1.85                     | 0.74              |
| 1:N:133:ARG:HE   | 1:N:190:ASN:ND2  | 1.84                     | 0.74              |
| 1:C:58:GLN:O     | 1:C:62:THR:HB    | 1.87                     | 0.74              |
| 1:A:122:PRO:HG2  | 1:C:59:LEU:HA    | 1.70                     | 0.74              |
| 1:E:133:ARG:NH1  | 1:E:190:ASN:ND2  | 2.33                     | 0.74              |
| 1:G:254:SER:CB   | 1:L:244:ILE:H    | 2.01                     | 0.74              |
| 1:O:80:ILE:HG22  | 1:O:81:ASP:O     | 1.87                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:129:LEU:HD23 | 1:B:191:PRO:CD   | 2.17                     | 0.74              |
| 1:C:185:PHE:CB   | 1:C:189:HIS:HD2  | 2.00                     | 0.74              |
| 1:N:59:LEU:HD13  | 1:O:122:PRO:HB2  | 1.68                     | 0.73              |
| 1:M:64:ILE:HG12  | 1:M:129:LEU:HD12 | 1.70                     | 0.73              |
| 1:I:40:TRP:CH2   | 1:I:57:TYR:HB2   | 2.24                     | 0.73              |
| 1:N:76:ARG:NH1   | 1:N:95:LEU:HD11  | 2.04                     | 0.73              |
| 1:B:129:LEU:HD23 | 1:B:191:PRO:HD3  | 1.70                     | 0.73              |
| 1:M:187:ARG:NH1  | 1:M:195:GLN:HG3  | 2.03                     | 0.73              |
| 1:J:129:LEU:CD2  | 1:J:191:PRO:HD3  | 2.18                     | 0.73              |
| 1:E:87:ILE:O     | 1:E:89:ILE:HG13  | 1.89                     | 0.73              |
| 1:F:79:THR:HB    | 1:F:176:PRO:HA   | 1.69                     | 0.73              |
| 1:K:262:LYS:HG2  | 1:K:270:TYR:HE1  | 1.53                     | 0.72              |
| 1:K:58:GLN:O     | 1:K:62:THR:HG23  | 1.89                     | 0.72              |
| 1:K:133:ARG:CB   | 1:K:191:PRO:HB3  | 2.20                     | 0.72              |
| 1:L:120:LEU:HG   | 1:L:122:PRO:HD3  | 1.71                     | 0.72              |
| 1:P:79:THR:OG1   | 1:P:176:PRO:HA   | 1.89                     | 0.72              |
| 1:N:84:THR:HB    | 1:N:86:GLN:HG2   | 1.72                     | 0.72              |
| 1:E:65:PRO:HB3   | 1:F:62:THR:O     | 1.90                     | 0.71              |
| 1:K:80:ILE:HG22  | 1:K:87:ILE:HD13  | 1.72                     | 0.71              |
| 1:E:156:THR:HG21 | 1:E:284:PRO:HG2  | 1.73                     | 0.71              |
| 1:O:76:ARG:HD3   | 1:O:198:ILE:HG13 | 1.71                     | 0.71              |
| 1:G:156:THR:HG21 | 1:G:284:PRO:HG2  | 1.72                     | 0.71              |
| 1:H:156:THR:HG21 | 1:H:284:PRO:HG2  | 1.73                     | 0.71              |
| 1:J:156:THR:HG21 | 1:J:284:PRO:HG2  | 1.73                     | 0.71              |
| 1:O:156:THR:HG21 | 1:O:284:PRO:HG2  | 1.72                     | 0.71              |
| 1:H:115:VAL:HG12 | 1:H:115:VAL:O    | 1.89                     | 0.71              |
| 1:P:65:PRO:HD3   | 1:P:129:LEU:CD1  | 2.21                     | 0.71              |
| 1:A:129:LEU:CD2  | 1:A:191:PRO:HD3  | 2.20                     | 0.71              |
| 1:A:156:THR:HG21 | 1:A:284:PRO:HG2  | 1.73                     | 0.71              |
| 1:F:129:LEU:HD23 | 1:F:191:PRO:HD3  | 1.73                     | 0.71              |
| 1:L:156:THR:HG21 | 1:L:284:PRO:HG2  | 1.72                     | 0.71              |
| 1:D:156:THR:HG21 | 1:D:284:PRO:HG2  | 1.73                     | 0.71              |
| 1:H:186:SER:N    | 1:H:188:ASN:OD1  | 2.24                     | 0.71              |
| 1:I:156:THR:HG21 | 1:I:284:PRO:HG2  | 1.73                     | 0.70              |
| 1:A:190:ASN:HA   | 1:A:192:PHE:N    | 2.06                     | 0.70              |
| 1:K:268:LEU:HD23 | 1:K:268:LEU:N    | 2.05                     | 0.70              |
| 1:B:156:THR:HG21 | 1:B:284:PRO:HG2  | 1.73                     | 0.70              |
| 1:E:87:ILE:HD11  | 1:E:176:PRO:HD3  | 1.73                     | 0.70              |
| 1:J:76:ARG:HD3   | 1:J:177:GLY:O    | 1.91                     | 0.70              |
| 1:N:156:THR:HG21 | 1:N:284:PRO:HG2  | 1.73                     | 0.70              |
| 1:K:156:THR:HG21 | 1:K:284:PRO:HG2  | 1.73                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:156:THR:HG21 | 1:C:284:PRO:HG2  | 1.73                     | 0.70              |
| 1:I:64:ILE:CG2   | 1:I:129:LEU:HD11 | 2.14                     | 0.70              |
| 1:K:135:ASN:ND2  | 1:K:271:ASN:HD21 | 1.90                     | 0.70              |
| 1:G:182:ASN:HB2  | 1:G:195:GLN:O    | 1.92                     | 0.70              |
| 1:B:40:TRP:HA    | 1:B:177:GLY:HA3  | 1.74                     | 0.70              |
| 1:D:40:TRP:CE3   | 1:D:41:ILE:HG23  | 2.27                     | 0.70              |
| 1:F:156:THR:HG21 | 1:F:284:PRO:HG2  | 1.73                     | 0.70              |
| 1:P:133:ARG:CB   | 1:P:191:PRO:HB3  | 2.22                     | 0.70              |
| 1:A:129:LEU:HD23 | 1:A:191:PRO:HG3  | 1.74                     | 0.70              |
| 1:G:182:ASN:HA   | 1:G:195:GLN:OE1  | 1.92                     | 0.70              |
| 1:J:194:ASN:HB3  | 1:J:197:GLU:HB2  | 1.72                     | 0.69              |
| 1:M:156:THR:HG21 | 1:M:284:PRO:HG2  | 1.73                     | 0.69              |
| 1:N:87:ILE:HD11  | 1:N:208:PHE:HE1  | 1.55                     | 0.69              |
| 1:H:264:PHE:HB3  | 1:P:248:PHE:CD2  | 2.27                     | 0.69              |
| 1:F:76:ARG:HD2   | 1:F:198:ILE:CG2  | 2.21                     | 0.69              |
| 1:N:120:LEU:HD12 | 1:N:120:LEU:O    | 1.92                     | 0.69              |
| 1:G:194:ASN:HD21 | 1:G:197:GLU:HB2  | 1.58                     | 0.69              |
| 1:J:190:ASN:CB   | 1:J:191:PRO:HA   | 2.18                     | 0.69              |
| 1:B:42:GLN:HE21  | 1:B:176:PRO:HG3  | 1.57                     | 0.69              |
| 1:P:156:THR:HG21 | 1:P:284:PRO:HG2  | 1.73                     | 0.69              |
| 1:N:76:ARG:HD2   | 1:N:198:ILE:HG23 | 1.74                     | 0.69              |
| 1:A:76:ARG:NH1   | 1:A:177:GLY:O    | 2.26                     | 0.69              |
| 1:K:44:ALA:O     | 1:K:205:ARG:NH1  | 2.26                     | 0.69              |
| 1:A:87:ILE:CD1   | 1:A:176:PRO:HD3  | 2.23                     | 0.68              |
| 1:I:63:ARG:NH2   | 1:I:123:VAL:O    | 2.26                     | 0.68              |
| 1:M:64:ILE:HG23  | 1:M:129:LEU:HD11 | 1.74                     | 0.68              |
| 1:G:254:SER:HB3  | 1:L:243:ASN:CA   | 2.24                     | 0.68              |
| 1:L:45:SER:HA    | 1:L:205:ARG:HG2  | 1.75                     | 0.68              |
| 1:P:57:TYR:CE1   | 1:P:73:LEU:HD23  | 2.29                     | 0.68              |
| 1:J:84:THR:CB    | 1:J:86:GLN:HG3   | 2.24                     | 0.68              |
| 1:J:43:ALA:O     | 1:J:205:ARG:HG3  | 1.94                     | 0.67              |
| 1:J:87:ILE:HD12  | 1:J:230:ILE:CG2  | 2.14                     | 0.67              |
| 1:L:116:THR:HG22 | 1:L:117:ASN:H    | 1.58                     | 0.67              |
| 1:I:129:LEU:CD2  | 1:I:191:PRO:HD3  | 2.24                     | 0.67              |
| 1:H:185:PHE:HB2  | 1:H:189:HIS:CD2  | 2.30                     | 0.67              |
| 1:L:116:THR:CG2  | 1:L:117:ASN:H    | 2.07                     | 0.67              |
| 1:F:79:THR:HG21  | 1:F:177:GLY:N    | 2.09                     | 0.67              |
| 1:B:129:LEU:CD2  | 1:B:191:PRO:HD3  | 2.25                     | 0.67              |
| 1:E:49:LEU:HD21  | 1:E:56:LEU:HD22  | 1.76                     | 0.67              |
| 1:A:70:PRO:HG2   | 1:A:71:ASN:H     | 1.58                     | 0.67              |
| 1:F:64:ILE:CG2   | 1:F:69:SER:HB3   | 2.24                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:264:PHE:O    | 1:L:266:LEU:HG   | 1.95                     | 0.67              |
| 1:E:283:ILE:HG22 | 1:H:268:LEU:HD21 | 1.76                     | 0.66              |
| 1:P:194:ASN:HB3  | 1:P:197:GLU:HB2  | 1.77                     | 0.66              |
| 1:G:116:THR:HG22 | 1:G:118:GLN:N    | 2.01                     | 0.66              |
| 1:N:48:TRP:HH2   | 1:N:120:LEU:HD23 | 1.57                     | 0.66              |
| 1:O:59:LEU:O     | 1:O:63:ARG:NH1   | 2.28                     | 0.66              |
| 1:D:254:SER:HB2  | 1:O:244:ILE:O    | 1.93                     | 0.66              |
| 1:I:188:ASN:OD1  | 1:K:119:ASN:ND2  | 2.28                     | 0.66              |
| 1:N:76:ARG:HD2   | 1:N:198:ILE:CG2  | 2.25                     | 0.66              |
| 1:I:48:TRP:HB2   | 1:I:118:GLN:HG3  | 1.79                     | 0.65              |
| 1:B:150:ASN:ND2  | 1:K:207:GLU:OE1  | 2.30                     | 0.65              |
| 1:H:59:LEU:O     | 1:H:63:ARG:NH1   | 2.29                     | 0.65              |
| 1:I:133:ARG:NH2  | 1:K:137:PRO:O    | 2.29                     | 0.65              |
| 1:L:44:ALA:O     | 1:L:205:ARG:NH1  | 2.30                     | 0.65              |
| 1:K:182:ASN:HB2  | 1:K:195:GLN:O    | 1.96                     | 0.65              |
| 1:L:116:THR:HG22 | 1:L:117:ASN:N    | 2.12                     | 0.65              |
| 1:N:87:ILE:HD11  | 1:N:208:PHE:CD1  | 2.32                     | 0.65              |
| 1:H:120:LEU:HD12 | 1:H:125:ASP:HB2  | 1.77                     | 0.65              |
| 1:A:129:LEU:HD23 | 1:A:191:PRO:CG   | 2.27                     | 0.65              |
| 1:O:63:ARG:CG    | 1:O:63:ARG:HH11  | 2.09                     | 0.65              |
| 1:O:69:SER:CB    | 1:O:72:GLY:HA2   | 2.25                     | 0.65              |
| 1:A:49:LEU:HD21  | 1:A:56:LEU:CD2   | 2.27                     | 0.65              |
| 1:I:87:ILE:HD11  | 1:I:208:PHE:HE1  | 1.62                     | 0.65              |
| 1:F:192:PHE:CG   | 1:G:137:PRO:HG2  | 2.32                     | 0.64              |
| 1:N:46:LEU:HD21  | 1:N:116:THR:HA   | 1.77                     | 0.64              |
| 1:A:48:TRP:CG    | 1:A:118:GLN:HG2  | 2.32                     | 0.64              |
| 1:M:190:ASN:CB   | 1:M:191:PRO:HA   | 2.26                     | 0.64              |
| 1:M:190:ASN:HB2  | 1:M:191:PRO:HA   | 1.77                     | 0.64              |
| 1:M:182:ASN:HB2  | 1:M:195:GLN:O    | 1.96                     | 0.64              |
| 1:F:63:ARG:O     | 1:F:65:PRO:HD3   | 1.96                     | 0.64              |
| 1:H:65:PRO:O     | 1:H:68:ALA:HB3   | 1.97                     | 0.64              |
| 1:B:194:ASN:O    | 1:B:197:GLU:N    | 2.28                     | 0.64              |
| 1:K:129:LEU:HD23 | 1:K:191:PRO:HD3  | 1.80                     | 0.64              |
| 1:E:46:LEU:HD11  | 1:E:113:PRO:HG2  | 1.79                     | 0.64              |
| 1:J:123:VAL:CB   | 1:K:63:ARG:HH21  | 2.10                     | 0.64              |
| 1:E:187:ARG:O    | 1:E:189:HIS:ND1  | 2.30                     | 0.64              |
| 1:H:84:THR:OG1   | 1:H:86:GLN:HB2   | 1.98                     | 0.64              |
| 1:I:87:ILE:HD11  | 1:I:208:PHE:CE1  | 2.33                     | 0.64              |
| 1:B:84:THR:CB    | 1:B:86:GLN:HG3   | 2.28                     | 0.64              |
| 1:E:68:ALA:HB1   | 1:E:129:LEU:HD21 | 1.78                     | 0.64              |
| 1:M:76:ARG:HB3   | 1:M:79:THR:CG2   | 2.28                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:81:ASP:HB3   | 1:C:84:THR:OG1   | 1.98                     | 0.64              |
| 1:E:55:LEU:HD23  | 1:G:55:LEU:HD23  | 1.80                     | 0.64              |
| 1:M:133:ARG:NH1  | 1:M:190:ASN:HB2  | 2.13                     | 0.64              |
| 1:F:87:ILE:HD12  | 1:F:230:ILE:CG1  | 2.25                     | 0.63              |
| 1:I:123:VAL:HG21 | 1:L:63:ARG:HH11  | 1.62                     | 0.63              |
| 1:I:43:ALA:HB2   | 1:I:176:PRO:CD   | 2.24                     | 0.63              |
| 1:N:133:ARG:NH2  | 1:P:125:ASP:OD1  | 2.30                     | 0.63              |
| 1:J:123:VAL:HB   | 1:K:63:ARG:HH21  | 1.64                     | 0.63              |
| 1:G:194:ASN:ND2  | 1:G:197:GLU:HB2  | 2.13                     | 0.63              |
| 1:I:48:TRP:CB    | 1:I:118:GLN:HG3  | 2.28                     | 0.63              |
| 1:N:64:ILE:HG23  | 1:N:129:LEU:HD11 | 1.79                     | 0.63              |
| 1:N:40:TRP:CZ2   | 1:N:57:TYR:HB2   | 2.33                     | 0.63              |
| 1:J:123:VAL:CG1  | 1:K:63:ARG:HH21  | 2.11                     | 0.63              |
| 1:E:283:ILE:HB   | 1:H:268:LEU:CD2  | 2.27                     | 0.63              |
| 1:K:74:HIS:HD2   | 1:K:183:ALA:O    | 1.81                     | 0.63              |
| 1:N:84:THR:CB    | 1:N:86:GLN:HG2   | 2.28                     | 0.63              |
| 1:B:76:ARG:NH1   | 1:B:95:LEU:HD11  | 2.12                     | 0.63              |
| 1:F:76:ARG:HD3   | 1:F:177:GLY:O    | 1.99                     | 0.63              |
| 1:B:64:ILE:HG23  | 1:B:129:LEU:HD11 | 1.79                     | 0.63              |
| 1:B:64:ILE:HG21  | 1:B:69:SER:HB3   | 1.81                     | 0.62              |
| 1:F:49:LEU:HD22  | 1:F:202:GLY:HA3  | 1.79                     | 0.62              |
| 1:M:194:ASN:O    | 1:M:197:GLU:N    | 2.28                     | 0.62              |
| 1:A:120:LEU:O    | 1:A:122:PRO:HD3  | 1.99                     | 0.62              |
| 1:A:55:LEU:HD12  | 1:A:55:LEU:O     | 1.98                     | 0.62              |
| 1:N:59:LEU:CA    | 1:O:122:PRO:HG2  | 2.28                     | 0.62              |
| 1:A:68:ALA:HB1   | 1:A:129:LEU:HD21 | 1.82                     | 0.62              |
| 1:C:120:LEU:HD21 | 1:C:122:PRO:HG3  | 1.80                     | 0.62              |
| 1:D:155:ILE:HG22 | 1:D:288:LEU:HD23 | 1.82                     | 0.62              |
| 1:E:155:ILE:HG22 | 1:E:288:LEU:HD23 | 1.82                     | 0.62              |
| 1:H:155:ILE:HG22 | 1:H:288:LEU:HD23 | 1.82                     | 0.62              |
| 1:H:38:ASN:OD1   | 1:H:42:GLN:NE2   | 2.32                     | 0.62              |
| 1:B:42:GLN:NE2   | 1:B:176:PRO:HG3  | 2.15                     | 0.62              |
| 1:N:155:ILE:HG22 | 1:N:288:LEU:HD23 | 1.82                     | 0.62              |
| 1:K:135:ASN:HD22 | 1:K:271:ASN:HD21 | 1.45                     | 0.62              |
| 1:A:155:ILE:HG22 | 1:A:288:LEU:HD23 | 1.82                     | 0.62              |
| 1:E:133:ARG:CD   | 1:E:190:ASN:HD21 | 2.05                     | 0.62              |
| 1:J:182:ASN:HB2  | 1:J:195:GLN:O    | 1.99                     | 0.62              |
| 1:M:155:ILE:HG22 | 1:M:288:LEU:HD23 | 1.82                     | 0.62              |
| 1:G:155:ILE:HG22 | 1:G:288:LEU:HD23 | 1.82                     | 0.62              |
| 1:G:264:PHE:HE2  | 1:L:236:ASN:HA   | 1.64                     | 0.62              |
| 1:O:63:ARG:HH11  | 1:O:63:ARG:HG3   | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:63:ARG:CG    | 1:A:63:ARG:HH11  | 2.03                     | 0.61              |
| 1:B:155:ILE:HG22 | 1:B:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:C:135:ASN:ND2  | 1:C:271:ASN:HD21 | 1.96                     | 0.61              |
| 1:I:133:ARG:NH1  | 1:I:190:ASN:ND2  | 2.47                     | 0.61              |
| 1:K:262:LYS:HG2  | 1:K:270:TYR:CE1  | 2.35                     | 0.61              |
| 1:I:40:TRP:CZ2   | 1:I:57:TYR:HB2   | 2.35                     | 0.61              |
| 1:B:133:ARG:HE   | 1:B:190:ASN:ND2  | 1.98                     | 0.61              |
| 1:F:129:LEU:CD2  | 1:F:191:PRO:HD3  | 2.30                     | 0.61              |
| 1:B:76:ARG:HD3   | 1:B:177:GLY:O    | 2.00                     | 0.61              |
| 1:F:155:ILE:HG22 | 1:F:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:J:155:ILE:HG22 | 1:J:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:D:39:THR:HA    | 1:D:42:GLN:HG3   | 1.83                     | 0.61              |
| 1:E:43:ALA:O     | 1:E:205:ARG:HG3  | 2.00                     | 0.61              |
| 1:M:64:ILE:HG12  | 1:M:129:LEU:CD1  | 2.31                     | 0.61              |
| 1:O:56:LEU:O     | 1:O:60:ILE:HD12  | 2.00                     | 0.61              |
| 1:E:39:THR:HG23  | 1:E:40:TRP:N     | 2.16                     | 0.61              |
| 1:H:87:ILE:HD13  | 1:H:87:ILE:N     | 2.16                     | 0.61              |
| 1:I:155:ILE:HG22 | 1:I:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:L:76:ARG:HD3   | 1:L:198:ILE:HG13 | 1.81                     | 0.61              |
| 1:L:155:ILE:HG22 | 1:L:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:P:155:ILE:HG22 | 1:P:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:F:87:ILE:HD12  | 1:F:230:ILE:CG2  | 2.31                     | 0.61              |
| 1:L:57:TYR:CE1   | 1:L:75:MET:HE3   | 2.36                     | 0.61              |
| 1:C:155:ILE:HG22 | 1:C:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:K:155:ILE:HG22 | 1:K:288:LEU:HD23 | 1.82                     | 0.61              |
| 1:C:62:THR:HG23  | 1:C:63:ARG:HG3   | 1.81                     | 0.60              |
| 1:A:133:ARG:NH1  | 1:A:190:ASN:HB2  | 2.17                     | 0.60              |
| 1:C:39:THR:HA    | 1:C:42:GLN:HG2   | 1.83                     | 0.60              |
| 1:E:40:TRP:CE3   | 1:E:41:ILE:HG23  | 2.36                     | 0.60              |
| 1:O:155:ILE:HG22 | 1:O:288:LEU:HD23 | 1.82                     | 0.60              |
| 1:G:116:THR:N    | 1:G:119:ASN:OD1  | 2.33                     | 0.60              |
| 1:O:78:GLN:O     | 1:O:88:GLN:HG3   | 2.00                     | 0.60              |
| 1:B:65:PRO:HD2   | 1:B:129:LEU:CD1  | 2.31                     | 0.60              |
| 1:F:64:ILE:HG21  | 1:F:69:SER:HB3   | 1.82                     | 0.60              |
| 1:J:64:ILE:HG21  | 1:J:69:SER:HB3   | 1.82                     | 0.60              |
| 1:B:65:PRO:HD2   | 1:B:129:LEU:HD13 | 1.82                     | 0.60              |
| 1:G:261:SER:O    | 1:G:264:PHE:HB2  | 2.02                     | 0.60              |
| 1:M:55:LEU:HD12  | 1:M:55:LEU:O     | 2.02                     | 0.60              |
| 1:E:283:ILE:CB   | 1:H:268:LEU:HD21 | 2.31                     | 0.60              |
| 1:I:190:ASN:ND2  | 1:I:191:PRO:HA   | 2.17                     | 0.60              |
| 1:N:133:ARG:NE   | 1:N:190:ASN:ND2  | 2.48                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:87:ILE:HG13  | 1:B:230:ILE:HG21 | 1.84                     | 0.59              |
| 1:P:84:THR:OG1   | 1:P:85:GLY:N     | 2.35                     | 0.59              |
| 1:J:87:ILE:HD11  | 1:J:208:PHE:HE1  | 1.65                     | 0.59              |
| 1:J:64:ILE:HG23  | 1:J:129:LEU:HD11 | 1.85                     | 0.59              |
| 1:P:65:PRO:HD3   | 1:P:129:LEU:HD11 | 1.83                     | 0.59              |
| 1:I:129:LEU:HD23 | 1:I:191:PRO:CD   | 2.33                     | 0.59              |
| 1:N:121:SER:HA   | 1:O:62:THR:HG21  | 1.84                     | 0.59              |
| 1:E:61:SER:HA    | 1:E:64:ILE:CD1   | 2.33                     | 0.59              |
| 1:O:63:ARG:NH1   | 1:O:63:ARG:HG3   | 2.17                     | 0.59              |
| 1:A:133:ARG:HD3  | 1:A:190:ASN:ND2  | 2.15                     | 0.59              |
| 1:J:123:VAL:HG11 | 1:K:63:ARG:HH21  | 1.68                     | 0.59              |
| 1:A:133:ARG:HH11 | 1:A:190:ASN:HB2  | 1.68                     | 0.58              |
| 1:H:135:ASN:HD22 | 1:H:271:ASN:HD21 | 1.50                     | 0.58              |
| 1:H:63:ARG:NH1   | 1:H:63:ARG:HG3   | 2.13                     | 0.58              |
| 1:N:55:LEU:HD23  | 1:O:55:LEU:HD23  | 1.85                     | 0.58              |
| 1:E:283:ILE:HB   | 1:H:268:LEU:HD21 | 1.83                     | 0.58              |
| 1:J:129:LEU:HD23 | 1:J:191:PRO:CD   | 2.30                     | 0.58              |
| 1:E:40:TRP:CD2   | 1:E:41:ILE:HG23  | 2.38                     | 0.58              |
| 1:D:252:ASN:O    | 1:O:245:SER:CA   | 2.51                     | 0.58              |
| 1:F:70:PRO:HG2   | 1:F:71:ASN:H     | 1.68                     | 0.58              |
| 1:E:77:GLU:O     | 1:E:78:GLN:HB2   | 2.02                     | 0.58              |
| 1:F:42:GLN:O     | 1:F:205:ARG:NH1  | 2.37                     | 0.58              |
| 1:I:65:PRO:HA    | 1:J:65:PRO:HA    | 1.84                     | 0.58              |
| 1:B:63:ARG:NH1   | 1:B:123:VAL:O    | 2.35                     | 0.58              |
| 1:F:70:PRO:CG    | 1:F:71:ASN:H     | 2.15                     | 0.58              |
| 1:O:58:GLN:O     | 1:O:62:THR:HG23  | 2.03                     | 0.58              |
| 1:B:55:LEU:HD12  | 1:B:55:LEU:O     | 2.03                     | 0.58              |
| 1:B:64:ILE:CD1   | 1:B:73:LEU:HD11  | 2.34                     | 0.58              |
| 1:F:123:VAL:HG21 | 1:H:63:ARG:HD3   | 1.85                     | 0.58              |
| 1:I:75:MET:HE2   | 1:I:75:MET:HA    | 1.85                     | 0.58              |
| 1:M:43:ALA:HB2   | 1:M:176:PRO:HD2  | 1.86                     | 0.58              |
| 1:B:43:ALA:O     | 1:B:205:ARG:HG3  | 2.04                     | 0.58              |
| 1:G:254:SER:OG   | 1:G:255:GLU:HG3  | 2.04                     | 0.58              |
| 1:H:190:ASN:CG   | 1:H:191:PRO:HD2  | 2.23                     | 0.58              |
| 1:A:254:SER:OG   | 1:A:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:B:288:LEU:HD13 | 1:K:86:GLN:NE2   | 2.19                     | 0.57              |
| 1:B:42:GLN:O     | 1:B:205:ARG:NH1  | 2.35                     | 0.57              |
| 1:H:194:ASN:OD1  | 1:H:196:ASP:HB2  | 2.04                     | 0.57              |
| 1:G:80:ILE:HG22  | 1:G:87:ILE:CD1   | 2.28                     | 0.57              |
| 1:H:254:SER:OG   | 1:H:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:H:264:PHE:HB3  | 1:P:248:PHE:HD2  | 1.70                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:254:SER:OG   | 1:I:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:B:87:ILE:CD1   | 1:B:208:PHE:HE1  | 2.16                     | 0.57              |
| 1:C:62:THR:CG2   | 1:C:63:ARG:HG3   | 2.34                     | 0.57              |
| 1:D:254:SER:OG   | 1:D:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:M:68:ALA:HB1   | 1:M:129:LEU:HD21 | 1.86                     | 0.57              |
| 1:B:122:PRO:HD2  | 1:B:123:VAL:H    | 1.70                     | 0.57              |
| 1:B:254:SER:OG   | 1:B:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:O:194:ASN:HD21 | 1:O:196:ASP:HB2  | 1.68                     | 0.57              |
| 1:E:254:SER:OG   | 1:E:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:I:84:THR:HB    | 1:I:86:GLN:HG2   | 1.87                     | 0.57              |
| 1:K:254:SER:OG   | 1:K:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:P:254:SER:OG   | 1:P:255:GLU:HG3  | 2.05                     | 0.57              |
| 1:B:49:LEU:CD1   | 1:B:202:GLY:HA3  | 2.35                     | 0.57              |
| 1:J:56:LEU:O     | 1:J:60:ILE:HG13  | 2.05                     | 0.57              |
| 1:A:79:THR:HG21  | 1:A:177:GLY:H    | 1.70                     | 0.57              |
| 1:J:254:SER:OG   | 1:J:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:M:254:SER:OG   | 1:M:255:GLU:HG3  | 2.04                     | 0.57              |
| 1:N:42:GLN:HG2   | 1:N:176:PRO:HG3  | 1.87                     | 0.57              |
| 1:C:120:LEU:CD2  | 1:C:122:PRO:HG3  | 2.35                     | 0.56              |
| 1:F:63:ARG:HE    | 1:F:127:HIS:CD2  | 2.22                     | 0.56              |
| 1:L:116:THR:CG2  | 1:L:117:ASN:N    | 2.68                     | 0.56              |
| 1:B:84:THR:HB    | 1:B:86:GLN:HG3   | 1.87                     | 0.56              |
| 1:A:61:SER:HB2   | 1:A:73:LEU:HD12  | 1.87                     | 0.56              |
| 1:C:40:TRP:CE2   | 1:C:41:ILE:HG23  | 2.39                     | 0.56              |
| 1:F:254:SER:OG   | 1:F:255:GLU:HG3  | 2.04                     | 0.56              |
| 1:N:254:SER:OG   | 1:N:255:GLU:HG3  | 2.04                     | 0.56              |
| 1:B:192:PHE:CE2  | 1:C:137:PRO:HB2  | 2.40                     | 0.56              |
| 1:C:254:SER:OG   | 1:C:255:GLU:HG3  | 2.05                     | 0.56              |
| 1:C:65:PRO:HG2   | 1:C:68:ALA:HB2   | 1.86                     | 0.56              |
| 1:K:61:SER:HA    | 1:K:64:ILE:HD12  | 1.86                     | 0.56              |
| 1:F:81:ASP:OD1   | 1:F:83:ASN:HB2   | 2.05                     | 0.56              |
| 1:O:254:SER:OG   | 1:O:255:GLU:HG3  | 2.04                     | 0.56              |
| 1:G:116:THR:HG22 | 1:G:117:ASN:N    | 2.21                     | 0.56              |
| 1:K:42:GLN:O     | 1:K:42:GLN:HG2   | 2.04                     | 0.56              |
| 1:L:254:SER:OG   | 1:L:255:GLU:HG3  | 2.04                     | 0.56              |
| 1:M:65:PRO:HA    | 1:N:64:ILE:O     | 2.06                     | 0.56              |
| 1:H:118:GLN:HG3  | 1:H:118:GLN:O    | 2.04                     | 0.56              |
| 1:B:133:ARG:HG3  | 1:B:190:ASN:HD21 | 1.71                     | 0.56              |
| 1:B:63:ARG:O     | 1:B:65:PRO:HD3   | 2.06                     | 0.56              |
| 1:K:129:LEU:HD23 | 1:K:191:PRO:CD   | 2.36                     | 0.56              |
| 1:C:76:ARG:HD3   | 1:C:198:ILE:HG13 | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:116:THR:CG2  | 1:D:117:ASN:N    | 2.69                     | 0.56              |
| 1:F:129:LEU:HD23 | 1:F:191:PRO:HG3  | 1.88                     | 0.56              |
| 1:C:264:PHE:HB3  | 1:K:248:PHE:CD2  | 2.41                     | 0.56              |
| 1:B:49:LEU:O     | 1:B:49:LEU:HD23  | 2.06                     | 0.56              |
| 1:I:123:VAL:HG21 | 1:L:63:ARG:NH1   | 2.20                     | 0.56              |
| 1:F:87:ILE:HD11  | 1:F:208:PHE:CE1  | 2.42                     | 0.55              |
| 1:A:65:PRO:HB3   | 1:B:62:THR:O     | 2.07                     | 0.55              |
| 1:B:84:THR:OG1   | 1:B:86:GLN:HG3   | 2.05                     | 0.55              |
| 1:C:264:PHE:HB3  | 1:K:248:PHE:HD2  | 1.70                     | 0.55              |
| 1:P:190:ASN:HA   | 1:P:192:PHE:H    | 1.72                     | 0.55              |
| 1:B:188:ASN:HD21 | 1:C:119:ASN:ND2  | 2.03                     | 0.55              |
| 1:I:59:LEU:HA    | 1:L:122:PRO:HG2  | 1.88                     | 0.55              |
| 1:O:87:ILE:HD11  | 1:O:208:PHE:HE1  | 1.70                     | 0.55              |
| 1:E:43:ALA:HB2   | 1:E:176:PRO:HD2  | 1.88                     | 0.55              |
| 1:F:45:SER:OG    | 1:F:112:ILE:HG12 | 2.06                     | 0.55              |
| 1:F:43:ALA:O     | 1:F:205:ARG:HG3  | 2.07                     | 0.55              |
| 1:F:55:LEU:HG    | 1:H:55:LEU:HD23  | 1.87                     | 0.55              |
| 1:A:87:ILE:HD12  | 1:A:176:PRO:HD3  | 1.88                     | 0.55              |
| 1:H:197:GLU:O    | 1:H:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:L:57:TYR:HE1   | 1:L:75:MET:HE3   | 1.72                     | 0.55              |
| 1:N:197:GLU:O    | 1:N:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:D:197:GLU:O    | 1:D:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:I:133:ARG:NH1  | 1:I:190:ASN:HD22 | 2.05                     | 0.55              |
| 1:I:197:GLU:O    | 1:I:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:J:197:GLU:O    | 1:J:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:K:158:TRP:CG   | 1:K:194:ASN:ND2  | 2.75                     | 0.55              |
| 1:L:197:GLU:O    | 1:L:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:D:116:THR:HG22 | 1:D:118:GLN:N    | 2.06                     | 0.55              |
| 1:E:87:ILE:HD11  | 1:E:208:PHE:HE1  | 1.72                     | 0.55              |
| 1:D:67:PHE:CD1   | 1:D:68:ALA:N     | 2.75                     | 0.55              |
| 1:F:197:GLU:O    | 1:F:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:F:64:ILE:HG21  | 1:F:69:SER:CB    | 2.37                     | 0.55              |
| 1:K:192:PHE:N    | 1:K:193:PRO:HD3  | 2.21                     | 0.55              |
| 1:N:158:TRP:CD1  | 1:N:194:ASN:ND2  | 2.75                     | 0.55              |
| 1:E:197:GLU:O    | 1:E:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:P:197:GLU:O    | 1:P:198:ILE:HD13 | 2.07                     | 0.55              |
| 1:B:80:ILE:HG13  | 1:B:80:ILE:O     | 2.06                     | 0.54              |
| 1:F:81:ASP:HB3   | 1:F:84:THR:HB    | 1.90                     | 0.54              |
| 1:K:197:GLU:O    | 1:K:198:ILE:HD13 | 2.07                     | 0.54              |
| 1:A:64:ILE:HG12  | 1:A:129:LEU:HD12 | 1.89                     | 0.54              |
| 1:C:278:ALA:HB3  | 1:C:279:PRO:HD3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:197:GLU:O    | 1:M:198:ILE:HD13 | 2.07                     | 0.54              |
| 1:N:120:LEU:O    | 1:N:122:PRO:HD3  | 2.06                     | 0.54              |
| 1:P:40:TRP:CE3   | 1:P:75:MET:HE1   | 2.42                     | 0.54              |
| 1:P:61:SER:HA    | 1:P:64:ILE:HD12  | 1.89                     | 0.54              |
| 1:B:197:GLU:O    | 1:B:198:ILE:HD13 | 2.07                     | 0.54              |
| 1:P:64:ILE:CD1   | 1:P:73:LEU:HD13  | 2.34                     | 0.54              |
| 1:A:48:TRP:CD2   | 1:A:118:GLN:HG2  | 2.43                     | 0.54              |
| 1:I:247:VAL:HG12 | 1:I:248:PHE:N    | 2.23                     | 0.54              |
| 1:K:247:VAL:HG12 | 1:K:248:PHE:N    | 2.23                     | 0.54              |
| 1:O:278:ALA:HB3  | 1:O:279:PRO:HD3  | 1.90                     | 0.54              |
| 1:C:186:SER:C    | 1:C:188:ASN:H    | 2.10                     | 0.54              |
| 1:I:182:ASN:HB2  | 1:I:195:GLN:O    | 2.07                     | 0.54              |
| 1:I:278:ALA:HB3  | 1:I:279:PRO:HD3  | 1.90                     | 0.54              |
| 1:O:197:GLU:O    | 1:O:198:ILE:HD13 | 2.07                     | 0.54              |
| 1:A:247:VAL:HG12 | 1:A:248:PHE:N    | 2.23                     | 0.54              |
| 1:B:192:PHE:CG   | 1:C:137:PRO:HG2  | 2.42                     | 0.54              |
| 1:C:247:VAL:HG12 | 1:C:248:PHE:N    | 2.23                     | 0.54              |
| 1:D:278:ALA:HB3  | 1:D:279:PRO:HD3  | 1.90                     | 0.54              |
| 1:G:197:GLU:O    | 1:G:198:ILE:HD13 | 2.07                     | 0.54              |
| 1:J:68:ALA:HB1   | 1:J:129:LEU:HD21 | 1.88                     | 0.54              |
| 1:J:283:ILE:O    | 1:L:268:LEU:HD13 | 2.07                     | 0.54              |
| 1:J:40:TRP:CE3   | 1:J:75:MET:HE2   | 2.43                     | 0.54              |
| 1:K:81:ASP:HB3   | 1:K:84:THR:OG1   | 2.07                     | 0.54              |
| 1:L:278:ALA:HB3  | 1:L:279:PRO:HD3  | 1.90                     | 0.54              |
| 1:P:65:PRO:CD    | 1:P:129:LEU:HD11 | 2.38                     | 0.54              |
| 1:A:79:THR:HG21  | 1:A:177:GLY:N    | 2.22                     | 0.54              |
| 1:E:116:THR:HG23 | 1:E:116:THR:O    | 2.08                     | 0.54              |
| 1:G:247:VAL:HG12 | 1:G:248:PHE:N    | 2.23                     | 0.54              |
| 1:K:278:ALA:HB3  | 1:K:279:PRO:HD3  | 1.90                     | 0.54              |
| 1:L:247:VAL:HG12 | 1:L:248:PHE:N    | 2.23                     | 0.54              |
| 1:M:247:VAL:HG12 | 1:M:248:PHE:N    | 2.23                     | 0.54              |
| 1:E:188:ASN:O    | 1:H:119:ASN:HB2  | 2.08                     | 0.54              |
| 1:F:192:PHE:CD1  | 1:G:137:PRO:HG2  | 2.43                     | 0.54              |
| 1:G:278:ALA:HB3  | 1:G:279:PRO:HD3  | 1.90                     | 0.54              |
| 1:A:49:LEU:HD13  | 1:A:202:GLY:HA3  | 1.89                     | 0.54              |
| 1:B:247:VAL:HG12 | 1:B:248:PHE:N    | 2.23                     | 0.54              |
| 1:C:118:GLN:HG3  | 1:C:118:GLN:O    | 2.08                     | 0.54              |
| 1:C:197:GLU:O    | 1:C:198:ILE:HD13 | 2.07                     | 0.54              |
| 1:E:40:TRP:HA    | 1:E:177:GLY:HA3  | 1.90                     | 0.54              |
| 1:N:74:HIS:HD2   | 1:N:183:ALA:O    | 1.91                     | 0.54              |
| 1:A:197:GLU:O    | 1:A:198:ILE:HD13 | 2.07                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:278:ALA:HB3  | 1:A:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:E:56:LEU:O     | 1:E:59:LEU:HB3   | 2.09                     | 0.53              |
| 1:F:278:ALA:HB3  | 1:F:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:I:122:PRO:O    | 1:I:126:THR:HG23 | 2.07                     | 0.53              |
| 1:K:40:TRP:CZ2   | 1:K:57:TYR:HB2   | 2.42                     | 0.53              |
| 1:E:79:THR:HG21  | 1:E:177:GLY:H    | 1.72                     | 0.53              |
| 1:E:97:ARG:NH1   | 1:E:99:ASP:OD2   | 2.41                     | 0.53              |
| 1:H:115:VAL:HB   | 1:H:138:SER:C    | 2.28                     | 0.53              |
| 1:C:194:ASN:C    | 1:C:196:ASP:H    | 2.10                     | 0.53              |
| 1:E:190:ASN:CG   | 1:E:191:PRO:HA   | 2.28                     | 0.53              |
| 1:H:97:ARG:NH1   | 1:H:99:ASP:OD2   | 2.41                     | 0.53              |
| 1:J:112:ILE:HG22 | 1:J:116:THR:HG22 | 1.90                     | 0.53              |
| 1:B:278:ALA:HB3  | 1:B:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:H:115:VAL:HB   | 1:H:138:SER:O    | 2.08                     | 0.53              |
| 1:H:278:ALA:HB3  | 1:H:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:C:87:ILE:HD11  | 1:C:230:ILE:HG21 | 1.87                     | 0.53              |
| 1:D:97:ARG:NH1   | 1:D:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:F:79:THR:CG2   | 1:F:177:GLY:H    | 2.20                     | 0.53              |
| 1:M:60:ILE:HG12  | 1:M:126:THR:HB   | 1.90                     | 0.53              |
| 1:N:247:VAL:HG12 | 1:N:248:PHE:N    | 2.23                     | 0.53              |
| 1:P:278:ALA:HB3  | 1:P:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:E:278:ALA:HB3  | 1:E:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:F:129:LEU:HD23 | 1:F:191:PRO:CD   | 2.38                     | 0.53              |
| 1:F:97:ARG:NH1   | 1:F:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:H:247:VAL:HG12 | 1:H:248:PHE:N    | 2.23                     | 0.53              |
| 1:K:120:LEU:HD12 | 1:K:125:ASP:HB2  | 1.91                     | 0.53              |
| 1:K:73:LEU:HD21  | 1:K:179:ILE:HG23 | 1.91                     | 0.53              |
| 1:L:97:ARG:NH1   | 1:L:99:ASP:OD2   | 2.41                     | 0.53              |
| 1:O:97:ARG:NH1   | 1:O:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:P:87:ILE:N     | 1:P:87:ILE:HD13  | 2.22                     | 0.53              |
| 1:E:49:LEU:HD23  | 1:E:49:LEU:C     | 2.29                     | 0.53              |
| 1:F:87:ILE:HD13  | 1:F:230:ILE:HG21 | 1.90                     | 0.53              |
| 1:J:247:VAL:HG12 | 1:J:248:PHE:N    | 2.23                     | 0.53              |
| 1:J:278:ALA:HB3  | 1:J:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:N:97:ARG:NH1   | 1:N:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:O:44:ALA:O     | 1:O:205:ARG:NH1  | 2.37                     | 0.53              |
| 1:O:63:ARG:HB2   | 1:O:63:ARG:HH11  | 1.73                     | 0.53              |
| 1:C:97:ARG:NH1   | 1:C:99:ASP:OD2   | 2.41                     | 0.53              |
| 1:P:97:ARG:NH1   | 1:P:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:I:64:ILE:O     | 1:J:65:PRO:HA    | 2.09                     | 0.53              |
| 1:I:97:ARG:NH1   | 1:I:99:ASP:OD2   | 2.41                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:97:ARG:NH1   | 1:K:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:O:247:VAL:HG12 | 1:O:248:PHE:N    | 2.23                     | 0.53              |
| 1:P:247:VAL:HG12 | 1:P:248:PHE:N    | 2.23                     | 0.53              |
| 1:B:97:ARG:NH1   | 1:B:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:F:46:LEU:HD11  | 1:F:115:VAL:O    | 2.09                     | 0.53              |
| 1:G:116:THR:CG2  | 1:G:117:ASN:N    | 2.72                     | 0.53              |
| 1:G:97:ARG:NH1   | 1:G:99:ASP:OD2   | 2.42                     | 0.53              |
| 1:I:63:ARG:CD    | 1:L:123:VAL:HG21 | 2.19                     | 0.53              |
| 1:M:278:ALA:HB3  | 1:M:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:D:254:SER:HB3  | 1:O:244:ILE:H    | 1.74                     | 0.53              |
| 1:A:80:ILE:HD11  | 1:A:176:PRO:HB3  | 1.91                     | 0.52              |
| 1:D:247:VAL:HG12 | 1:D:248:PHE:N    | 2.23                     | 0.52              |
| 1:J:97:ARG:NH1   | 1:J:99:ASP:OD2   | 2.42                     | 0.52              |
| 1:N:80:ILE:HD13  | 1:N:87:ILE:HA    | 1.91                     | 0.52              |
| 1:C:76:ARG:NH2   | 1:C:175:ALA:O    | 2.42                     | 0.52              |
| 1:E:247:VAL:HG12 | 1:E:248:PHE:N    | 2.23                     | 0.52              |
| 1:K:76:ARG:NH2   | 1:K:79:THR:HG22  | 2.24                     | 0.52              |
| 1:M:59:LEU:HD13  | 1:P:122:PRO:HB2  | 1.91                     | 0.52              |
| 1:A:97:ARG:NH1   | 1:A:99:ASP:OD2   | 2.41                     | 0.52              |
| 1:E:63:ARG:NH1   | 1:E:123:VAL:O    | 2.28                     | 0.52              |
| 1:I:55:LEU:HD23  | 1:L:55:LEU:HD23  | 1.90                     | 0.52              |
| 1:M:97:ARG:NH1   | 1:M:99:ASP:OD2   | 2.41                     | 0.52              |
| 1:O:78:GLN:OE1   | 1:O:78:GLN:HA    | 2.09                     | 0.52              |
| 1:C:70:PRO:HG2   | 1:C:71:ASN:H     | 1.74                     | 0.52              |
| 1:L:40:TRP:CE3   | 1:L:41:ILE:HG23  | 2.43                     | 0.52              |
| 1:M:45:SER:HA    | 1:M:205:ARG:HG2  | 1.90                     | 0.52              |
| 1:P:115:VAL:HG11 | 1:P:120:LEU:HD12 | 1.90                     | 0.52              |
| 1:I:79:THR:OG1   | 1:I:176:PRO:HA   | 2.09                     | 0.52              |
| 1:K:192:PHE:N    | 1:K:192:PHE:CD2  | 2.77                     | 0.52              |
| 1:N:278:ALA:HB3  | 1:N:279:PRO:HD3  | 1.90                     | 0.52              |
| 1:C:40:TRP:CZ2   | 1:C:41:ILE:HD13  | 2.44                     | 0.52              |
| 1:E:120:LEU:O    | 1:E:122:PRO:HD3  | 2.10                     | 0.52              |
| 1:F:247:VAL:HG12 | 1:F:248:PHE:N    | 2.23                     | 0.52              |
| 1:A:189:HIS:CD2  | 1:D:119:ASN:HB2  | 2.45                     | 0.52              |
| 1:D:70:PRO:CG    | 1:D:71:ASN:H     | 2.22                     | 0.52              |
| 1:G:40:TRP:HB3   | 1:G:75:MET:HG3   | 1.91                     | 0.52              |
| 1:I:46:LEU:CD1   | 1:I:202:GLY:HA2  | 2.31                     | 0.52              |
| 1:D:44:ALA:O     | 1:D:205:ARG:NH1  | 2.41                     | 0.52              |
| 1:F:64:ILE:HG22  | 1:F:69:SER:HB3   | 1.91                     | 0.52              |
| 1:L:56:LEU:HD12  | 1:L:56:LEU:C     | 2.28                     | 0.52              |
| 1:L:57:TYR:CE1   | 1:L:75:MET:CE    | 2.93                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:79:THR:HG21  | 1:M:177:GLY:H    | 1.75                     | 0.52              |
| 1:B:58:GLN:NE2   | 1:D:120:LEU:O    | 2.43                     | 0.51              |
| 1:L:40:TRP:CD2   | 1:L:41:ILE:HG23  | 2.45                     | 0.51              |
| 1:M:48:TRP:HH2   | 1:M:120:LEU:HD23 | 1.75                     | 0.51              |
| 1:H:265:ILE:HG22 | 1:H:267:ASP:HB2  | 1.92                     | 0.51              |
| 1:N:42:GLN:HG2   | 1:N:176:PRO:CG   | 2.40                     | 0.51              |
| 1:A:79:THR:HB    | 1:A:176:PRO:HA   | 1.91                     | 0.51              |
| 1:F:46:LEU:HG    | 1:F:113:PRO:HD2  | 1.93                     | 0.51              |
| 1:F:122:PRO:HG2  | 1:H:59:LEU:HA    | 1.93                     | 0.51              |
| 1:E:65:PRO:HA    | 1:F:65:PRO:HA    | 1.92                     | 0.51              |
| 1:G:87:ILE:HD11  | 1:G:176:PRO:CB   | 2.38                     | 0.51              |
| 1:I:48:TRP:CG    | 1:I:118:GLN:HG3  | 2.46                     | 0.51              |
| 1:I:76:ARG:HD2   | 1:I:198:ILE:HG13 | 1.93                     | 0.51              |
| 1:N:56:LEU:HD11  | 1:N:60:ILE:HD11  | 1.93                     | 0.51              |
| 1:O:66:SER:O     | 1:O:69:SER:O     | 2.28                     | 0.51              |
| 1:A:122:PRO:HG2  | 1:C:59:LEU:CA    | 2.39                     | 0.51              |
| 1:B:45:SER:HA    | 1:B:205:ARG:HG2  | 1.92                     | 0.51              |
| 1:H:133:ARG:HG3  | 1:H:133:ARG:O    | 2.09                     | 0.51              |
| 1:I:150:ASN:OD1  | 1:I:150:ASN:N    | 2.44                     | 0.51              |
| 1:J:122:PRO:HB2  | 1:K:59:LEU:HD13  | 1.93                     | 0.51              |
| 1:J:40:TRP:HB2   | 1:J:75:MET:HE2   | 1.93                     | 0.51              |
| 1:K:133:ARG:HG3  | 1:K:191:PRO:CB   | 2.25                     | 0.51              |
| 1:N:181:ILE:HG21 | 1:N:193:PRO:HB2  | 1.92                     | 0.51              |
| 1:P:181:ILE:HG21 | 1:P:193:PRO:HB2  | 1.92                     | 0.51              |
| 1:A:150:ASN:N    | 1:A:150:ASN:OD1  | 2.44                     | 0.51              |
| 1:H:194:ASN:C    | 1:H:196:ASP:H    | 2.12                     | 0.51              |
| 1:K:150:ASN:OD1  | 1:K:150:ASN:N    | 2.44                     | 0.51              |
| 1:J:69:SER:HB2   | 1:J:184:SER:O    | 2.11                     | 0.51              |
| 1:I:46:LEU:HD12  | 1:I:202:GLY:CA   | 2.33                     | 0.51              |
| 1:J:67:PHE:CZ    | 1:J:189:HIS:CD2  | 2.99                     | 0.51              |
| 1:N:150:ASN:OD1  | 1:N:150:ASN:N    | 2.44                     | 0.51              |
| 1:B:181:ILE:HG21 | 1:B:193:PRO:HB2  | 1.93                     | 0.50              |
| 1:B:87:ILE:HD12  | 1:B:208:PHE:HE1  | 1.76                     | 0.50              |
| 1:F:250:HIS:O    | 1:F:253:HIS:HB2  | 2.12                     | 0.50              |
| 1:E:250:HIS:O    | 1:E:253:HIS:HB2  | 2.12                     | 0.50              |
| 1:H:264:PHE:CB   | 1:P:248:PHE:CD2  | 2.93                     | 0.50              |
| 1:M:129:LEU:HD23 | 1:M:191:PRO:HD3  | 1.94                     | 0.50              |
| 1:D:254:SER:HA   | 1:O:246:LYS:HB2  | 1.93                     | 0.50              |
| 1:A:48:TRP:CG    | 1:A:118:GLN:CG   | 2.94                     | 0.50              |
| 1:C:120:LEU:HD12 | 1:C:125:ASP:HB2  | 1.93                     | 0.50              |
| 1:E:288:LEU:HD13 | 1:P:86:GLN:HE21  | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:40:TRP:HA    | 1:J:177:GLY:HA3  | 1.94                     | 0.50              |
| 1:K:250:HIS:O    | 1:K:253:HIS:HB2  | 2.12                     | 0.50              |
| 1:K:73:LEU:HD21  | 1:K:179:ILE:CG2  | 2.41                     | 0.50              |
| 1:N:250:HIS:O    | 1:N:253:HIS:HB2  | 2.12                     | 0.50              |
| 1:F:87:ILE:O     | 1:F:89:ILE:HG13  | 2.12                     | 0.50              |
| 1:I:250:HIS:O    | 1:I:253:HIS:HB2  | 2.12                     | 0.50              |
| 1:G:264:PHE:CE2  | 1:L:236:ASN:HA   | 2.45                     | 0.50              |
| 1:M:250:HIS:O    | 1:M:253:HIS:HB2  | 2.12                     | 0.50              |
| 1:O:45:SER:HA    | 1:O:205:ARG:HG2  | 1.94                     | 0.50              |
| 1:P:63:ARG:NH2   | 1:P:126:THR:OG1  | 2.44                     | 0.50              |
| 1:C:150:ASN:N    | 1:C:150:ASN:OD1  | 2.44                     | 0.50              |
| 1:G:250:HIS:O    | 1:G:253:HIS:HB2  | 2.12                     | 0.50              |
| 1:H:262:LYS:C    | 1:H:264:PHE:H    | 2.14                     | 0.50              |
| 1:L:182:ASN:HB2  | 1:L:195:GLN:O    | 2.11                     | 0.50              |
| 1:N:49:LEU:HD13  | 1:N:202:GLY:HA3  | 1.93                     | 0.50              |
| 1:C:39:THR:HA    | 1:C:42:GLN:CG    | 2.41                     | 0.49              |
| 1:E:129:LEU:HD23 | 1:E:191:PRO:CG   | 2.42                     | 0.49              |
| 1:E:192:PHE:CD1  | 1:H:137:PRO:HG2  | 2.47                     | 0.49              |
| 1:E:49:LEU:HD21  | 1:E:56:LEU:CD2   | 2.40                     | 0.49              |
| 1:F:181:ILE:HG21 | 1:F:193:PRO:HB2  | 1.93                     | 0.49              |
| 1:H:185:PHE:CB   | 1:H:189:HIS:HD2  | 2.18                     | 0.49              |
| 1:B:49:LEU:C     | 1:B:49:LEU:HD23  | 2.33                     | 0.49              |
| 1:D:40:TRP:HA    | 1:D:177:GLY:HA3  | 1.94                     | 0.49              |
| 1:J:250:HIS:O    | 1:J:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:L:250:HIS:O    | 1:L:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:M:79:THR:HB    | 1:M:176:PRO:HA   | 1.94                     | 0.49              |
| 1:F:61:SER:HB3   | 1:F:73:LEU:HD23  | 1.95                     | 0.49              |
| 1:P:250:HIS:O    | 1:P:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:D:250:HIS:O    | 1:D:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:I:63:ARG:NH1   | 1:I:63:ARG:HG2   | 2.28                     | 0.49              |
| 1:J:75:MET:HE3   | 1:J:179:ILE:HG13 | 1.95                     | 0.49              |
| 1:K:158:TRP:CD1  | 1:K:194:ASN:ND2  | 2.80                     | 0.49              |
| 1:I:123:VAL:CG2  | 1:L:63:ARG:NH1   | 2.75                     | 0.49              |
| 1:O:250:HIS:O    | 1:O:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:P:39:THR:HA    | 1:P:42:GLN:HB2   | 1.93                     | 0.49              |
| 1:M:74:HIS:HD2   | 1:M:183:ALA:O    | 1.95                     | 0.49              |
| 1:B:232:PRO:HA   | 1:B:235:LEU:HG   | 1.95                     | 0.49              |
| 1:E:192:PHE:N    | 1:E:193:PRO:HD3  | 2.28                     | 0.49              |
| 1:F:87:ILE:HD11  | 1:F:208:PHE:HE1  | 1.78                     | 0.49              |
| 1:M:57:TYR:CD2   | 1:M:57:TYR:C     | 2.86                     | 0.49              |
| 1:I:76:ARG:HH21  | 1:I:93:HIS:HB3   | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:64:ILE:HG12  | 1:J:129:LEU:CD1  | 2.43                     | 0.49              |
| 1:K:232:PRO:HA   | 1:K:235:LEU:HG   | 1.95                     | 0.49              |
| 1:P:40:TRP:CE3   | 1:P:75:MET:CE    | 2.96                     | 0.49              |
| 1:A:250:HIS:O    | 1:A:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:B:250:HIS:O    | 1:B:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:F:232:PRO:HA   | 1:F:235:LEU:HG   | 1.95                     | 0.49              |
| 1:H:250:HIS:O    | 1:H:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:H:104:ASN:HB2  | 1:H:256:GLY:O    | 2.13                     | 0.49              |
| 1:H:265:ILE:HG22 | 1:H:267:ASP:CB   | 2.42                     | 0.49              |
| 1:L:150:ASN:OD1  | 1:L:150:ASN:N    | 2.44                     | 0.49              |
| 1:L:232:PRO:HA   | 1:L:235:LEU:HG   | 1.95                     | 0.49              |
| 1:A:70:PRO:HG2   | 1:A:71:ASN:ND2   | 2.28                     | 0.49              |
| 1:A:77:GLU:O     | 1:A:78:GLN:HB2   | 2.13                     | 0.49              |
| 1:B:104:ASN:HB2  | 1:B:256:GLY:O    | 2.13                     | 0.49              |
| 1:C:250:HIS:O    | 1:C:253:HIS:HB2  | 2.12                     | 0.49              |
| 1:G:254:SER:OG   | 1:L:242:SER:HA   | 2.12                     | 0.49              |
| 1:I:59:LEU:HD21  | 1:I:126:THR:HG21 | 1.93                     | 0.49              |
| 1:J:115:VAL:HG23 | 1:J:138:SER:O    | 2.13                     | 0.49              |
| 1:J:69:SER:OG    | 1:J:69:SER:O     | 2.27                     | 0.49              |
| 1:K:104:ASN:HB2  | 1:K:256:GLY:O    | 2.13                     | 0.49              |
| 1:O:232:PRO:HA   | 1:O:235:LEU:HG   | 1.95                     | 0.49              |
| 1:N:55:LEU:CD2   | 1:O:55:LEU:HD23  | 2.43                     | 0.49              |
| 1:A:192:PHE:CG   | 1:D:137:PRO:HG2  | 2.48                     | 0.48              |
| 1:B:48:TRP:HB2   | 1:B:118:GLN:HG3  | 1.95                     | 0.48              |
| 1:E:79:THR:HG21  | 1:E:177:GLY:N    | 2.28                     | 0.48              |
| 1:I:232:PRO:HA   | 1:I:235:LEU:HG   | 1.95                     | 0.48              |
| 1:J:112:ILE:HG22 | 1:J:116:THR:CG2  | 2.42                     | 0.48              |
| 1:O:84:THR:OG1   | 1:O:86:GLN:HG2   | 2.13                     | 0.48              |
| 1:P:232:PRO:HA   | 1:P:235:LEU:HG   | 1.95                     | 0.48              |
| 1:P:59:LEU:HD12  | 1:P:63:ARG:HH12  | 1.77                     | 0.48              |
| 1:E:104:ASN:HB2  | 1:E:256:GLY:O    | 2.13                     | 0.48              |
| 1:E:79:THR:OG1   | 1:E:176:PRO:HA   | 2.13                     | 0.48              |
| 1:G:76:ARG:HD3   | 1:G:198:ILE:HG13 | 1.94                     | 0.48              |
| 1:K:81:ASP:HB3   | 1:K:84:THR:HG1   | 1.78                     | 0.48              |
| 1:M:63:ARG:NH1   | 1:M:123:VAL:O    | 2.34                     | 0.48              |
| 1:P:190:ASN:HB2  | 1:P:191:PRO:CA   | 2.32                     | 0.48              |
| 1:E:232:PRO:HA   | 1:E:235:LEU:HG   | 1.95                     | 0.48              |
| 1:J:60:ILE:HG12  | 1:J:126:THR:HB   | 1.95                     | 0.48              |
| 1:F:63:ARG:HH11  | 1:H:123:VAL:HG21 | 1.79                     | 0.48              |
| 1:O:63:ARG:CB    | 1:O:63:ARG:HH11  | 2.25                     | 0.48              |
| 1:C:104:ASN:HB2  | 1:C:256:GLY:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:40:TRP:CE3   | 1:D:41:ILE:CG2   | 2.96                     | 0.48              |
| 1:G:158:TRP:CD1  | 1:G:194:ASN:HB3  | 2.48                     | 0.48              |
| 1:J:123:VAL:HG11 | 1:K:63:ARG:NH2   | 2.29                     | 0.48              |
| 1:K:81:ASP:OD1   | 1:K:84:THR:HG23  | 2.14                     | 0.48              |
| 1:M:104:ASN:HB2  | 1:M:256:GLY:O    | 2.13                     | 0.48              |
| 1:M:49:LEU:HD22  | 1:M:202:GLY:HA3  | 1.95                     | 0.48              |
| 1:P:182:ASN:HB2  | 1:P:195:GLN:O    | 2.11                     | 0.48              |
| 1:P:242:SER:O    | 1:P:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:B:69:SER:OG    | 1:B:69:SER:O     | 2.26                     | 0.48              |
| 1:D:129:LEU:HD23 | 1:D:191:PRO:CD   | 2.44                     | 0.48              |
| 1:F:242:SER:O    | 1:F:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:H:242:SER:O    | 1:H:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:H:40:TRP:CH2   | 1:H:57:TYR:HA    | 2.48                     | 0.48              |
| 1:I:45:SER:CB    | 1:I:205:ARG:HG2  | 2.43                     | 0.48              |
| 1:B:46:LEU:HA    | 1:B:46:LEU:HD23  | 1.53                     | 0.48              |
| 1:D:40:TRP:CZ3   | 1:D:41:ILE:CG2   | 2.97                     | 0.48              |
| 1:G:242:SER:O    | 1:G:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:H:259:MET:CG   | 1:H:264:PHE:CE2  | 2.96                     | 0.48              |
| 1:I:242:SER:O    | 1:I:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:M:242:SER:O    | 1:M:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:P:104:ASN:HB2  | 1:P:256:GLY:O    | 2.13                     | 0.48              |
| 1:B:242:SER:O    | 1:B:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:C:65:PRO:HB3   | 1:C:67:PHE:CE2   | 2.48                     | 0.48              |
| 1:G:39:THR:CA    | 1:G:42:GLN:HG3   | 2.42                     | 0.48              |
| 1:N:104:ASN:HB2  | 1:N:256:GLY:O    | 2.13                     | 0.48              |
| 1:H:265:ILE:C    | 1:H:267:ASP:H    | 2.16                     | 0.48              |
| 1:K:192:PHE:N    | 1:K:192:PHE:HD2  | 2.12                     | 0.48              |
| 1:D:232:PRO:HA   | 1:D:235:LEU:HG   | 1.95                     | 0.48              |
| 1:F:104:ASN:HB2  | 1:F:256:GLY:O    | 2.13                     | 0.48              |
| 1:G:232:PRO:HA   | 1:G:235:LEU:HG   | 1.95                     | 0.48              |
| 1:H:232:PRO:HA   | 1:H:235:LEU:HG   | 1.95                     | 0.48              |
| 1:I:104:ASN:HB2  | 1:I:256:GLY:O    | 2.13                     | 0.48              |
| 1:J:242:SER:O    | 1:J:243:ASN:HB2  | 2.14                     | 0.48              |
| 1:J:104:ASN:HB2  | 1:J:256:GLY:O    | 2.13                     | 0.48              |
| 1:L:104:ASN:HB2  | 1:L:256:GLY:O    | 2.13                     | 0.48              |
| 1:M:133:ARG:NH1  | 1:M:190:ASN:CB   | 2.75                     | 0.48              |
| 1:N:80:ILE:CG2   | 1:N:81:ASP:N     | 2.76                     | 0.48              |
| 1:O:104:ASN:HB2  | 1:O:256:GLY:O    | 2.13                     | 0.48              |
| 1:P:64:ILE:HA    | 1:P:129:LEU:HD11 | 1.96                     | 0.48              |
| 1:C:264:PHE:CB   | 1:K:248:PHE:CD2  | 2.97                     | 0.47              |
| 1:J:232:PRO:HA   | 1:J:235:LEU:HG   | 1.95                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:48:TRP:HB2  | 1:A:118:GLN:HE21 | 1.79                     | 0.47              |
| 1:C:242:SER:O   | 1:C:243:ASN:HB2  | 2.14                     | 0.47              |
| 1:F:120:LEU:O   | 1:F:120:LEU:HD13 | 2.13                     | 0.47              |
| 1:K:40:TRP:CE3  | 1:K:75:MET:CE    | 2.97                     | 0.47              |
| 1:P:150:ASN:N   | 1:P:150:ASN:OD1  | 2.44                     | 0.47              |
| 1:P:40:TRP:CE3  | 1:P:41:ILE:HG23  | 2.50                     | 0.47              |
| 1:B:87:ILE:HD12 | 1:B:208:PHE:CE1  | 2.49                     | 0.47              |
| 1:N:80:ILE:HG22 | 1:N:81:ASP:N     | 2.28                     | 0.47              |
| 1:P:65:PRO:HD3  | 1:P:129:LEU:HD13 | 1.95                     | 0.47              |
| 1:C:232:PRO:HA  | 1:C:235:LEU:HG   | 1.95                     | 0.47              |
| 1:D:39:THR:HA   | 1:D:42:GLN:CG    | 2.44                     | 0.47              |
| 1:G:120:LEU:CD1 | 1:G:125:ASP:HB2  | 2.44                     | 0.47              |
| 1:G:104:ASN:HB2 | 1:G:256:GLY:O    | 2.13                     | 0.47              |
| 1:I:63:ARG:HH11 | 1:I:63:ARG:HG2   | 1.78                     | 0.47              |
| 1:N:242:SER:O   | 1:N:243:ASN:HB2  | 2.14                     | 0.47              |
| 1:A:242:SER:O   | 1:A:243:ASN:HB2  | 2.14                     | 0.47              |
| 1:A:60:ILE:HG22 | 1:A:73:LEU:HD11  | 1.95                     | 0.47              |
| 1:B:41:ILE:HG22 | 1:B:201:PRO:O    | 2.15                     | 0.47              |
| 1:C:70:PRO:CG   | 1:C:71:ASN:H     | 2.26                     | 0.47              |
| 1:D:242:SER:O   | 1:D:243:ASN:HB2  | 2.14                     | 0.47              |
| 1:E:133:ARG:NH1 | 1:E:190:ASN:HD22 | 2.10                     | 0.47              |
| 1:I:43:ALA:H    | 1:I:176:PRO:HG2  | 1.79                     | 0.47              |
| 1:I:189:HIS:CD2 | 1:K:119:ASN:HB2  | 2.50                     | 0.47              |
| 1:K:89:ILE:O    | 1:K:89:ILE:HG22  | 2.15                     | 0.47              |
| 1:O:65:PRO:HG2  | 1:O:68:ALA:HB3   | 1.96                     | 0.47              |
| 1:O:89:ILE:HG22 | 1:O:89:ILE:O     | 2.15                     | 0.47              |
| 1:A:188:ASN:O   | 1:D:119:ASN:ND2  | 2.43                     | 0.47              |
| 1:A:190:ASN:ND2 | 1:A:191:PRO:HA   | 2.30                     | 0.47              |
| 1:A:104:ASN:HB2 | 1:A:256:GLY:O    | 2.13                     | 0.47              |
| 1:D:104:ASN:HB2 | 1:D:256:GLY:O    | 2.13                     | 0.47              |
| 1:F:41:ILE:HG22 | 1:F:201:PRO:HB2  | 1.97                     | 0.47              |
| 1:F:89:ILE:HG22 | 1:F:89:ILE:O     | 2.15                     | 0.47              |
| 1:G:70:PRO:HD2  | 1:G:71:ASN:H     | 1.80                     | 0.47              |
| 1:I:89:ILE:HG22 | 1:I:89:ILE:O     | 2.15                     | 0.47              |
| 1:J:40:TRP:CE3  | 1:J:75:MET:CE    | 2.97                     | 0.47              |
| 1:K:60:ILE:HG22 | 1:K:61:SER:N     | 2.29                     | 0.47              |
| 1:B:288:LEU:CD1 | 1:K:86:GLN:NE2   | 2.78                     | 0.47              |
| 1:M:232:PRO:HA  | 1:M:235:LEU:HG   | 1.95                     | 0.47              |
| 1:N:124:GLU:HG2 | 1:N:124:GLU:H    | 1.57                     | 0.47              |
| 1:C:120:LEU:HG  | 1:C:121:SER:N    | 2.29                     | 0.47              |
| 1:E:89:ILE:HG22 | 1:E:89:ILE:O     | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:188:ASN:C    | 1:I:189:HIS:HD2  | 2.18                     | 0.47              |
| 1:L:242:SER:O    | 1:L:243:ASN:HB2  | 2.14                     | 0.47              |
| 1:L:89:ILE:HG22  | 1:L:89:ILE:O     | 2.15                     | 0.47              |
| 1:N:48:TRP:CZ3   | 1:N:120:LEU:HD23 | 2.49                     | 0.47              |
| 1:P:115:VAL:CG1  | 1:P:120:LEU:HD12 | 2.44                     | 0.47              |
| 1:A:232:PRO:HA   | 1:A:235:LEU:HG   | 1.95                     | 0.47              |
| 1:D:142:SER:OG   | 1:D:197:GLU:OE2  | 2.27                     | 0.47              |
| 1:H:89:ILE:HG22  | 1:H:89:ILE:O     | 2.15                     | 0.47              |
| 1:N:40:TRP:HA    | 1:N:177:GLY:HA3  | 1.97                     | 0.47              |
| 1:N:232:PRO:HA   | 1:N:235:LEU:HG   | 1.95                     | 0.47              |
| 1:N:89:ILE:O     | 1:N:89:ILE:HG22  | 2.15                     | 0.47              |
| 1:C:190:ASN:OD1  | 1:C:191:PRO:HD2  | 2.15                     | 0.47              |
| 1:D:89:ILE:O     | 1:D:89:ILE:HG22  | 2.15                     | 0.47              |
| 1:F:73:LEU:HG    | 1:F:75:MET:HE2   | 1.95                     | 0.47              |
| 1:J:133:ARG:NH1  | 1:J:192:PHE:HE2  | 2.12                     | 0.47              |
| 1:J:89:ILE:HG22  | 1:J:89:ILE:O     | 2.15                     | 0.47              |
| 1:O:242:SER:O    | 1:O:243:ASN:HB2  | 2.14                     | 0.47              |
| 1:E:242:SER:O    | 1:E:243:ASN:HB2  | 2.14                     | 0.47              |
| 1:E:64:ILE:H     | 1:E:64:ILE:HD12  | 1.79                     | 0.47              |
| 1:F:129:LEU:HD23 | 1:F:191:PRO:CG   | 2.44                     | 0.47              |
| 1:H:150:ASN:N    | 1:H:150:ASN:OD1  | 2.44                     | 0.47              |
| 1:L:43:ALA:O     | 1:L:205:ARG:HG3  | 2.15                     | 0.47              |
| 1:M:40:TRP:CZ2   | 1:M:57:TYR:HB2   | 2.49                     | 0.47              |
| 1:O:150:ASN:N    | 1:O:150:ASN:OD1  | 2.44                     | 0.47              |
| 1:P:133:ARG:HB2  | 1:P:191:PRO:HB3  | 1.97                     | 0.47              |
| 1:C:98:TRP:CH2   | 1:C:170:ARG:HD2  | 2.50                     | 0.46              |
| 1:D:70:PRO:HG2   | 1:D:71:ASN:H     | 1.80                     | 0.46              |
| 1:G:147:ARG:HD3  | 1:G:156:THR:O    | 2.16                     | 0.46              |
| 1:H:98:TRP:CH2   | 1:H:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:I:142:SER:OG   | 1:I:197:GLU:OE2  | 2.27                     | 0.46              |
| 1:I:68:ALA:O     | 1:I:185:PHE:HA   | 2.15                     | 0.46              |
| 1:K:147:ARG:HD3  | 1:K:156:THR:O    | 2.16                     | 0.46              |
| 1:O:81:ASP:OD1   | 1:O:82:SER:N     | 2.47                     | 0.46              |
| 1:P:64:ILE:HA    | 1:P:129:LEU:CD1  | 2.46                     | 0.46              |
| 1:A:122:PRO:HB2  | 1:C:59:LEU:HD13  | 1.97                     | 0.46              |
| 1:C:89:ILE:HG22  | 1:C:89:ILE:O     | 2.15                     | 0.46              |
| 1:D:40:TRP:HB2   | 1:D:75:MET:SD    | 2.55                     | 0.46              |
| 1:E:147:ARG:HD3  | 1:E:156:THR:O    | 2.16                     | 0.46              |
| 1:E:133:ARG:CD   | 1:E:190:ASN:ND2  | 2.73                     | 0.46              |
| 1:H:59:LEU:HD21  | 1:H:122:PRO:HB3  | 1.96                     | 0.46              |
| 1:I:188:ASN:O    | 1:I:189:HIS:HD2  | 1.99                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:98:TRP:CH2   | 1:K:170:ARG:HD2  | 2.50                     | 0.46              |
| 1:K:190:ASN:CB   | 1:K:191:PRO:HA   | 2.29                     | 0.46              |
| 1:J:59:LEU:HD13  | 1:K:59:LEU:HD21  | 1.97                     | 0.46              |
| 1:L:147:ARG:HD3  | 1:L:156:THR:O    | 2.16                     | 0.46              |
| 1:L:45:SER:HA    | 1:L:205:ARG:CG   | 2.44                     | 0.46              |
| 1:O:120:LEU:HD12 | 1:O:125:ASP:HB2  | 1.97                     | 0.46              |
| 1:O:98:TRP:CH2   | 1:O:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:O:81:ASP:HB3   | 1:O:84:THR:OG1   | 2.15                     | 0.46              |
| 1:A:55:LEU:HG    | 1:C:55:LEU:HD23  | 1.97                     | 0.46              |
| 1:D:98:TRP:CH2   | 1:D:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:E:153:LEU:HD13 | 1:P:86:GLN:HG2   | 1.97                     | 0.46              |
| 1:F:98:TRP:CH2   | 1:F:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:H:147:ARG:HD3  | 1:H:156:THR:O    | 2.16                     | 0.46              |
| 1:J:98:TRP:CH2   | 1:J:170:ARG:HD2  | 2.50                     | 0.46              |
| 1:N:87:ILE:CD1   | 1:N:208:PHE:CD1  | 2.99                     | 0.46              |
| 1:N:98:TRP:CH2   | 1:N:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:B:192:PHE:CZ   | 1:C:137:PRO:HB2  | 2.51                     | 0.46              |
| 1:D:150:ASN:OD1  | 1:D:150:ASN:N    | 2.44                     | 0.46              |
| 1:E:123:VAL:HG21 | 1:G:63:ARG:HD2   | 1.98                     | 0.46              |
| 1:F:150:ASN:N    | 1:F:150:ASN:OD1  | 2.44                     | 0.46              |
| 1:G:98:TRP:CH2   | 1:G:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:I:147:ARG:HD3  | 1:I:156:THR:O    | 2.16                     | 0.46              |
| 1:M:98:TRP:CH2   | 1:M:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:N:46:LEU:HD22  | 1:N:48:TRP:CE2   | 2.51                     | 0.46              |
| 1:A:147:ARG:HD3  | 1:A:156:THR:O    | 2.16                     | 0.46              |
| 1:B:98:TRP:CH2   | 1:B:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:D:147:ARG:HD3  | 1:D:156:THR:O    | 2.16                     | 0.46              |
| 1:I:121:SER:HA   | 1:I:122:PRO:HD3  | 1.68                     | 0.46              |
| 1:I:98:TRP:CH2   | 1:I:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:B:153:LEU:HD21 | 1:K:84:THR:O     | 2.16                     | 0.46              |
| 1:L:158:TRP:CD1  | 1:L:194:ASN:ND2  | 2.84                     | 0.46              |
| 1:M:68:ALA:CB    | 1:M:129:LEU:HD21 | 2.46                     | 0.46              |
| 1:N:147:ARG:HD3  | 1:N:156:THR:O    | 2.16                     | 0.46              |
| 1:N:46:LEU:HD22  | 1:N:48:TRP:NE1   | 2.30                     | 0.46              |
| 1:N:40:TRP:HB3   | 1:N:75:MET:HG3   | 1.98                     | 0.46              |
| 1:C:147:ARG:HD3  | 1:C:156:THR:O    | 2.16                     | 0.46              |
| 1:E:49:LEU:HD23  | 1:E:49:LEU:O     | 2.15                     | 0.46              |
| 1:F:147:ARG:HD3  | 1:F:156:THR:O    | 2.16                     | 0.46              |
| 1:H:259:MET:HG2  | 1:H:264:PHE:CZ   | 2.50                     | 0.46              |
| 1:H:135:ASN:ND2  | 1:H:271:ASN:HD21 | 2.13                     | 0.46              |
| 1:I:58:GLN:O     | 1:I:62:THR:HG22  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:133:ARG:HB2  | 1:K:191:PRO:CG   | 2.46                     | 0.46              |
| 1:K:242:SER:O    | 1:K:243:ASN:HB2  | 2.14                     | 0.46              |
| 1:N:37:ASP:OD1   | 1:N:39:THR:OG1   | 2.32                     | 0.46              |
| 1:D:254:SER:HB3  | 1:O:244:ILE:N    | 2.29                     | 0.46              |
| 1:A:98:TRP:CH2   | 1:A:170:ARG:HD2  | 2.51                     | 0.46              |
| 1:B:133:ARG:O    | 1:B:277:PHE:HZ   | 1.98                     | 0.46              |
| 1:B:192:PHE:HZ   | 1:C:115:VAL:HG22 | 1.80                     | 0.46              |
| 1:C:65:PRO:CB    | 1:C:67:PHE:CE2   | 2.99                     | 0.46              |
| 1:G:73:LEU:HD22  | 1:G:179:ILE:CG2  | 2.46                     | 0.46              |
| 1:G:37:ASP:HB2   | 1:G:38:ASN:H     | 1.56                     | 0.46              |
| 1:G:40:TRP:CB    | 1:G:75:MET:HG3   | 2.45                     | 0.46              |
| 1:J:147:ARG:HD3  | 1:J:156:THR:O    | 2.16                     | 0.46              |
| 1:M:55:LEU:HD12  | 1:M:55:LEU:C     | 2.35                     | 0.46              |
| 1:A:122:PRO:O    | 1:A:126:THR:HG23 | 2.16                     | 0.46              |
| 1:A:89:ILE:HG22  | 1:A:89:ILE:O     | 2.15                     | 0.46              |
| 1:B:89:ILE:HG22  | 1:B:89:ILE:O     | 2.15                     | 0.46              |
| 1:C:186:SER:O    | 1:C:188:ASN:N    | 2.45                     | 0.46              |
| 1:E:81:ASP:HB3   | 1:E:84:THR:OG1   | 2.15                     | 0.46              |
| 1:H:189:HIS:CE1  | 1:H:193:PRO:HB3  | 2.51                     | 0.46              |
| 1:H:247:VAL:CG1  | 1:H:248:PHE:N    | 2.79                     | 0.46              |
| 1:I:48:TRP:CD1   | 1:I:118:GLN:HB2  | 2.50                     | 0.46              |
| 1:I:247:VAL:CG1  | 1:I:248:PHE:N    | 2.79                     | 0.46              |
| 1:N:64:ILE:HA    | 1:N:65:PRO:HD3   | 1.80                     | 0.46              |
| 1:O:147:ARG:HD3  | 1:O:156:THR:O    | 2.16                     | 0.46              |
| 1:P:247:VAL:CG1  | 1:P:248:PHE:N    | 2.79                     | 0.46              |
| 1:A:133:ARG:HH11 | 1:A:190:ASN:HD22 | 1.64                     | 0.46              |
| 1:C:187:ARG:HB3  | 1:C:193:PRO:HG3  | 1.97                     | 0.46              |
| 1:E:150:ASN:OD1  | 1:E:150:ASN:N    | 2.44                     | 0.46              |
| 1:O:40:TRP:HB2   | 1:O:75:MET:SD    | 2.56                     | 0.46              |
| 1:P:147:ARG:HD3  | 1:P:156:THR:O    | 2.16                     | 0.46              |
| 1:P:89:ILE:O     | 1:P:89:ILE:HG22  | 2.15                     | 0.46              |
| 1:B:147:ARG:HD3  | 1:B:156:THR:O    | 2.16                     | 0.46              |
| 1:D:192:PHE:N    | 1:D:193:PRO:HD3  | 2.31                     | 0.46              |
| 1:G:74:HIS:O     | 1:G:180:ASP:HB3  | 2.16                     | 0.46              |
| 1:K:84:THR:OG1   | 1:K:85:GLY:N     | 2.48                     | 0.46              |
| 1:M:283:ILE:O    | 1:O:268:LEU:HD13 | 2.16                     | 0.46              |
| 1:A:123:VAL:HG21 | 1:C:63:ARG:HD2   | 1.97                     | 0.45              |
| 1:D:80:ILE:HG12  | 1:D:87:ILE:HD13  | 1.97                     | 0.45              |
| 1:M:133:ARG:HH11 | 1:M:190:ASN:CB   | 2.21                     | 0.45              |
| 1:M:147:ARG:HD3  | 1:M:156:THR:O    | 2.16                     | 0.45              |
| 1:M:89:ILE:HG22  | 1:M:89:ILE:O     | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:247:VAL:CG1  | 1:N:248:PHE:N    | 2.79                     | 0.45              |
| 1:A:226:ASN:HA   | 1:A:227:PRO:HD2  | 1.82                     | 0.45              |
| 1:B:142:SER:OG   | 1:B:197:GLU:OE2  | 2.27                     | 0.45              |
| 1:C:247:VAL:CG1  | 1:C:248:PHE:N    | 2.79                     | 0.45              |
| 1:E:57:TYR:CD2   | 1:E:58:GLN:N     | 2.84                     | 0.45              |
| 1:F:87:ILE:CD1   | 1:F:208:PHE:CE1  | 3.00                     | 0.45              |
| 1:F:65:PRO:HD2   | 1:F:129:LEU:HD13 | 1.96                     | 0.45              |
| 1:F:61:SER:HB3   | 1:F:73:LEU:CD2   | 2.47                     | 0.45              |
| 1:K:64:ILE:HA    | 1:K:129:LEU:HD11 | 1.98                     | 0.45              |
| 1:K:190:ASN:CA   | 1:K:192:PHE:CD2  | 2.93                     | 0.45              |
| 1:N:48:TRP:CZ3   | 1:N:120:LEU:CD2  | 2.99                     | 0.45              |
| 1:E:40:TRP:CZ2   | 1:E:57:TYR:HB2   | 2.51                     | 0.45              |
| 1:F:70:PRO:CG    | 1:F:71:ASN:N     | 2.78                     | 0.45              |
| 1:G:247:VAL:CG1  | 1:G:248:PHE:N    | 2.79                     | 0.45              |
| 1:N:192:PHE:CG   | 1:P:137:PRO:HG2  | 2.51                     | 0.45              |
| 1:P:61:SER:C     | 1:P:63:ARG:H     | 2.20                     | 0.45              |
| 1:I:56:LEU:CD2   | 1:I:60:ILE:HD11  | 2.46                     | 0.45              |
| 1:I:75:MET:HE2   | 1:I:75:MET:CA    | 2.46                     | 0.45              |
| 1:K:247:VAL:CG1  | 1:K:248:PHE:N    | 2.79                     | 0.45              |
| 1:L:247:VAL:CG1  | 1:L:248:PHE:N    | 2.79                     | 0.45              |
| 1:L:73:LEU:CD2   | 1:L:75:MET:HE1   | 2.46                     | 0.45              |
| 1:M:121:SER:HA   | 1:M:122:PRO:HD3  | 1.63                     | 0.45              |
| 1:O:247:VAL:CG1  | 1:O:248:PHE:N    | 2.79                     | 0.45              |
| 1:D:182:ASN:HB2  | 1:D:195:GLN:O    | 2.15                     | 0.45              |
| 1:E:98:TRP:CH2   | 1:E:170:ARG:HD2  | 2.51                     | 0.45              |
| 1:G:89:ILE:HG22  | 1:G:89:ILE:O     | 2.15                     | 0.45              |
| 1:I:129:LEU:HD23 | 1:I:191:PRO:CG   | 2.47                     | 0.45              |
| 1:L:98:TRP:CH2   | 1:L:170:ARG:HD2  | 2.51                     | 0.45              |
| 1:B:247:VAL:CG1  | 1:B:248:PHE:N    | 2.79                     | 0.45              |
| 1:B:57:TYR:C     | 1:B:57:TYR:CD2   | 2.88                     | 0.45              |
| 1:B:64:ILE:HD13  | 1:B:73:LEU:HD11  | 1.98                     | 0.45              |
| 1:D:264:PHE:O    | 1:D:266:LEU:HD13 | 2.17                     | 0.45              |
| 1:F:247:VAL:CG1  | 1:F:248:PHE:N    | 2.79                     | 0.45              |
| 1:K:268:LEU:CD2  | 1:K:268:LEU:N    | 2.76                     | 0.45              |
| 1:M:113:PRO:O    | 1:M:116:THR:HG22 | 2.17                     | 0.45              |
| 1:M:192:PHE:CG   | 1:O:137:PRO:HG2  | 2.51                     | 0.45              |
| 1:P:98:TRP:CH2   | 1:P:170:ARG:HD2  | 2.50                     | 0.45              |
| 1:G:67:PHE:CD1   | 1:G:68:ALA:N     | 2.85                     | 0.45              |
| 1:H:56:LEU:HD12  | 1:H:56:LEU:HA    | 1.60                     | 0.45              |
| 1:J:247:VAL:CG1  | 1:J:248:PHE:N    | 2.79                     | 0.45              |
| 1:K:40:TRP:CE3   | 1:K:75:MET:HE3   | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:150:ASN:OD1  | 1:M:150:ASN:N    | 2.44                     | 0.45              |
| 1:C:65:PRO:O     | 1:C:68:ALA:HB3   | 2.17                     | 0.45              |
| 1:D:116:THR:HG22 | 1:D:117:ASN:N    | 2.32                     | 0.45              |
| 1:G:41:ILE:O     | 1:G:41:ILE:HG12  | 2.17                     | 0.45              |
| 1:G:55:LEU:O     | 1:G:58:GLN:N     | 2.50                     | 0.45              |
| 1:H:115:VAL:HG12 | 1:H:139:ILE:HG22 | 1.97                     | 0.45              |
| 1:H:42:GLN:HB3   | 1:H:176:PRO:CG   | 2.47                     | 0.45              |
| 1:I:117:ASN:OD1  | 1:I:117:ASN:N    | 2.43                     | 0.45              |
| 1:I:226:ASN:HA   | 1:I:227:PRO:HD2  | 1.82                     | 0.45              |
| 1:A:48:TRP:HB2   | 1:A:118:GLN:NE2  | 2.32                     | 0.45              |
| 1:A:156:THR:HG21 | 1:A:284:PRO:CG   | 2.46                     | 0.45              |
| 1:A:247:VAL:CG1  | 1:A:248:PHE:N    | 2.79                     | 0.45              |
| 1:D:282:GLU:O    | 1:D:284:PRO:HD3  | 2.17                     | 0.45              |
| 1:F:282:GLU:O    | 1:F:284:PRO:HD3  | 2.17                     | 0.45              |
| 1:K:73:LEU:CD2   | 1:K:179:ILE:HG23 | 2.47                     | 0.45              |
| 1:N:49:LEU:HD13  | 1:N:202:GLY:CA   | 2.47                     | 0.45              |
| 1:P:72:GLY:O     | 1:P:74:HIS:HD2   | 1.99                     | 0.45              |
| 1:A:87:ILE:HD11  | 1:A:176:PRO:HD3  | 1.98                     | 0.45              |
| 1:B:156:THR:HG21 | 1:B:284:PRO:CG   | 2.46                     | 0.45              |
| 1:D:247:VAL:CG1  | 1:D:248:PHE:N    | 2.79                     | 0.45              |
| 1:E:46:LEU:HD12  | 1:E:202:GLY:CA   | 2.28                     | 0.45              |
| 1:K:156:THR:HG21 | 1:K:284:PRO:CG   | 2.46                     | 0.45              |
| 1:E:182:ASN:HB2  | 1:E:195:GLN:O    | 2.17                     | 0.44              |
| 1:E:247:VAL:CG1  | 1:E:248:PHE:N    | 2.79                     | 0.44              |
| 1:E:282:GLU:O    | 1:E:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:F:133:ARG:HH11 | 1:F:190:ASN:HD22 | 1.64                     | 0.44              |
| 1:M:63:ARG:C     | 1:M:64:ILE:HG13  | 2.37                     | 0.44              |
| 1:A:69:SER:HB2   | 1:A:185:PHE:CE1  | 2.52                     | 0.44              |
| 1:A:282:GLU:O    | 1:A:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:A:72:GLY:O     | 1:A:74:HIS:HD2   | 2.01                     | 0.44              |
| 1:G:150:ASN:OD1  | 1:G:150:ASN:N    | 2.44                     | 0.44              |
| 1:G:156:THR:HG21 | 1:G:284:PRO:CG   | 2.46                     | 0.44              |
| 1:H:282:GLU:O    | 1:H:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:I:64:ILE:HA    | 1:I:65:PRO:HD3   | 1.92                     | 0.44              |
| 1:L:226:ASN:HA   | 1:L:227:PRO:HD2  | 1.82                     | 0.44              |
| 1:E:41:ILE:HD12  | 1:E:49:LEU:HD22  | 1.97                     | 0.44              |
| 1:K:226:ASN:HA   | 1:K:227:PRO:HD2  | 1.82                     | 0.44              |
| 1:L:282:GLU:O    | 1:L:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:M:37:ASP:OD2   | 1:M:39:THR:OG1   | 2.35                     | 0.44              |
| 1:N:120:LEU:C    | 1:N:120:LEU:HD12 | 2.37                     | 0.44              |
| 1:P:282:GLU:O    | 1:P:284:PRO:HD3  | 2.17                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:142:SER:OG  | 1:H:197:GLU:OE2  | 2.27                     | 0.44              |
| 1:M:84:THR:HB   | 1:M:86:GLN:H     | 1.82                     | 0.44              |
| 1:O:282:GLU:O   | 1:O:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:M:122:PRO:HG2 | 1:P:59:LEU:HA    | 1.99                     | 0.44              |
| 1:B:182:ASN:HB2 | 1:B:195:GLN:O    | 2.18                     | 0.44              |
| 1:C:195:GLN:HB2 | 1:C:195:GLN:HE21 | 1.48                     | 0.44              |
| 1:C:259:MET:HG2 | 1:C:264:PHE:CZ   | 2.52                     | 0.44              |
| 1:H:70:PRO:CD   | 1:H:71:ASN:H     | 2.31                     | 0.44              |
| 1:J:81:ASP:HB3  | 1:J:84:THR:OG1   | 2.18                     | 0.44              |
| 1:M:247:VAL:CG1 | 1:M:248:PHE:N    | 2.79                     | 0.44              |
| 1:N:282:GLU:O   | 1:N:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:P:261:SER:O   | 1:P:264:PHE:HB2  | 2.18                     | 0.44              |
| 1:B:122:PRO:HG2 | 1:D:59:LEU:HA    | 1.99                     | 0.44              |
| 1:E:87:ILE:HD11 | 1:E:208:PHE:CE1  | 2.53                     | 0.44              |
| 1:G:262:LYS:C   | 1:G:264:PHE:H    | 2.20                     | 0.44              |
| 1:G:282:GLU:O   | 1:G:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:G:87:ILE:HG22 | 1:G:87:ILE:O     | 2.17                     | 0.44              |
| 1:H:59:LEU:HD23 | 1:H:126:THR:HG21 | 2.00                     | 0.44              |
| 1:K:129:LEU:CD2 | 1:K:191:PRO:HD3  | 2.45                     | 0.44              |
| 1:K:190:ASN:HA  | 1:K:192:PHE:N    | 2.32                     | 0.44              |
| 1:L:140:PHE:HB3 | 1:L:199:THR:CG2  | 2.48                     | 0.44              |
| 1:N:58:GLN:NE2  | 1:O:120:LEU:O    | 2.50                     | 0.44              |
| 1:B:81:ASP:OD1  | 1:B:83:ASN:HB2   | 2.17                     | 0.44              |
| 1:E:140:PHE:HB3 | 1:E:199:THR:CG2  | 2.48                     | 0.44              |
| 1:F:140:PHE:HB3 | 1:F:199:THR:CG2  | 2.48                     | 0.44              |
| 1:H:140:PHE:HB3 | 1:H:199:THR:CG2  | 2.48                     | 0.44              |
| 1:K:282:GLU:O   | 1:K:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:M:61:SER:OG   | 1:M:62:THR:N     | 2.50                     | 0.44              |
| 1:B:140:PHE:HB3 | 1:B:199:THR:CG2  | 2.48                     | 0.44              |
| 1:B:282:GLU:O   | 1:B:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:C:69:SER:HB2  | 1:C:184:SER:O    | 2.17                     | 0.44              |
| 1:C:190:ASN:CG  | 1:C:191:PRO:HD2  | 2.37                     | 0.44              |
| 1:O:81:ASP:OD2  | 1:O:84:THR:HG23  | 2.18                     | 0.44              |
| 1:B:283:ILE:CG2 | 1:C:268:LEU:HD21 | 2.48                     | 0.44              |
| 1:E:64:ILE:HG21 | 1:E:69:SER:HB2   | 1.99                     | 0.44              |
| 1:F:186:SER:OG  | 1:F:189:HIS:HB2  | 2.18                     | 0.44              |
| 1:I:140:PHE:HB3 | 1:I:199:THR:CG2  | 2.48                     | 0.44              |
| 1:K:102:PRO:HB2 | 1:K:256:GLY:O    | 2.18                     | 0.44              |
| 1:M:140:PHE:HB3 | 1:M:199:THR:CG2  | 2.48                     | 0.44              |
| 1:M:282:GLU:O   | 1:M:284:PRO:HD3  | 2.17                     | 0.44              |
| 1:M:76:ARG:NH1  | 1:M:177:GLY:O    | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:84:THR:HB    | 1:N:86:GLN:H     | 1.83                     | 0.44              |
| 1:A:140:PHE:HB3  | 1:A:199:THR:CG2  | 2.48                     | 0.43              |
| 1:B:112:ILE:HA   | 1:B:113:PRO:HD3  | 1.91                     | 0.43              |
| 1:B:46:LEU:HD13  | 1:B:48:TRP:CZ2   | 2.53                     | 0.43              |
| 1:B:64:ILE:HD12  | 1:B:73:LEU:CD1   | 2.48                     | 0.43              |
| 1:D:102:PRO:HB2  | 1:D:256:GLY:O    | 2.18                     | 0.43              |
| 1:F:120:LEU:O    | 1:F:122:PRO:HD3  | 2.18                     | 0.43              |
| 1:F:64:ILE:HA    | 1:F:65:PRO:HD2   | 1.94                     | 0.43              |
| 1:I:102:PRO:HB2  | 1:I:256:GLY:O    | 2.18                     | 0.43              |
| 1:I:56:LEU:O     | 1:I:56:LEU:HD23  | 2.18                     | 0.43              |
| 1:J:102:PRO:HB2  | 1:J:256:GLY:O    | 2.18                     | 0.43              |
| 1:J:37:ASP:OD1   | 1:J:37:ASP:N     | 2.51                     | 0.43              |
| 1:P:188:ASN:O    | 1:P:192:PHE:HE1  | 2.00                     | 0.43              |
| 1:H:192:PHE:N    | 1:H:193:PRO:CD   | 2.81                     | 0.43              |
| 1:J:140:PHE:HB3  | 1:J:199:THR:CG2  | 2.48                     | 0.43              |
| 1:L:102:PRO:HB2  | 1:L:256:GLY:O    | 2.18                     | 0.43              |
| 1:N:45:SER:N     | 1:N:202:GLY:O    | 2.51                     | 0.43              |
| 1:N:76:ARG:HH12  | 1:N:95:LEU:HD11  | 1.81                     | 0.43              |
| 1:O:154:GLU:CG   | 1:O:289:LEU:HD22 | 2.43                     | 0.43              |
| 1:B:122:PRO:HG2  | 1:D:59:LEU:HD23  | 2.00                     | 0.43              |
| 1:C:282:GLU:O    | 1:C:284:PRO:HD3  | 2.17                     | 0.43              |
| 1:E:122:PRO:O    | 1:E:126:THR:HG23 | 2.18                     | 0.43              |
| 1:E:102:PRO:HB2  | 1:E:256:GLY:O    | 2.18                     | 0.43              |
| 1:G:102:PRO:HB2  | 1:G:256:GLY:O    | 2.18                     | 0.43              |
| 1:H:56:LEU:HG    | 1:H:60:ILE:HD12  | 1.99                     | 0.43              |
| 1:J:133:ARG:HG3  | 1:J:133:ARG:O    | 2.16                     | 0.43              |
| 1:K:120:LEU:HG   | 1:K:121:SER:N    | 2.33                     | 0.43              |
| 1:N:102:PRO:HB2  | 1:N:256:GLY:O    | 2.18                     | 0.43              |
| 1:N:156:THR:HG21 | 1:N:284:PRO:CG   | 2.46                     | 0.43              |
| 1:A:69:SER:HA    | 1:A:70:PRO:HD2   | 1.83                     | 0.43              |
| 1:C:84:THR:HB    | 1:C:86:GLN:HG3   | 2.00                     | 0.43              |
| 1:E:68:ALA:CB    | 1:E:129:LEU:HD21 | 2.46                     | 0.43              |
| 1:F:76:ARG:NH1   | 1:F:177:GLY:O    | 2.48                     | 0.43              |
| 1:G:194:ASN:HD21 | 1:G:197:GLU:CB   | 2.30                     | 0.43              |
| 1:H:76:ARG:HD3   | 1:H:198:ILE:HG13 | 2.00                     | 0.43              |
| 1:I:133:ARG:HD2  | 1:I:190:ASN:HD21 | 1.84                     | 0.43              |
| 1:M:129:LEU:HD23 | 1:M:191:PRO:HG3  | 2.00                     | 0.43              |
| 1:M:102:PRO:HB2  | 1:M:256:GLY:O    | 2.18                     | 0.43              |
| 1:O:102:PRO:HB2  | 1:O:256:GLY:O    | 2.18                     | 0.43              |
| 1:A:154:GLU:CG   | 1:A:289:LEU:HD22 | 2.43                     | 0.43              |
| 1:D:120:LEU:HG   | 1:D:121:SER:N    | 2.27                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:65:PRO:HB2   | 1:D:67:PHE:CD2   | 2.53                     | 0.43              |
| 1:H:156:THR:HG21 | 1:H:284:PRO:CG   | 2.46                     | 0.43              |
| 1:I:63:ARG:CG    | 1:I:63:ARG:HH11  | 2.31                     | 0.43              |
| 1:J:282:GLU:O    | 1:J:284:PRO:HD3  | 2.17                     | 0.43              |
| 1:M:112:ILE:HA   | 1:M:113:PRO:HD3  | 1.91                     | 0.43              |
| 1:O:140:PHE:HB3  | 1:O:199:THR:CG2  | 2.48                     | 0.43              |
| 1:A:102:PRO:HB2  | 1:A:256:GLY:O    | 2.18                     | 0.43              |
| 1:D:140:PHE:HB3  | 1:D:199:THR:CG2  | 2.48                     | 0.43              |
| 1:E:283:ILE:O    | 1:H:268:LEU:HD23 | 2.19                     | 0.43              |
| 1:G:44:ALA:O     | 1:G:205:ARG:NH1  | 2.50                     | 0.43              |
| 1:H:124:GLU:N    | 1:H:124:GLU:OE1  | 2.52                     | 0.43              |
| 1:I:43:ALA:CB    | 1:I:176:PRO:HD2  | 2.33                     | 0.43              |
| 1:I:282:GLU:O    | 1:I:284:PRO:HD3  | 2.17                     | 0.43              |
| 1:K:76:ARG:NH2   | 1:K:79:THR:CG2   | 2.82                     | 0.43              |
| 1:C:186:SER:C    | 1:C:188:ASN:N    | 2.72                     | 0.43              |
| 1:I:45:SER:HB3   | 1:I:204:ILE:C    | 2.39                     | 0.43              |
| 1:K:140:PHE:HB3  | 1:K:199:THR:CG2  | 2.48                     | 0.43              |
| 1:K:40:TRP:HA    | 1:K:177:GLY:HA3  | 1.99                     | 0.43              |
| 1:M:283:ILE:HB   | 1:O:268:LEU:HD21 | 1.97                     | 0.43              |
| 1:P:190:ASN:HA   | 1:P:192:PHE:N    | 2.33                     | 0.43              |
| 1:P:140:PHE:HB3  | 1:P:199:THR:CG2  | 2.48                     | 0.43              |
| 1:P:40:TRP:HB3   | 1:P:75:MET:HG3   | 2.01                     | 0.43              |
| 1:B:69:SER:HA    | 1:B:184:SER:O    | 2.18                     | 0.43              |
| 1:B:64:ILE:CG2   | 1:B:69:SER:HB3   | 2.48                     | 0.43              |
| 1:C:102:PRO:HB2  | 1:C:256:GLY:O    | 2.18                     | 0.43              |
| 1:D:154:GLU:CG   | 1:D:289:LEU:HD22 | 2.43                     | 0.43              |
| 1:E:46:LEU:CD1   | 1:E:113:PRO:HG2  | 2.48                     | 0.43              |
| 1:E:39:THR:CG2   | 1:E:40:TRP:N     | 2.81                     | 0.43              |
| 1:K:267:ASP:HB2  | 1:K:268:LEU:HD23 | 2.00                     | 0.43              |
| 1:M:79:THR:HG21  | 1:M:177:GLY:N    | 2.33                     | 0.43              |
| 1:O:156:THR:HG21 | 1:O:284:PRO:CG   | 2.46                     | 0.43              |
| 1:N:284:PRO:O    | 1:P:262:LYS:HD3  | 2.18                     | 0.43              |
| 1:B:102:PRO:HB2  | 1:B:256:GLY:O    | 2.18                     | 0.43              |
| 1:C:140:PHE:HB3  | 1:C:199:THR:CG2  | 2.48                     | 0.43              |
| 1:E:190:ASN:ND2  | 1:E:191:PRO:HA   | 2.34                     | 0.43              |
| 1:F:120:LEU:HD12 | 1:F:120:LEU:H    | 1.84                     | 0.43              |
| 1:F:189:HIS:HD2  | 1:G:119:ASN:HB2  | 1.84                     | 0.43              |
| 1:E:59:LEU:HA    | 1:G:122:PRO:HG2  | 2.01                     | 0.43              |
| 1:F:192:PHE:CZ   | 1:G:137:PRO:HB2  | 2.54                     | 0.43              |
| 1:G:80:ILE:CG2   | 1:G:87:ILE:HD13  | 2.33                     | 0.43              |
| 1:D:88:GLN:NE2   | 1:D:90:ASP:OD2   | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:64:ILE:HA    | 1:F:129:LEU:CD1  | 2.48                     | 0.43              |
| 1:G:140:PHE:HB3  | 1:G:199:THR:CG2  | 2.48                     | 0.43              |
| 1:J:87:ILE:CD1   | 1:J:208:PHE:CD1  | 3.01                     | 0.43              |
| 1:E:288:LEU:CD1  | 1:P:86:GLN:NE2   | 2.76                     | 0.43              |
| 1:D:120:LEU:HD12 | 1:D:125:ASP:HB2  | 2.01                     | 0.42              |
| 1:D:80:ILE:HG22  | 1:D:81:ASP:N     | 2.34                     | 0.42              |
| 1:L:76:ARG:HD3   | 1:L:198:ILE:CG1  | 2.46                     | 0.42              |
| 1:N:140:PHE:HB3  | 1:N:199:THR:CG2  | 2.48                     | 0.42              |
| 1:N:226:ASN:HA   | 1:N:227:PRO:HD2  | 1.82                     | 0.42              |
| 1:P:102:PRO:HB2  | 1:P:256:GLY:O    | 2.18                     | 0.42              |
| 1:A:133:ARG:O    | 1:A:133:ARG:HG3  | 2.19                     | 0.42              |
| 1:A:192:PHE:CD1  | 1:D:137:PRO:HG2  | 2.54                     | 0.42              |
| 1:B:49:LEU:HD21  | 1:B:56:LEU:HD22  | 2.01                     | 0.42              |
| 1:J:226:ASN:HA   | 1:J:227:PRO:HD2  | 1.82                     | 0.42              |
| 1:A:39:THR:O     | 1:A:42:GLN:HB3   | 2.19                     | 0.42              |
| 1:A:65:PRO:HA    | 1:B:65:PRO:HA    | 2.01                     | 0.42              |
| 1:B:192:PHE:CD1  | 1:C:137:PRO:HG2  | 2.55                     | 0.42              |
| 1:D:159:THR:HA   | 1:D:160:PRO:HD3  | 1.93                     | 0.42              |
| 1:D:65:PRO:HB2   | 1:D:67:PHE:CE2   | 2.55                     | 0.42              |
| 1:E:79:THR:CB    | 1:E:176:PRO:HA   | 2.49                     | 0.42              |
| 1:F:59:LEU:HD23  | 1:F:126:THR:HG21 | 2.01                     | 0.42              |
| 1:G:55:LEU:O     | 1:G:59:LEU:N     | 2.41                     | 0.42              |
| 1:H:102:PRO:HB2  | 1:H:256:GLY:O    | 2.18                     | 0.42              |
| 1:J:87:ILE:CD1   | 1:J:208:PHE:CE1  | 2.97                     | 0.42              |
| 1:J:64:ILE:HA    | 1:J:65:PRO:HD3   | 1.67                     | 0.42              |
| 1:K:80:ILE:HG22  | 1:K:87:ILE:CD1   | 2.47                     | 0.42              |
| 1:N:190:ASN:CG   | 1:N:191:PRO:HA   | 2.40                     | 0.42              |
| 1:N:37:ASP:OD1   | 1:N:39:THR:N     | 2.40                     | 0.42              |
| 1:N:81:ASP:OD1   | 1:N:83:ASN:HB2   | 2.19                     | 0.42              |
| 1:B:288:LEU:HD13 | 1:K:86:GLN:HE21  | 1.85                     | 0.42              |
| 1:D:56:LEU:C     | 1:D:56:LEU:HD23  | 2.38                     | 0.42              |
| 1:E:156:THR:HG21 | 1:E:284:PRO:CG   | 2.46                     | 0.42              |
| 1:G:194:ASN:ND2  | 1:G:197:GLU:N    | 2.67                     | 0.42              |
| 1:E:283:ILE:HG21 | 1:H:268:LEU:HD21 | 1.94                     | 0.42              |
| 1:J:77:GLU:HB3   | 1:J:78:GLN:NE2   | 2.34                     | 0.42              |
| 1:N:48:TRP:HB3   | 1:N:118:GLN:OE1  | 2.19                     | 0.42              |
| 1:D:158:TRP:CD1  | 1:D:194:ASN:HB3  | 2.55                     | 0.42              |
| 1:D:40:TRP:CD1   | 1:D:40:TRP:N     | 2.81                     | 0.42              |
| 1:I:47:THR:HG23  | 1:I:48:TRP:H     | 1.84                     | 0.42              |
| 1:L:115:VAL:HG12 | 1:L:116:THR:O    | 2.19                     | 0.42              |
| 1:N:57:TYR:CD2   | 1:N:57:TYR:C     | 2.92                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:186:SER:HB2  | 1:D:189:HIS:CB   | 2.43                     | 0.42              |
| 1:H:123:VAL:HG23 | 1:H:123:VAL:H    | 1.62                     | 0.42              |
| 1:H:84:THR:C     | 1:H:86:GLN:H     | 2.23                     | 0.42              |
| 1:P:188:ASN:O    | 1:P:192:PHE:CE1  | 2.72                     | 0.42              |
| 1:F:226:ASN:HA   | 1:F:227:PRO:HD2  | 1.82                     | 0.42              |
| 1:F:84:THR:HG21  | 1:F:86:GLN:HB2   | 2.02                     | 0.42              |
| 1:H:112:ILE:HA   | 1:H:113:PRO:HD3  | 1.91                     | 0.42              |
| 1:I:56:LEU:HD21  | 1:I:60:ILE:HD11  | 2.02                     | 0.42              |
| 1:M:156:THR:HG21 | 1:M:284:PRO:CG   | 2.46                     | 0.42              |
| 1:E:61:SER:HA    | 1:E:64:ILE:HD12  | 2.00                     | 0.42              |
| 1:F:159:THR:HA   | 1:F:160:PRO:HD3  | 1.93                     | 0.42              |
| 1:L:73:LEU:HD23  | 1:L:75:MET:CE    | 2.50                     | 0.42              |
| 1:O:42:GLN:HB3   | 1:O:42:GLN:HE21  | 1.69                     | 0.42              |
| 1:O:65:PRO:HG2   | 1:O:68:ALA:CB    | 2.50                     | 0.42              |
| 1:A:68:ALA:CB    | 1:A:129:LEU:HD21 | 2.47                     | 0.42              |
| 1:C:67:PHE:C     | 1:C:67:PHE:CD1   | 2.93                     | 0.42              |
| 1:F:102:PRO:HB2  | 1:F:256:GLY:O    | 2.18                     | 0.42              |
| 1:F:55:LEU:CD2   | 1:H:55:LEU:HD23  | 2.49                     | 0.42              |
| 1:I:70:PRO:HD2   | 1:I:71:ASN:H     | 1.84                     | 0.42              |
| 1:L:78:GLN:OE1   | 1:L:78:GLN:HA    | 2.19                     | 0.42              |
| 1:N:142:SER:OG   | 1:N:197:GLU:OE2  | 2.27                     | 0.42              |
| 1:B:226:ASN:HA   | 1:B:227:PRO:HD2  | 1.82                     | 0.42              |
| 1:B:64:ILE:CD1   | 1:B:73:LEU:CD1   | 2.97                     | 0.42              |
| 1:D:149:ASN:HD21 | 1:D:153:LEU:HD12 | 1.85                     | 0.42              |
| 1:M:73:LEU:HD23  | 1:M:73:LEU:HA    | 1.83                     | 0.42              |
| 1:H:60:ILE:HG22  | 1:H:73:LEU:HD11  | 2.01                     | 0.41              |
| 1:I:74:HIS:HD2   | 1:I:183:ALA:O    | 2.03                     | 0.41              |
| 1:J:166:ASN:H    | 1:J:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:J:87:ILE:HD11  | 1:J:208:PHE:CD1  | 2.54                     | 0.41              |
| 1:L:116:THR:HG22 | 1:L:118:GLN:H    | 1.85                     | 0.41              |
| 1:L:156:THR:HG21 | 1:L:284:PRO:CG   | 2.46                     | 0.41              |
| 1:M:133:ARG:O    | 1:M:277:PHE:HZ   | 2.03                     | 0.41              |
| 1:M:192:PHE:N    | 1:M:193:PRO:HD3  | 2.35                     | 0.41              |
| 1:O:166:ASN:H    | 1:O:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:B:98:TRP:CD1   | 1:B:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:B:87:ILE:HD11  | 1:B:208:PHE:HE1  | 1.84                     | 0.41              |
| 1:F:166:ASN:H    | 1:F:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:F:81:ASP:HB3   | 1:F:85:GLY:H     | 1.85                     | 0.41              |
| 1:H:166:ASN:H    | 1:H:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:I:159:THR:HA   | 1:I:160:PRO:HD3  | 1.93                     | 0.41              |
| 1:I:166:ASN:H    | 1:I:217:ASN:ND2  | 2.18                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:98:TRP:CD1   | 1:J:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:L:80:ILE:HD11  | 1:L:176:PRO:HB3  | 2.02                     | 0.41              |
| 1:L:142:SER:OG   | 1:L:197:GLU:OE2  | 2.27                     | 0.41              |
| 1:M:129:LEU:HD23 | 1:M:191:PRO:CG   | 2.51                     | 0.41              |
| 1:M:149:ASN:HD21 | 1:M:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:A:98:TRP:CD1   | 1:A:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:C:156:THR:HG21 | 1:C:284:PRO:CG   | 2.46                     | 0.41              |
| 1:D:156:THR:HG21 | 1:D:284:PRO:CG   | 2.46                     | 0.41              |
| 1:G:69:SER:OG    | 1:G:184:SER:O    | 2.28                     | 0.41              |
| 1:H:55:LEU:O     | 1:H:58:GLN:HB2   | 2.20                     | 0.41              |
| 1:L:124:GLU:C    | 1:L:126:THR:H    | 2.24                     | 0.41              |
| 1:A:48:TRP:O     | 1:A:48:TRP:HE3   | 2.03                     | 0.41              |
| 1:D:98:TRP:CD1   | 1:D:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:D:194:ASN:OD1  | 1:D:194:ASN:N    | 2.53                     | 0.41              |
| 1:E:59:LEU:CA    | 1:G:122:PRO:HG2  | 2.50                     | 0.41              |
| 1:G:98:TRP:CD1   | 1:G:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:H:149:ASN:HD21 | 1:H:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:N:98:TRP:CD1   | 1:N:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:O:112:ILE:HA   | 1:O:113:PRO:HD3  | 1.91                     | 0.41              |
| 1:O:76:ARG:HD3   | 1:O:198:ILE:CG1  | 2.45                     | 0.41              |
| 1:P:166:ASN:H    | 1:P:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:B:166:ASN:H    | 1:B:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:E:37:ASP:OD1   | 1:E:37:ASP:N     | 2.54                     | 0.41              |
| 1:E:64:ILE:HG21  | 1:E:69:SER:CB    | 2.51                     | 0.41              |
| 1:F:190:ASN:HA   | 1:F:191:PRO:HA   | 1.83                     | 0.41              |
| 1:H:241:PRO:HB2  | 1:H:244:ILE:HD11 | 2.00                     | 0.41              |
| 1:I:149:ASN:HD21 | 1:I:153:LEU:HD12 | 1.86                     | 0.41              |
| 1:L:58:GLN:O     | 1:L:62:THR:OG1   | 2.28                     | 0.41              |
| 1:M:73:LEU:HD22  | 1:M:179:ILE:HG23 | 2.01                     | 0.41              |
| 1:P:98:TRP:CD1   | 1:P:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:P:69:SER:HA    | 1:P:70:PRO:HD2   | 1.77                     | 0.41              |
| 1:A:60:ILE:HG22  | 1:A:61:SER:N     | 2.36                     | 0.41              |
| 1:B:149:ASN:HD21 | 1:B:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:C:154:GLU:CG   | 1:C:289:LEU:HD22 | 2.43                     | 0.41              |
| 1:D:80:ILE:CG2   | 1:D:81:ASP:N     | 2.83                     | 0.41              |
| 1:E:187:ARG:HG2  | 1:E:195:GLN:NE2  | 2.35                     | 0.41              |
| 1:E:241:PRO:HB2  | 1:E:244:ILE:HD11 | 2.00                     | 0.41              |
| 1:H:98:TRP:CD1   | 1:H:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:I:98:TRP:CD1   | 1:I:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:L:98:TRP:CD1   | 1:L:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:L:166:ASN:H    | 1:L:217:ASN:ND2  | 2.18                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:129:LEU:CD2  | 1:M:191:PRO:HD3  | 2.51                     | 0.41              |
| 1:B:48:TRP:CD2   | 1:B:118:GLN:HA   | 2.55                     | 0.41              |
| 1:C:98:TRP:CD1   | 1:C:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:D:56:LEU:HD23  | 1:D:56:LEU:O     | 2.21                     | 0.41              |
| 1:F:76:ARG:HD2   | 1:F:198:ILE:HG23 | 2.02                     | 0.41              |
| 1:G:254:SER:HB3  | 1:L:243:ASN:C    | 2.39                     | 0.41              |
| 1:I:74:HIS:C     | 1:I:75:MET:HE3   | 2.41                     | 0.41              |
| 1:I:75:MET:HE2   | 1:I:179:ILE:HA   | 2.01                     | 0.41              |
| 1:K:98:TRP:CD1   | 1:K:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:L:69:SER:HA    | 1:L:70:PRO:HD2   | 1.49                     | 0.41              |
| 1:N:159:THR:HA   | 1:N:160:PRO:HD3  | 1.93                     | 0.41              |
| 1:B:64:ILE:HD12  | 1:B:73:LEU:HD13  | 2.01                     | 0.41              |
| 1:A:123:VAL:HG11 | 1:C:63:ARG:NH1   | 2.36                     | 0.41              |
| 1:D:166:ASN:H    | 1:D:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:E:40:TRP:N     | 1:E:40:TRP:CD1   | 2.89                     | 0.41              |
| 1:F:156:THR:HG21 | 1:F:284:PRO:CG   | 2.46                     | 0.41              |
| 1:F:98:TRP:CD1   | 1:F:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:E:59:LEU:N     | 1:G:122:PRO:HG2  | 2.36                     | 0.41              |
| 1:G:120:LEU:HD11 | 1:G:125:ASP:HB2  | 2.01                     | 0.41              |
| 1:G:61:SER:HA    | 1:G:64:ILE:HD12  | 2.02                     | 0.41              |
| 1:H:159:THR:HA   | 1:H:160:PRO:HD3  | 1.93                     | 0.41              |
| 1:H:59:LEU:HA    | 1:H:59:LEU:HD12  | 1.90                     | 0.41              |
| 1:J:151:LEU:HD23 | 1:J:151:LEU:HA   | 1.90                     | 0.41              |
| 1:P:112:ILE:HA   | 1:P:113:PRO:HD3  | 1.91                     | 0.41              |
| 1:A:149:ASN:HD21 | 1:A:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:E:192:PHE:CG   | 1:H:137:PRO:HG2  | 2.56                     | 0.41              |
| 1:F:148:TYR:CE1  | 1:F:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:F:149:ASN:HD21 | 1:F:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:H:262:LYS:O    | 1:H:264:PHE:N    | 2.53                     | 0.41              |
| 1:I:43:ALA:N     | 1:I:176:PRO:HG2  | 2.35                     | 0.41              |
| 1:K:148:TYR:CE1  | 1:K:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:K:166:ASN:H    | 1:K:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:L:149:ASN:HD21 | 1:L:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:L:148:TYR:CE1  | 1:L:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:A:42:GLN:HG3   | 1:A:42:GLN:O     | 2.21                     | 0.41              |
| 1:C:100:ARG:HH11 | 1:C:100:ARG:HD3  | 1.75                     | 0.41              |
| 1:C:124:GLU:C    | 1:C:126:THR:H    | 2.24                     | 0.41              |
| 1:E:133:ARG:HB2  | 1:E:191:PRO:HB2  | 2.03                     | 0.41              |
| 1:E:98:TRP:CD1   | 1:E:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:F:154:GLU:CG   | 1:F:289:LEU:HD22 | 2.43                     | 0.41              |
| 1:F:40:TRP:CZ2   | 1:F:57:TYR:HB2   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:148:TYR:CE1  | 1:H:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:I:148:TYR:CE1  | 1:I:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:I:79:THR:HG23  | 1:I:80:ILE:N     | 2.36                     | 0.41              |
| 1:O:43:ALA:HB2   | 1:O:176:PRO:O    | 2.21                     | 0.41              |
| 1:A:166:ASN:H    | 1:A:217:ASN:ND2  | 2.18                     | 0.41              |
| 1:C:41:ILE:HG23  | 1:C:41:ILE:HD13  | 1.89                     | 0.41              |
| 1:D:129:LEU:HD23 | 1:D:191:PRO:HD3  | 2.02                     | 0.41              |
| 1:D:88:GLN:HG2   | 1:D:93:HIS:ND1   | 2.36                     | 0.41              |
| 1:E:149:ASN:HD21 | 1:E:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:G:142:SER:OG   | 1:G:197:GLU:OE2  | 2.27                     | 0.41              |
| 1:I:42:GLN:HE21  | 1:I:176:PRO:HG3  | 1.84                     | 0.41              |
| 1:J:112:ILE:HA   | 1:J:113:PRO:HD3  | 1.91                     | 0.41              |
| 1:J:149:ASN:HD21 | 1:J:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:J:148:TYR:CE1  | 1:J:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:J:156:THR:HG21 | 1:J:284:PRO:CG   | 2.46                     | 0.41              |
| 1:M:129:LEU:HD23 | 1:M:191:PRO:CD   | 2.50                     | 0.41              |
| 1:M:98:TRP:CD1   | 1:M:160:PRO:HD3  | 2.56                     | 0.41              |
| 1:N:148:TYR:CE1  | 1:N:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:P:149:ASN:HD21 | 1:P:153:LEU:HD12 | 1.85                     | 0.41              |
| 1:P:156:THR:HG21 | 1:P:284:PRO:CG   | 2.46                     | 0.41              |
| 1:P:44:ALA:O     | 1:P:205:ARG:NH1  | 2.42                     | 0.41              |
| 1:B:122:PRO:CD   | 1:B:123:VAL:H    | 2.34                     | 0.40              |
| 1:D:64:ILE:HD12  | 1:D:73:LEU:HG    | 2.03                     | 0.40              |
| 1:F:76:ARG:CD    | 1:F:198:ILE:HG21 | 2.45                     | 0.40              |
| 1:G:231:ASN:HA   | 1:G:232:PRO:HD3  | 1.85                     | 0.40              |
| 1:G:73:LEU:HD23  | 1:G:184:SER:HB3  | 2.01                     | 0.40              |
| 1:N:127:HIS:CE1  | 1:N:130:ASN:HB2  | 2.55                     | 0.40              |
| 1:N:166:ASN:H    | 1:N:217:ASN:ND2  | 2.18                     | 0.40              |
| 1:O:63:ARG:HH21  | 1:O:123:VAL:HA   | 1.85                     | 0.40              |
| 1:P:148:TYR:CE1  | 1:P:154:GLU:HB2  | 2.56                     | 0.40              |
| 1:C:226:ASN:HA   | 1:C:227:PRO:HD2  | 1.82                     | 0.40              |
| 1:E:148:TYR:CE1  | 1:E:154:GLU:HB2  | 2.56                     | 0.40              |
| 1:E:166:ASN:H    | 1:E:217:ASN:ND2  | 2.18                     | 0.40              |
| 1:F:120:LEU:C    | 1:F:120:LEU:HD13 | 2.42                     | 0.40              |
| 1:G:81:ASP:OD2   | 1:G:84:THR:OG1   | 2.40                     | 0.40              |
| 1:J:68:ALA:CB    | 1:J:129:LEU:HD21 | 2.51                     | 0.40              |
| 1:M:166:ASN:H    | 1:M:217:ASN:ND2  | 2.18                     | 0.40              |
| 1:N:234:THR:C    | 1:N:236:ASN:N    | 2.75                     | 0.40              |
| 1:P:262:LYS:NZ   | 1:P:268:LEU:HB3  | 2.37                     | 0.40              |
| 1:P:79:THR:HG23  | 1:P:80:ILE:HG23  | 2.02                     | 0.40              |
| 1:B:190:ASN:ND2  | 1:B:191:PRO:HA   | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:40:TRP:CD2   | 1:C:41:ILE:CG2   | 2.98                     | 0.40              |
| 1:H:259:MET:HG2  | 1:H:264:PHE:CE2  | 2.56                     | 0.40              |
| 1:K:40:TRP:CE3   | 1:K:75:MET:HE1   | 2.57                     | 0.40              |
| 1:K:40:TRP:CD2   | 1:K:41:ILE:HG23  | 2.56                     | 0.40              |
| 1:L:77:GLU:O     | 1:L:78:GLN:HB2   | 2.20                     | 0.40              |
| 1:O:149:ASN:HD21 | 1:O:153:LEU:HD12 | 1.85                     | 0.40              |
| 1:A:120:LEU:O    | 1:A:120:LEU:HD12 | 2.21                     | 0.40              |
| 1:A:148:TYR:CE1  | 1:A:154:GLU:HB2  | 2.56                     | 0.40              |
| 1:B:234:THR:C    | 1:B:236:ASN:N    | 2.75                     | 0.40              |
| 1:C:149:ASN:HD21 | 1:C:153:LEU:HD12 | 1.85                     | 0.40              |
| 1:C:166:ASN:H    | 1:C:217:ASN:ND2  | 2.18                     | 0.40              |
| 1:C:185:PHE:CB   | 1:C:189:HIS:CD2  | 2.89                     | 0.40              |
| 1:G:226:ASN:HA   | 1:G:227:PRO:HD2  | 1.82                     | 0.40              |
| 1:H:43:ALA:O     | 1:H:204:ILE:HA   | 2.22                     | 0.40              |
| 1:J:150:ASN:N    | 1:J:150:ASN:OD1  | 2.44                     | 0.40              |
| 1:O:231:ASN:HA   | 1:O:232:PRO:HD3  | 1.85                     | 0.40              |
| 1:A:133:ARG:HB2  | 1:A:191:PRO:HB3  | 2.02                     | 0.40              |
| 1:A:48:TRP:O     | 1:A:48:TRP:CE3   | 2.74                     | 0.40              |
| 1:E:112:ILE:HA   | 1:E:113:PRO:HD3  | 1.91                     | 0.40              |
| 1:E:127:HIS:CE1  | 1:E:130:ASN:HB2  | 2.55                     | 0.40              |
| 1:F:44:ALA:HA    | 1:F:202:GLY:O    | 2.22                     | 0.40              |
| 1:G:149:ASN:HD21 | 1:G:153:LEU:HD12 | 1.85                     | 0.40              |
| 1:G:159:THR:HA   | 1:G:160:PRO:HD3  | 1.93                     | 0.40              |
| 1:G:79:THR:O     | 1:G:88:GLN:HB3   | 2.21                     | 0.40              |
| 1:H:154:GLU:CG   | 1:H:289:LEU:HD22 | 2.43                     | 0.40              |
| 1:J:40:TRP:CZ2   | 1:J:57:TYR:HB2   | 2.57                     | 0.40              |
| 1:I:192:PHE:CG   | 1:K:137:PRO:HG2  | 2.56                     | 0.40              |
| 1:M:235:LEU:HA   | 1:M:235:LEU:HD23 | 1.91                     | 0.40              |
| 1:N:149:ASN:HD21 | 1:N:153:LEU:HD12 | 1.85                     | 0.40              |
| 1:N:63:ARG:HE    | 1:N:63:ARG:HB2   | 1.37                     | 0.40              |
| 1:P:234:THR:C    | 1:P:236:ASN:N    | 2.75                     | 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:150:ASN:O | 1:H:148:TYR:N[2_664] | 1.96                     | 0.24              |

## 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     | 232/291 (80%)   | 202 (87%)  | 29 (12%)  | 1 (0%)   | 38          | 78  |
| 1   | B     | 232/291 (80%)   | 205 (88%)  | 27 (12%)  | 0        | 100         | 100 |
| 1   | C     | 240/291 (82%)   | 211 (88%)  | 28 (12%)  | 1 (0%)   | 38          | 78  |
| 1   | D     | 240/291 (82%)   | 216 (90%)  | 21 (9%)   | 3 (1%)   | 14          | 51  |
| 1   | E     | 232/291 (80%)   | 200 (86%)  | 30 (13%)  | 2 (1%)   | 20          | 62  |
| 1   | F     | 232/291 (80%)   | 205 (88%)  | 25 (11%)  | 2 (1%)   | 20          | 62  |
| 1   | G     | 230/291 (79%)   | 208 (90%)  | 22 (10%)  | 0        | 100         | 100 |
| 1   | H     | 241/291 (83%)   | 211 (88%)  | 27 (11%)  | 3 (1%)   | 15          | 53  |
| 1   | I     | 232/291 (80%)   | 208 (90%)  | 21 (9%)   | 3 (1%)   | 14          | 51  |
| 1   | J     | 232/291 (80%)   | 208 (90%)  | 23 (10%)  | 1 (0%)   | 38          | 78  |
| 1   | K     | 240/291 (82%)   | 211 (88%)  | 28 (12%)  | 1 (0%)   | 38          | 78  |
| 1   | L     | 230/291 (79%)   | 202 (88%)  | 26 (11%)  | 2 (1%)   | 20          | 62  |
| 1   | M     | 232/291 (80%)   | 206 (89%)  | 25 (11%)  | 1 (0%)   | 38          | 78  |
| 1   | N     | 232/291 (80%)   | 206 (89%)  | 23 (10%)  | 3 (1%)   | 14          | 51  |
| 1   | O     | 230/291 (79%)   | 201 (87%)  | 27 (12%)  | 2 (1%)   | 20          | 62  |
| 1   | P     | 240/291 (82%)   | 212 (88%)  | 25 (10%)  | 3 (1%)   | 14          | 51  |
| All | All   | 3747/4656 (80%) | 3312 (88%) | 407 (11%) | 28 (1%)  | 25          | 67  |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 70  | PRO  |
| 1   | O     | 70  | PRO  |
| 1   | A     | 70  | PRO  |
| 1   | N     | 62  | THR  |
| 1   | P     | 83  | ASN  |
| 1   | C     | 125 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 39  | THR  |
| 1   | K     | 62  | THR  |
| 1   | L     | 125 | ASP  |
| 1   | D     | 122 | PRO  |
| 1   | E     | 70  | PRO  |
| 1   | E     | 121 | SER  |
| 1   | I     | 43  | ALA  |
| 1   | I     | 47  | THR  |
| 1   | M     | 195 | GLN  |
| 1   | N     | 122 | PRO  |
| 1   | O     | 44  | ALA  |
| 1   | P     | 62  | THR  |
| 1   | D     | 82  | SER  |
| 1   | H     | 195 | GLN  |
| 1   | P     | 193 | PRO  |
| 1   | D     | 70  | PRO  |
| 1   | F     | 44  | ALA  |
| 1   | H     | 263 | GLY  |
| 1   | I     | 48  | TRP  |
| 1   | J     | 122 | PRO  |
| 1   | N     | 121 | SER  |
| 1   | L     | 122 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 218/262 (83%) | 207 (95%) | 11 (5%)  | 28          | 67 |
| 1   | B     | 218/262 (83%) | 205 (94%) | 13 (6%)  | 22          | 60 |
| 1   | C     | 223/262 (85%) | 212 (95%) | 11 (5%)  | 29          | 68 |
| 1   | D     | 223/262 (85%) | 213 (96%) | 10 (4%)  | 32          | 71 |
| 1   | E     | 218/262 (83%) | 206 (94%) | 12 (6%)  | 25          | 63 |
| 1   | F     | 218/262 (83%) | 205 (94%) | 13 (6%)  | 22          | 60 |
| 1   | G     | 215/262 (82%) | 201 (94%) | 14 (6%)  | 20          | 56 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | H     | 224/262 (86%)   | 210 (94%)  | 14 (6%)  | 21          | 57 |
| 1   | I     | 218/262 (83%)   | 205 (94%)  | 13 (6%)  | 22          | 60 |
| 1   | J     | 218/262 (83%)   | 207 (95%)  | 11 (5%)  | 28          | 67 |
| 1   | K     | 223/262 (85%)   | 210 (94%)  | 13 (6%)  | 23          | 61 |
| 1   | L     | 215/262 (82%)   | 206 (96%)  | 9 (4%)   | 34          | 73 |
| 1   | M     | 218/262 (83%)   | 204 (94%)  | 14 (6%)  | 20          | 57 |
| 1   | N     | 218/262 (83%)   | 207 (95%)  | 11 (5%)  | 28          | 67 |
| 1   | O     | 215/262 (82%)   | 206 (96%)  | 9 (4%)   | 34          | 73 |
| 1   | P     | 223/262 (85%)   | 215 (96%)  | 8 (4%)   | 40          | 77 |
| All | All   | 3505/4192 (84%) | 3319 (95%) | 186 (5%) | 26          | 65 |

All (186) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | ILE  |
| 1   | A     | 63  | ARG  |
| 1   | A     | 97  | ARG  |
| 1   | A     | 120 | LEU  |
| 1   | A     | 121 | SER  |
| 1   | A     | 150 | ASN  |
| 1   | A     | 188 | ASN  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 233 | SER  |
| 1   | A     | 242 | SER  |
| 1   | A     | 248 | PHE  |
| 1   | B     | 41  | ILE  |
| 1   | B     | 81  | ASP  |
| 1   | B     | 82  | SER  |
| 1   | B     | 87  | ILE  |
| 1   | B     | 97  | ARG  |
| 1   | B     | 116 | THR  |
| 1   | B     | 120 | LEU  |
| 1   | B     | 133 | ARG  |
| 1   | B     | 150 | ASN  |
| 1   | B     | 189 | HIS  |
| 1   | B     | 233 | SER  |
| 1   | B     | 242 | SER  |
| 1   | B     | 248 | PHE  |
| 1   | C     | 38  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 41  | ILE  |
| 1   | C     | 45  | SER  |
| 1   | C     | 59  | LEU  |
| 1   | C     | 97  | ARG  |
| 1   | C     | 150 | ASN  |
| 1   | C     | 186 | SER  |
| 1   | C     | 195 | GLN  |
| 1   | C     | 233 | SER  |
| 1   | C     | 242 | SER  |
| 1   | C     | 248 | PHE  |
| 1   | D     | 66  | SER  |
| 1   | D     | 74  | HIS  |
| 1   | D     | 97  | ARG  |
| 1   | D     | 150 | ASN  |
| 1   | D     | 187 | ARG  |
| 1   | D     | 190 | ASN  |
| 1   | D     | 192 | PHE  |
| 1   | D     | 233 | SER  |
| 1   | D     | 242 | SER  |
| 1   | D     | 248 | PHE  |
| 1   | E     | 37  | ASP  |
| 1   | E     | 61  | SER  |
| 1   | E     | 66  | SER  |
| 1   | E     | 73  | LEU  |
| 1   | E     | 97  | ARG  |
| 1   | E     | 120 | LEU  |
| 1   | E     | 133 | ARG  |
| 1   | E     | 150 | ASN  |
| 1   | E     | 195 | GLN  |
| 1   | E     | 233 | SER  |
| 1   | E     | 242 | SER  |
| 1   | E     | 248 | PHE  |
| 1   | F     | 39  | THR  |
| 1   | F     | 75  | MET  |
| 1   | F     | 97  | ARG  |
| 1   | F     | 120 | LEU  |
| 1   | F     | 124 | GLU  |
| 1   | F     | 150 | ASN  |
| 1   | F     | 186 | SER  |
| 1   | F     | 188 | ASN  |
| 1   | F     | 190 | ASN  |
| 1   | F     | 194 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 233 | SER  |
| 1   | F     | 242 | SER  |
| 1   | F     | 248 | PHE  |
| 1   | G     | 37  | ASP  |
| 1   | G     | 59  | LEU  |
| 1   | G     | 66  | SER  |
| 1   | G     | 74  | HIS  |
| 1   | G     | 83  | ASN  |
| 1   | G     | 84  | THR  |
| 1   | G     | 87  | ILE  |
| 1   | G     | 97  | ARG  |
| 1   | G     | 133 | ARG  |
| 1   | G     | 150 | ASN  |
| 1   | G     | 233 | SER  |
| 1   | G     | 242 | SER  |
| 1   | G     | 248 | PHE  |
| 1   | G     | 269 | ASP  |
| 1   | H     | 42  | GLN  |
| 1   | H     | 84  | THR  |
| 1   | H     | 87  | ILE  |
| 1   | H     | 97  | ARG  |
| 1   | H     | 116 | THR  |
| 1   | H     | 119 | ASN  |
| 1   | H     | 133 | ARG  |
| 1   | H     | 150 | ASN  |
| 1   | H     | 186 | SER  |
| 1   | H     | 195 | GLN  |
| 1   | H     | 233 | SER  |
| 1   | H     | 242 | SER  |
| 1   | H     | 248 | PHE  |
| 1   | H     | 267 | ASP  |
| 1   | I     | 39  | THR  |
| 1   | I     | 56  | LEU  |
| 1   | I     | 63  | ARG  |
| 1   | I     | 69  | SER  |
| 1   | I     | 75  | MET  |
| 1   | I     | 97  | ARG  |
| 1   | I     | 117 | ASN  |
| 1   | I     | 120 | LEU  |
| 1   | I     | 133 | ARG  |
| 1   | I     | 150 | ASN  |
| 1   | I     | 233 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 242 | SER  |
| 1   | I     | 248 | PHE  |
| 1   | J     | 49  | LEU  |
| 1   | J     | 61  | SER  |
| 1   | J     | 69  | SER  |
| 1   | J     | 83  | ASN  |
| 1   | J     | 97  | ARG  |
| 1   | J     | 120 | LEU  |
| 1   | J     | 150 | ASN  |
| 1   | J     | 190 | ASN  |
| 1   | J     | 233 | SER  |
| 1   | J     | 242 | SER  |
| 1   | J     | 248 | PHE  |
| 1   | K     | 41  | ILE  |
| 1   | K     | 59  | LEU  |
| 1   | K     | 73  | LEU  |
| 1   | K     | 76  | ARG  |
| 1   | K     | 97  | ARG  |
| 1   | K     | 150 | ASN  |
| 1   | K     | 192 | PHE  |
| 1   | K     | 193 | PRO  |
| 1   | K     | 233 | SER  |
| 1   | K     | 242 | SER  |
| 1   | K     | 248 | PHE  |
| 1   | K     | 268 | LEU  |
| 1   | K     | 269 | ASP  |
| 1   | L     | 37  | ASP  |
| 1   | L     | 56  | LEU  |
| 1   | L     | 71  | ASN  |
| 1   | L     | 97  | ARG  |
| 1   | L     | 133 | ARG  |
| 1   | L     | 150 | ASN  |
| 1   | L     | 233 | SER  |
| 1   | L     | 242 | SER  |
| 1   | L     | 248 | PHE  |
| 1   | M     | 45  | SER  |
| 1   | M     | 47  | THR  |
| 1   | M     | 71  | ASN  |
| 1   | M     | 76  | ARG  |
| 1   | M     | 81  | ASP  |
| 1   | M     | 97  | ARG  |
| 1   | M     | 116 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 117 | ASN  |
| 1   | M     | 150 | ASN  |
| 1   | M     | 188 | ASN  |
| 1   | M     | 190 | ASN  |
| 1   | M     | 233 | SER  |
| 1   | M     | 242 | SER  |
| 1   | M     | 248 | PHE  |
| 1   | N     | 47  | THR  |
| 1   | N     | 58  | GLN  |
| 1   | N     | 63  | ARG  |
| 1   | N     | 79  | THR  |
| 1   | N     | 97  | ARG  |
| 1   | N     | 124 | GLU  |
| 1   | N     | 133 | ARG  |
| 1   | N     | 150 | ASN  |
| 1   | N     | 233 | SER  |
| 1   | N     | 242 | SER  |
| 1   | N     | 248 | PHE  |
| 1   | O     | 63  | ARG  |
| 1   | O     | 66  | SER  |
| 1   | O     | 75  | MET  |
| 1   | O     | 97  | ARG  |
| 1   | O     | 120 | LEU  |
| 1   | O     | 150 | ASN  |
| 1   | O     | 233 | SER  |
| 1   | O     | 242 | SER  |
| 1   | O     | 248 | PHE  |
| 1   | P     | 80  | ILE  |
| 1   | P     | 97  | ARG  |
| 1   | P     | 121 | SER  |
| 1   | P     | 150 | ASN  |
| 1   | P     | 233 | SER  |
| 1   | P     | 242 | SER  |
| 1   | P     | 248 | PHE  |
| 1   | P     | 265 | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 71  | ASN  |
| 1   | A     | 74  | HIS  |
| 1   | A     | 118 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 119 | ASN  |
| 1   | A     | 189 | HIS  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 217 | ASN  |
| 1   | B     | 42  | GLN  |
| 1   | B     | 58  | GLN  |
| 1   | B     | 188 | ASN  |
| 1   | B     | 190 | ASN  |
| 1   | B     | 217 | ASN  |
| 1   | C     | 83  | ASN  |
| 1   | C     | 119 | ASN  |
| 1   | C     | 135 | ASN  |
| 1   | C     | 189 | HIS  |
| 1   | C     | 195 | GLN  |
| 1   | C     | 217 | ASN  |
| 1   | D     | 189 | HIS  |
| 1   | D     | 217 | ASN  |
| 1   | E     | 86  | GLN  |
| 1   | E     | 190 | ASN  |
| 1   | E     | 217 | ASN  |
| 1   | F     | 86  | GLN  |
| 1   | F     | 182 | ASN  |
| 1   | F     | 189 | HIS  |
| 1   | F     | 190 | ASN  |
| 1   | F     | 217 | ASN  |
| 1   | G     | 135 | ASN  |
| 1   | G     | 182 | ASN  |
| 1   | G     | 194 | ASN  |
| 1   | G     | 217 | ASN  |
| 1   | H     | 135 | ASN  |
| 1   | H     | 189 | HIS  |
| 1   | H     | 195 | GLN  |
| 1   | H     | 217 | ASN  |
| 1   | I     | 42  | GLN  |
| 1   | I     | 58  | GLN  |
| 1   | I     | 74  | HIS  |
| 1   | I     | 189 | HIS  |
| 1   | I     | 190 | ASN  |
| 1   | I     | 217 | ASN  |
| 1   | J     | 74  | HIS  |
| 1   | J     | 78  | GLN  |
| 1   | J     | 83  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 182 | ASN  |
| 1   | J     | 189 | HIS  |
| 1   | J     | 195 | GLN  |
| 1   | J     | 217 | ASN  |
| 1   | K     | 74  | HIS  |
| 1   | K     | 86  | GLN  |
| 1   | K     | 135 | ASN  |
| 1   | K     | 217 | ASN  |
| 1   | L     | 42  | GLN  |
| 1   | L     | 194 | ASN  |
| 1   | L     | 217 | ASN  |
| 1   | M     | 74  | HIS  |
| 1   | M     | 188 | ASN  |
| 1   | M     | 190 | ASN  |
| 1   | M     | 217 | ASN  |
| 1   | N     | 42  | GLN  |
| 1   | N     | 58  | GLN  |
| 1   | N     | 74  | HIS  |
| 1   | N     | 182 | ASN  |
| 1   | N     | 189 | HIS  |
| 1   | N     | 190 | ASN  |
| 1   | N     | 194 | ASN  |
| 1   | N     | 195 | GLN  |
| 1   | N     | 217 | ASN  |
| 1   | O     | 42  | GLN  |
| 1   | O     | 217 | ASN  |
| 1   | P     | 74  | HIS  |
| 1   | P     | 135 | ASN  |
| 1   | P     | 182 | ASN  |
| 1   | P     | 217 | 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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     | 238/291 (81%)   | -0.07  | 2 (0%) 86 64  | 15, 35, 66, 84        | 0       |
| 1   | B     | 238/291 (81%)   | 0.16   | 10 (4%) 37 15 | 17, 41, 71, 84        | 0       |
| 1   | C     | 244/291 (83%)   | -0.20  | 2 (0%) 86 64  | 13, 32, 58, 78        | 0       |
| 1   | D     | 244/291 (83%)   | -0.09  | 3 (1%) 79 53  | 14, 36, 65, 92        | 0       |
| 1   | E     | 238/291 (81%)   | 0.06   | 4 (1%) 70 42  | 15, 40, 71, 83        | 0       |
| 1   | F     | 238/291 (81%)   | 0.14   | 8 (3%) 46 20  | 14, 36, 67, 86        | 0       |
| 1   | G     | 236/291 (81%)   | -0.09  | 1 (0%) 92 77  | 18, 37, 66, 77        | 0       |
| 1   | H     | 245/291 (84%)   | -0.02  | 2 (0%) 86 64  | 13, 30, 57, 71        | 0       |
| 1   | I     | 238/291 (81%)   | 0.08   | 8 (3%) 46 20  | 23, 42, 72, 85        | 0       |
| 1   | J     | 238/291 (81%)   | -0.13  | 3 (1%) 77 51  | 16, 39, 68, 81        | 0       |
| 1   | K     | 244/291 (83%)   | -0.22  | 1 (0%) 92 77  | 10, 35, 68, 85        | 0       |
| 1   | L     | 236/291 (81%)   | -0.05  | 4 (1%) 70 42  | 18, 34, 64, 76        | 0       |
| 1   | M     | 238/291 (81%)   | 0.19   | 11 (4%) 33 13 | 17, 40, 71, 87        | 0       |
| 1   | N     | 238/291 (81%)   | -0.18  | 4 (1%) 70 42  | 14, 40, 69, 83        | 0       |
| 1   | O     | 236/291 (81%)   | -0.17  | 3 (1%) 77 51  | 9, 34, 64, 79         | 0       |
| 1   | P     | 244/291 (83%)   | -0.13  | 1 (0%) 92 77  | 12, 35, 67, 87        | 0       |
| All | All   | 3833/4656 (82%) | -0.05  | 67 (1%) 70 42 | 9, 37, 67, 92         | 0       |

All (67) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 261 | SER  | 4.4  |
| 1   | M     | 83  | ASN  | 4.0  |
| 1   | D     | 150 | ASN  | 3.9  |
| 1   | I     | 83  | ASN  | 3.7  |
| 1   | L     | 243 | ASN  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 83  | ASN  | 3.6  |
| 1   | L     | 262 | LYS  | 3.6  |
| 1   | M     | 151 | LEU  | 3.5  |
| 1   | A     | 245 | SER  | 3.5  |
| 1   | N     | 243 | ASN  | 3.5  |
| 1   | J     | 245 | SER  | 3.4  |
| 1   | M     | 243 | ASN  | 3.2  |
| 1   | M     | 244 | ILE  | 3.2  |
| 1   | L     | 242 | SER  | 3.1  |
| 1   | M     | 239 | SER  | 3.1  |
| 1   | M     | 236 | ASN  | 3.0  |
| 1   | M     | 247 | VAL  | 3.0  |
| 1   | B     | 247 | VAL  | 3.0  |
| 1   | N     | 82  | SER  | 2.9  |
| 1   | E     | 241 | PRO  | 2.9  |
| 1   | F     | 256 | GLY  | 2.9  |
| 1   | B     | 246 | LYS  | 2.8  |
| 1   | I     | 254 | SER  | 2.8  |
| 1   | P     | 150 | ASN  | 2.8  |
| 1   | N     | 84  | THR  | 2.7  |
| 1   | D     | 243 | ASN  | 2.7  |
| 1   | F     | 254 | SER  | 2.7  |
| 1   | H     | 83  | ASN  | 2.7  |
| 1   | M     | 241 | PRO  | 2.6  |
| 1   | L     | 245 | SER  | 2.6  |
| 1   | O     | 244 | ILE  | 2.6  |
| 1   | E     | 261 | SER  | 2.5  |
| 1   | B     | 239 | SER  | 2.5  |
| 1   | F     | 245 | SER  | 2.5  |
| 1   | I     | 239 | SER  | 2.5  |
| 1   | M     | 245 | SER  | 2.5  |
| 1   | H     | 242 | SER  | 2.4  |
| 1   | A     | 244 | ILE  | 2.4  |
| 1   | K     | 266 | LEU  | 2.4  |
| 1   | F     | 252 | ASN  | 2.4  |
| 1   | J     | 243 | ASN  | 2.3  |
| 1   | I     | 86  | GLN  | 2.3  |
| 1   | E     | 239 | SER  | 2.3  |
| 1   | I     | 82  | SER  | 2.3  |
| 1   | B     | 248 | PHE  | 2.3  |
| 1   | O     | 262 | LYS  | 2.3  |
| 1   | G     | 82  | SER  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 247 | VAL  | 2.3  |
| 1   | I     | 221 | VAL  | 2.2  |
| 1   | F     | 261 | SER  | 2.2  |
| 1   | F     | 241 | PRO  | 2.2  |
| 1   | M     | 255 | GLU  | 2.2  |
| 1   | I     | 84  | THR  | 2.2  |
| 1   | C     | 186 | SER  | 2.2  |
| 1   | B     | 238 | VAL  | 2.2  |
| 1   | F     | 83  | ASN  | 2.2  |
| 1   | I     | 167 | ILE  | 2.1  |
| 1   | F     | 104 | ASN  | 2.1  |
| 1   | N     | 83  | ASN  | 2.1  |
| 1   | B     | 177 | GLY  | 2.1  |
| 1   | B     | 234 | THR  | 2.1  |
| 1   | C     | 84  | THR  | 2.1  |
| 1   | O     | 242 | SER  | 2.0  |
| 1   | B     | 84  | THR  | 2.0  |
| 1   | B     | 245 | SER  | 2.0  |
| 1   | M     | 81  | ASP  | 2.0  |
| 1   | D     | 286 | ASN  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.