



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:00 am BST

PDB ID : 1PD5  
Title : Crystal structure of E.coli chloramphenicol acetyltransferase type I at 2.5 Angstrom resolution  
Authors : Roidis, A.; Kokkinidis, M.  
Deposited on : 2003-05-19  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

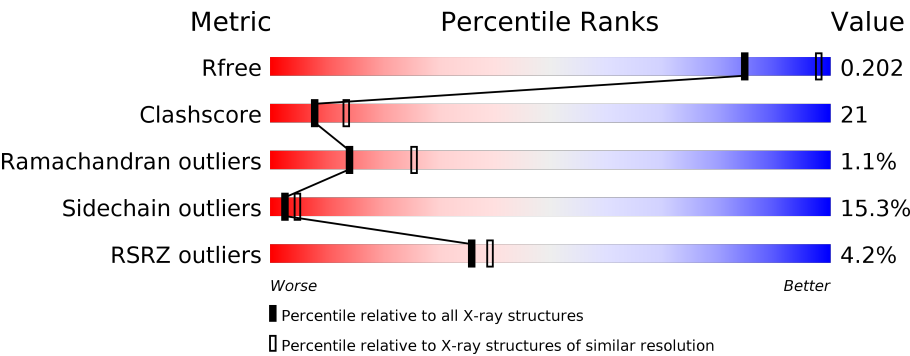
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 4661 (2.50-2.50)                                      |
| Clashscore            | 141614                      | 5346 (2.50-2.50)                                      |
| Ramachandran outliers | 138981                      | 5231 (2.50-2.50)                                      |
| Sidechain outliers    | 138945                      | 5233 (2.50-2.50)                                      |
| RSRZ outliers         | 127900                      | 4559 (2.50-2.50)                                      |

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

| Mol | Chain | Length | Quality of chain                                 |
|-----|-------|--------|--|
| 1   | A     | 219    | <div><div></div><div>45%37%12% . .</div></div>   |
| 1   | B     | 219    | <div><div></div><div>57%29%9% . .</div></div>    |
| 1   | C     | 219    | <div><div>%</div><div>47%38%9% . .</div></div>   |
| 1   | D     | 219    | <div><div>%</div><div>46%40%8% . .</div></div>   |
| 1   | E     | 219    | <div><div>%</div><div>54%35%8% . .</div></div>   |
| 1   | F     | 219    | <div><div>2%</div><div>48%38%10% . .</div></div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 219    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%51%35%8% . .</div></div>   |
| 1   | H     | 219    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%49%40%8% . .</div></div>   |
| 1   | I     | 219    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%44%41%10% . .</div></div>   |
| 1   | J     | 219    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>12%43%36%13% . .</div></div> |
| 1   | K     | 219    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>11%47%39%10% . .</div></div> |
| 1   | L     | 219    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%41%39%16% .</div></div>   |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 21418 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 Chloramphenicol acetyltransferase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1763  | 1144 | 290 | 316 | 13 |         |         |       |
| 1   | B     | 216      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1789  | 1162 | 295 | 319 | 13 |         |         |       |
| 1   | C     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1763  | 1144 | 290 | 316 | 13 |         |         |       |
| 1   | D     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1763  | 1144 | 290 | 316 | 13 |         |         |       |
| 1   | E     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1785  | 1160 | 294 | 318 | 13 |         |         |       |
| 1   | F     | 212      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1759  | 1142 | 289 | 315 | 13 |         |         |       |
| 1   | G     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1763  | 1144 | 290 | 316 | 13 |         |         |       |
| 1   | H     | 216      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1785  | 1159 | 294 | 319 | 13 |         |         |       |
| 1   | I     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1776  | 1154 | 292 | 317 | 13 |         |         |       |
| 1   | J     | 211      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1755  | 1140 | 288 | 314 | 13 |         |         |       |
| 1   | K     | 212      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1763  | 1147 | 289 | 314 | 13 |         |         |       |
| 1   | L     | 210      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1746  | 1135 | 286 | 312 | 13 |         |         |       |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 2   | B     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |

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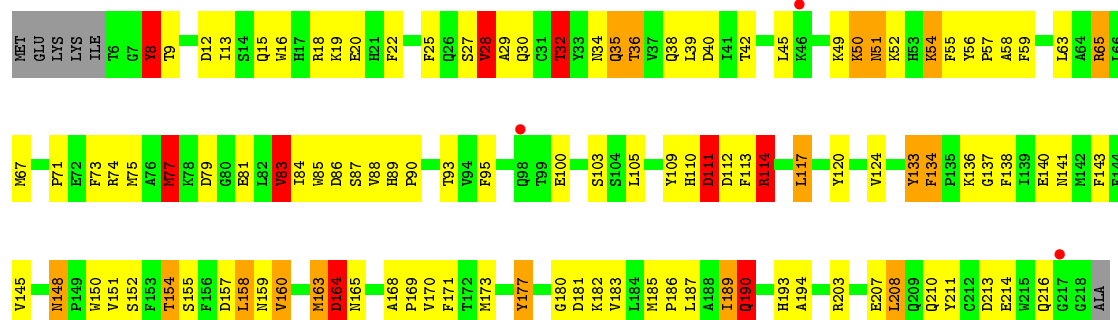
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | C     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 2   | D     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 2   | E     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 2   | F     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 2   | G     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 2   | H     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |
| 2   | I     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 2   | J     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 2   | K     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 2   | L     | 8        | Total | O  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |

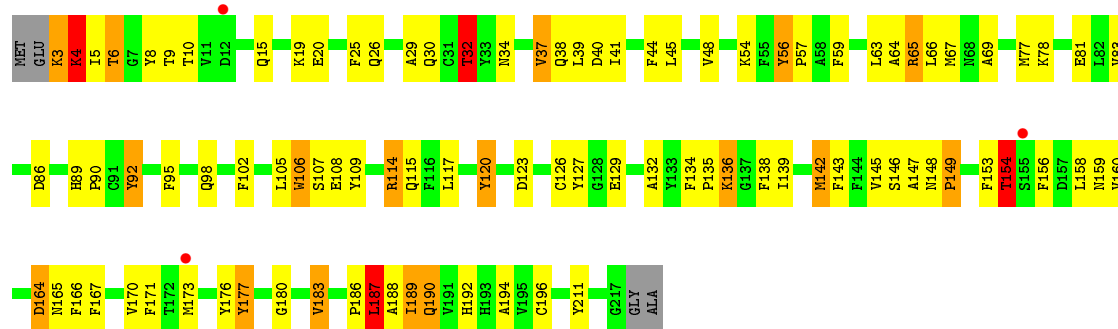




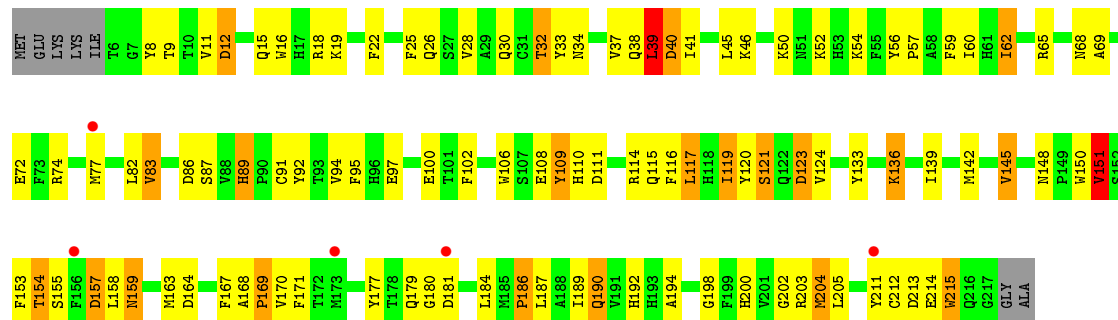
• Molecule 1: Chloramphenicol acetyltransferase



• Molecule 1: Chloramphenicol acetyltransferase

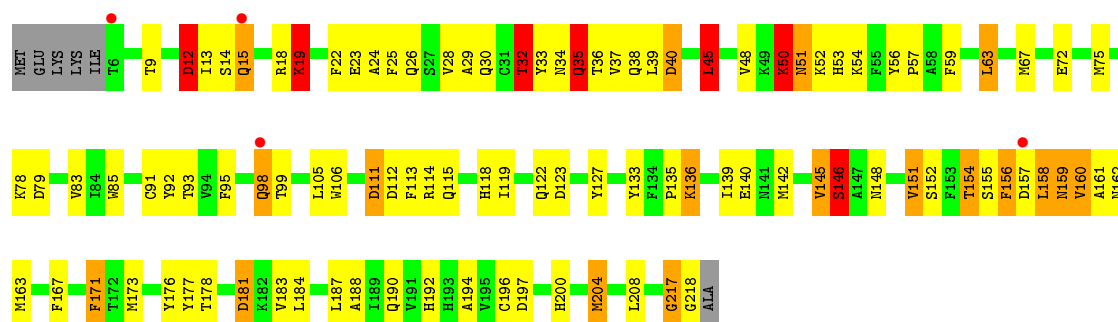


• Molecule 1: Chloramphenicol acetyltransferase

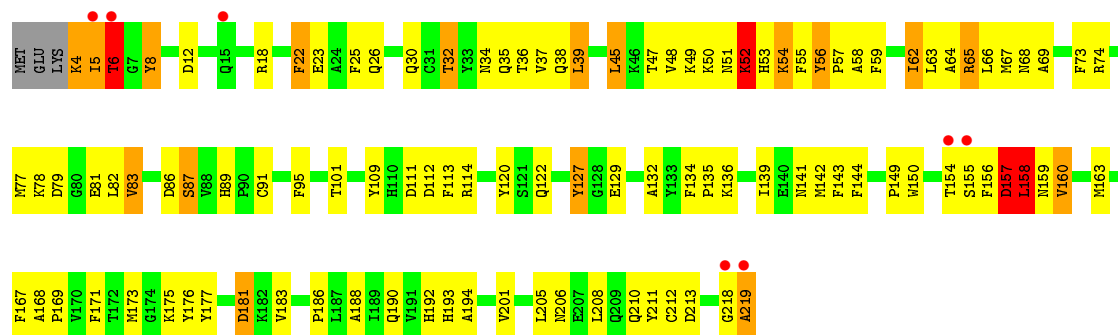


• Molecule 1: Chloramphenicol acetyltransferase

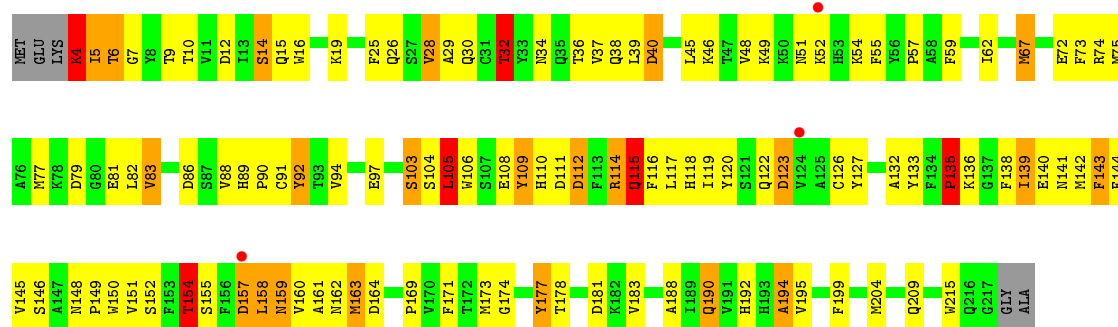
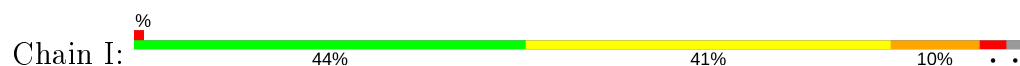




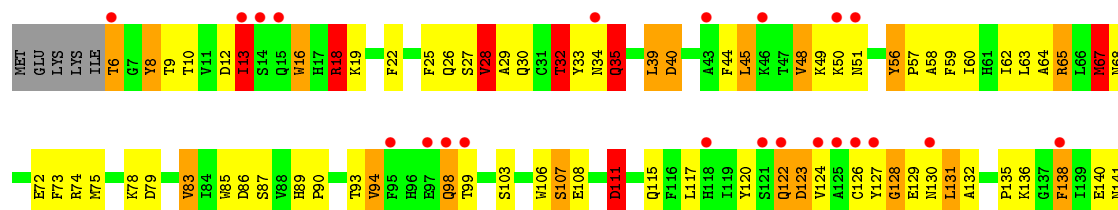
• Molecule 1: Chloramphenicol acetyltransferase



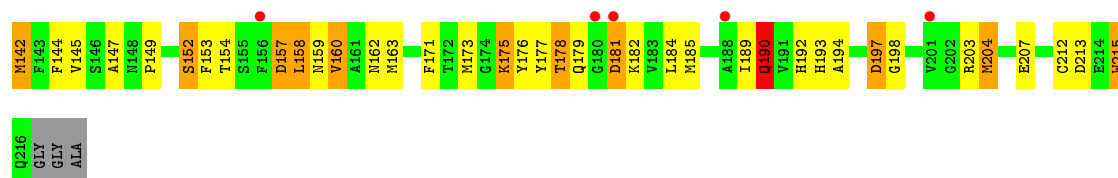
• Molecule 1: Chloramphenicol acetyltransferase



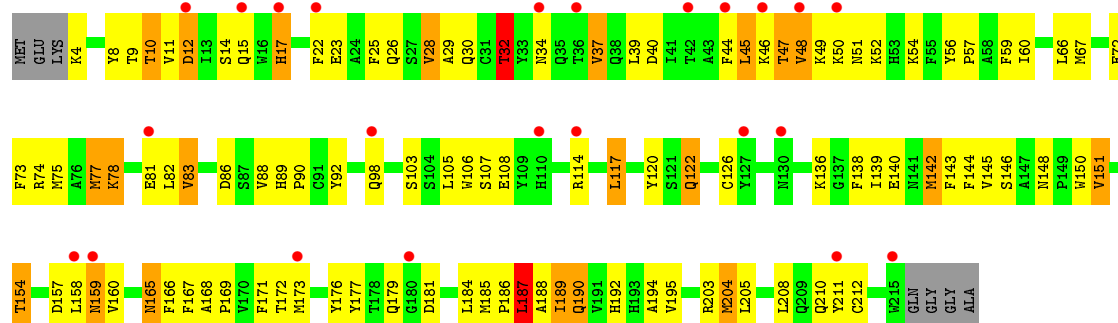
• Molecule 1: Chloramphenicol acetyltransferase



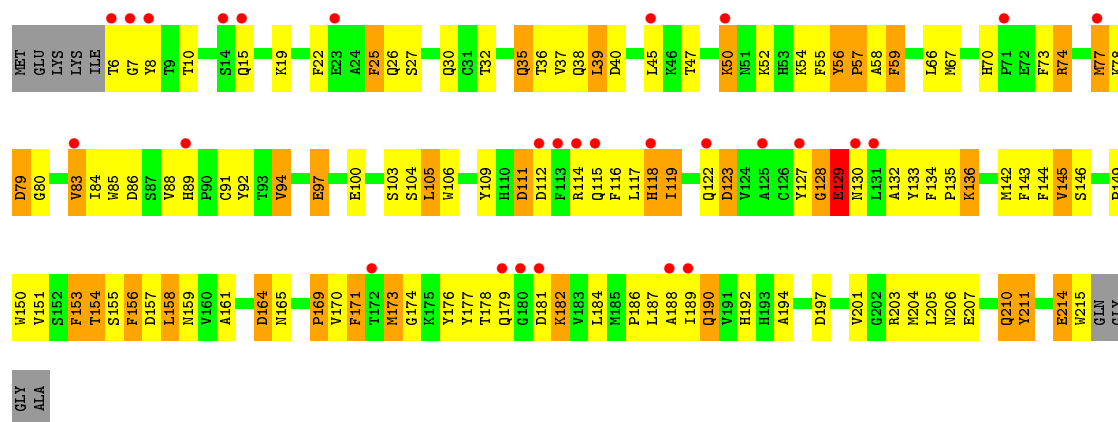




• Molecule 1: Chloramphenicol acetyltransferase



• Molecule 1: Chloramphenicol acetyltransferase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 115.74Å 129.70Å 117.98Å<br>90.00° 108.38° 90.00°            | Depositor        |
| Resolution (Å)  | 10.00 – 2.50<br>39.33 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.6 (10.00-2.50)<br>98.7 (39.33-2.50)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | 0.06  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.61 (at 2.51Å)   | Xtriage          |
| Refinement program  | REFMAC 5.1.24   | Depositor        |
| R, $R_{free}$   | 0.195 , 0.281<br>0.211 , 0.202                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5684 reflections (5.04%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 37.9  | Xtriage          |
| Anisotropy  | 0.643   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 51.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction   | 0.012 for l,-k,h  | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 21418   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 46.0  | 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 21.31 % 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 7.2096e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 1   | A     | 2.04         | 58/1822 (3.2%)   | 1.62        | 38/2473 (1.5%)   |
| 1   | B     | 1.76         | 22/1848 (1.2%)   | 1.59        | 34/2506 (1.4%)   |
| 1   | C     | 1.84         | 35/1822 (1.9%)   | 1.58        | 36/2473 (1.5%)   |
| 1   | D     | 1.83         | 38/1822 (2.1%)   | 1.52        | 25/2473 (1.0%)   |
| 1   | E     | 1.67         | 20/1844 (1.1%)   | 1.39        | 14/2501 (0.6%)   |
| 1   | F     | 1.76         | 26/1818 (1.4%)   | 1.53        | 31/2468 (1.3%)   |
| 1   | G     | 1.71         | 18/1822 (1.0%)   | 1.53        | 30/2473 (1.2%)   |
| 1   | H     | 1.85         | 33/1844 (1.8%)   | 1.55        | 30/2502 (1.2%)   |
| 1   | I     | 1.85         | 38/1835 (2.1%)   | 1.50        | 23/2490 (0.9%)   |
| 1   | J     | 1.57         | 15/1814 (0.8%)   | 1.47        | 26/2463 (1.1%)   |
| 1   | K     | 1.55         | 14/1822 (0.8%)   | 1.35        | 9/2473 (0.4%)    |
| 1   | L     | 1.67         | 21/1805 (1.2%)   | 1.41        | 19/2451 (0.8%)   |
| All | All   | 1.76         | 338/21918 (1.5%) | 1.51        | 315/29746 (1.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 2                   |
| 1   | G     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 1   | J     | 0                   | 3                   |
| 1   | K     | 0                   | 1                   |
| 1   | L     | 0                   | 1                   |
| All | All   | 0                   | 10                  |

All (338) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 150 | TRP  | CE3-CZ3 | 10.79 | 1.56        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 95  | PHE  | CE2-CZ  | 10.43  | 1.57        | 1.37     |
| 1   | A     | 87  | SER  | CB-OG   | -10.09 | 1.29        | 1.42     |
| 1   | I     | 127 | TYR  | CD1-CE1 | 10.07  | 1.54        | 1.39     |
| 1   | I     | 140 | GLU  | CD-OE1  | 9.99   | 1.36        | 1.25     |
| 1   | E     | 146 | SER  | CB-OG   | 9.66   | 1.54        | 1.42     |
| 1   | G     | 151 | VAL  | CB-CG2  | 9.36   | 1.72        | 1.52     |
| 1   | I     | 28  | VAL  | CB-CG2  | 9.03   | 1.71        | 1.52     |
| 1   | I     | 183 | VAL  | CB-CG1  | 9.00   | 1.71        | 1.52     |
| 1   | F     | 171 | PHE  | CE2-CZ  | 8.93   | 1.54        | 1.37     |
| 1   | A     | 28  | VAL  | CB-CG1  | 8.76   | 1.71        | 1.52     |
| 1   | F     | 145 | VAL  | CB-CG1  | 8.62   | 1.71        | 1.52     |
| 1   | K     | 151 | VAL  | CB-CG2  | 8.49   | 1.70        | 1.52     |
| 1   | C     | 95  | PHE  | CE1-CZ  | 8.35   | 1.53        | 1.37     |
| 1   | C     | 28  | VAL  | CB-CG2  | 8.33   | 1.70        | 1.52     |
| 1   | F     | 116 | PHE  | CE2-CZ  | 8.24   | 1.53        | 1.37     |
| 1   | I     | 144 | PHE  | CD1-CE1 | 8.23   | 1.55        | 1.39     |
| 1   | A     | 35  | GLN  | CB-CG   | -8.21  | 1.30        | 1.52     |
| 1   | J     | 94  | VAL  | CB-CG2  | 8.21   | 1.70        | 1.52     |
| 1   | A     | 177 | TYR  | CE1-CZ  | 8.19   | 1.49        | 1.38     |
| 1   | J     | 177 | TYR  | CD2-CE2 | -8.13  | 1.27        | 1.39     |
| 1   | H     | 69  | ALA  | CA-CB   | 8.12   | 1.69        | 1.52     |
| 1   | B     | 159 | ASN  | CB-CG   | 8.07   | 1.69        | 1.51     |
| 1   | F     | 211 | TYR  | CD2-CE2 | 8.05   | 1.51        | 1.39     |
| 1   | D     | 58  | ALA  | CA-CB   | 8.04   | 1.69        | 1.52     |
| 1   | A     | 33  | TYR  | CD1-CE1 | 8.03   | 1.51        | 1.39     |
| 1   | D     | 35  | GLN  | CB-CG   | -7.99  | 1.30        | 1.52     |
| 1   | A     | 162 | ASN  | CB-CG   | 7.94   | 1.69        | 1.51     |
| 1   | A     | 129 | GLU  | CD-OE1  | 7.81   | 1.34        | 1.25     |
| 1   | J     | 198 | GLY  | C-O     | 7.71   | 1.35        | 1.23     |
| 1   | E     | 160 | VAL  | CB-CG1  | -7.67  | 1.36        | 1.52     |
| 1   | L     | 143 | PHE  | CE1-CZ  | 7.66   | 1.51        | 1.37     |
| 1   | A     | 24  | ALA  | C-O     | 7.63   | 1.37        | 1.23     |
| 1   | A     | 86  | ASP  | CB-CG   | 7.62   | 1.67        | 1.51     |
| 1   | A     | 156 | PHE  | CE2-CZ  | 7.62   | 1.51        | 1.37     |
| 1   | F     | 211 | TYR  | CD1-CE1 | 7.61   | 1.50        | 1.39     |
| 1   | I     | 109 | TYR  | CB-CG   | -7.59  | 1.40        | 1.51     |
| 1   | C     | 162 | ASN  | CB-CG   | -7.49  | 1.33        | 1.51     |
| 1   | F     | 170 | VAL  | CB-CG2  | 7.47   | 1.68        | 1.52     |
| 1   | C     | 98  | GLN  | CG-CD   | 7.45   | 1.68        | 1.51     |
| 1   | C     | 195 | VAL  | CB-CG1  | 7.44   | 1.68        | 1.52     |
| 1   | J     | 160 | VAL  | CB-CG2  | 7.42   | 1.68        | 1.52     |
| 1   | B     | 160 | VAL  | CB-CG1  | -7.39  | 1.37        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 157 | ASP  | CB-CG   | -7.38 | 1.36        | 1.51     |
| 1   | B     | 28  | VAL  | CB-CG2  | 7.38  | 1.68        | 1.52     |
| 1   | I     | 111 | ASP  | CB-CG   | 7.38  | 1.67        | 1.51     |
| 1   | F     | 150 | TRP  | CB-CG   | -7.26 | 1.37        | 1.50     |
| 1   | C     | 87  | SER  | CB-OG   | -7.22 | 1.32        | 1.42     |
| 1   | B     | 102 | PHE  | CE2-CZ  | 7.17  | 1.50        | 1.37     |
| 1   | E     | 166 | PHE  | CD1-CE1 | 7.16  | 1.53        | 1.39     |
| 1   | A     | 69  | ALA  | CA-CB   | 7.14  | 1.67        | 1.52     |
| 1   | A     | 81  | GLU  | CG-CD   | 7.14  | 1.62        | 1.51     |
| 1   | K     | 211 | TYR  | CD1-CE1 | 7.13  | 1.50        | 1.39     |
| 1   | I     | 162 | ASN  | C-O     | -7.12 | 1.09        | 1.23     |
| 1   | H     | 81  | GLU  | CD-OE2  | 7.11  | 1.33        | 1.25     |
| 1   | A     | 195 | VAL  | CB-CG1  | 7.11  | 1.67        | 1.52     |
| 1   | I     | 152 | SER  | CB-OG   | 7.10  | 1.51        | 1.42     |
| 1   | B     | 199 | PHE  | CE1-CZ  | 7.08  | 1.50        | 1.37     |
| 1   | F     | 102 | PHE  | CD1-CE1 | 7.08  | 1.53        | 1.39     |
| 1   | G     | 176 | TYR  | CD1-CE1 | 7.08  | 1.50        | 1.39     |
| 1   | I     | 55  | PHE  | CE2-CZ  | 7.07  | 1.50        | 1.37     |
| 1   | F     | 167 | PHE  | CG-CD2  | 7.06  | 1.49        | 1.38     |
| 1   | A     | 8   | TYR  | CD1-CE1 | -7.04 | 1.28        | 1.39     |
| 1   | A     | 95  | PHE  | CE2-CZ  | 7.02  | 1.50        | 1.37     |
| 1   | A     | 161 | ALA  | CA-CB   | -6.97 | 1.37        | 1.52     |
| 1   | C     | 156 | PHE  | CE2-CZ  | 6.96  | 1.50        | 1.37     |
| 1   | I     | 116 | PHE  | CE1-CZ  | 6.92  | 1.50        | 1.37     |
| 1   | H     | 134 | PHE  | CD1-CE1 | 6.91  | 1.53        | 1.39     |
| 1   | L     | 174 | GLY  | C-O     | 6.90  | 1.34        | 1.23     |
| 1   | K     | 98  | GLN  | CG-CD   | 6.89  | 1.66        | 1.51     |
| 1   | I     | 103 | SER  | C-O     | 6.88  | 1.36        | 1.23     |
| 1   | L     | 176 | TYR  | CG-CD1  | 6.86  | 1.48        | 1.39     |
| 1   | K     | 144 | PHE  | CD1-CE1 | 6.85  | 1.52        | 1.39     |
| 1   | I     | 106 | TRP  | CB-CG   | 6.84  | 1.62        | 1.50     |
| 1   | I     | 199 | PHE  | CE1-CZ  | 6.80  | 1.50        | 1.37     |
| 1   | H     | 22  | PHE  | CE1-CZ  | 6.79  | 1.50        | 1.37     |
| 1   | I     | 6   | THR  | CB-CG2  | 6.79  | 1.74        | 1.52     |
| 1   | H     | 143 | PHE  | CE2-CZ  | 6.78  | 1.50        | 1.37     |
| 1   | D     | 190 | GLN  | CB-CG   | -6.75 | 1.34        | 1.52     |
| 1   | G     | 159 | ASN  | CB-CG   | 6.74  | 1.66        | 1.51     |
| 1   | B     | 215 | TRP  | CG-CD1  | 6.71  | 1.46        | 1.36     |
| 1   | L     | 171 | PHE  | CE2-CZ  | 6.71  | 1.50        | 1.37     |
| 1   | C     | 176 | TYR  | CG-CD1  | 6.71  | 1.47        | 1.39     |
| 1   | E     | 143 | PHE  | CD2-CE2 | 6.70  | 1.52        | 1.39     |
| 1   | E     | 37  | VAL  | CB-CG1  | -6.65 | 1.38        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 54  | LYS  | CE-NZ   | 6.64  | 1.65        | 1.49     |
| 1   | B     | 28  | VAL  | CB-CG1  | 6.64  | 1.66        | 1.52     |
| 1   | L     | 177 | TYR  | CE1-CZ  | 6.62  | 1.47        | 1.38     |
| 1   | I     | 215 | TRP  | CB-CG   | -6.60 | 1.38        | 1.50     |
| 1   | H     | 176 | TYR  | CG-CD1  | 6.60  | 1.47        | 1.39     |
| 1   | E     | 102 | PHE  | CE2-CZ  | 6.53  | 1.49        | 1.37     |
| 1   | B     | 170 | VAL  | CB-CG2  | 6.52  | 1.66        | 1.52     |
| 1   | C     | 15  | GLN  | CG-CD   | 6.51  | 1.66        | 1.51     |
| 1   | H     | 78  | LYS  | CE-NZ   | 6.51  | 1.65        | 1.49     |
| 1   | G     | 181 | ASP  | CB-CG   | 6.51  | 1.65        | 1.51     |
| 1   | D     | 95  | PHE  | CG-CD1  | 6.47  | 1.48        | 1.38     |
| 1   | L     | 116 | PHE  | CE1-CZ  | 6.47  | 1.49        | 1.37     |
| 1   | E     | 143 | PHE  | CD1-CE1 | 6.47  | 1.52        | 1.39     |
| 1   | I     | 72  | GLU  | CD-OE2  | 6.46  | 1.32        | 1.25     |
| 1   | A     | 54  | LYS  | CD-CE   | 6.45  | 1.67        | 1.51     |
| 1   | D     | 177 | TYR  | CD1-CE1 | 6.40  | 1.49        | 1.39     |
| 1   | F     | 95  | PHE  | CE1-CZ  | 6.37  | 1.49        | 1.37     |
| 1   | C     | 33  | TYR  | CB-CG   | -6.36 | 1.42        | 1.51     |
| 1   | C     | 81  | GLU  | CD-OE2  | 6.36  | 1.32        | 1.25     |
| 1   | G     | 176 | TYR  | CE1-CZ  | 6.34  | 1.46        | 1.38     |
| 1   | E     | 196 | CYS  | CB-SG   | -6.31 | 1.71        | 1.82     |
| 1   | A     | 150 | TRP  | CE3-CZ3 | 6.28  | 1.49        | 1.38     |
| 1   | F     | 69  | ALA  | CA-CB   | 6.27  | 1.65        | 1.52     |
| 1   | E     | 56  | TYR  | CG-CD1  | -6.27 | 1.31        | 1.39     |
| 1   | A     | 74  | ARG  | CB-CG   | 6.26  | 1.69        | 1.52     |
| 1   | H     | 183 | VAL  | CB-CG2  | 6.26  | 1.66        | 1.52     |
| 1   | H     | 55  | PHE  | CE1-CZ  | 6.26  | 1.49        | 1.37     |
| 1   | I     | 37  | VAL  | CB-CG2  | -6.25 | 1.39        | 1.52     |
| 1   | D     | 54  | LYS  | CD-CE   | 6.24  | 1.66        | 1.51     |
| 1   | L     | 153 | PHE  | CE1-CZ  | 6.23  | 1.49        | 1.37     |
| 1   | H     | 167 | PHE  | CB-CG   | 6.23  | 1.61        | 1.51     |
| 1   | B     | 176 | TYR  | CG-CD1  | 6.22  | 1.47        | 1.39     |
| 1   | I     | 55  | PHE  | CD1-CE1 | 6.22  | 1.51        | 1.39     |
| 1   | C     | 176 | TYR  | CD1-CE1 | 6.22  | 1.48        | 1.39     |
| 1   | G     | 146 | SER  | CB-OG   | -6.19 | 1.34        | 1.42     |
| 1   | B     | 16  | TRP  | CG-CD1  | 6.19  | 1.45        | 1.36     |
| 1   | J     | 190 | GLN  | CB-CG   | 6.17  | 1.69        | 1.52     |
| 1   | H     | 206 | ASN  | C-O     | 6.16  | 1.35        | 1.23     |
| 1   | H     | 160 | VAL  | CA-CB   | 6.15  | 1.67        | 1.54     |
| 1   | F     | 151 | VAL  | CB-CG2  | -6.14 | 1.40        | 1.52     |
| 1   | A     | 166 | PHE  | CE1-CZ  | 6.13  | 1.49        | 1.37     |
| 1   | A     | 153 | PHE  | CD1-CE1 | 6.13  | 1.51        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 126 | CYS  | CB-SG   | -6.12 | 1.71        | 1.82     |
| 1   | B     | 67  | MET  | CB-CG   | 6.11  | 1.70        | 1.51     |
| 1   | A     | 22  | PHE  | CE2-CZ  | 6.10  | 1.49        | 1.37     |
| 1   | D     | 211 | TYR  | CB-CG   | -6.10 | 1.42        | 1.51     |
| 1   | H     | 157 | ASP  | CA-CB   | -6.10 | 1.40        | 1.53     |
| 1   | C     | 23  | GLU  | CG-CD   | 6.09  | 1.61        | 1.51     |
| 1   | C     | 27  | SER  | C-O     | 6.09  | 1.34        | 1.23     |
| 1   | D     | 22  | PHE  | CE1-CZ  | 6.09  | 1.49        | 1.37     |
| 1   | I     | 92  | TYR  | CE2-CZ  | 6.08  | 1.46        | 1.38     |
| 1   | D     | 138 | PHE  | CE2-CZ  | 6.07  | 1.48        | 1.37     |
| 1   | K     | 177 | TYR  | CE2-CZ  | 6.07  | 1.46        | 1.38     |
| 1   | L     | 97  | GLU  | CD-OE1  | 6.07  | 1.32        | 1.25     |
| 1   | D     | 8   | TYR  | CG-CD1  | 6.07  | 1.47        | 1.39     |
| 1   | J     | 140 | GLU  | CD-OE2  | 6.05  | 1.32        | 1.25     |
| 1   | L     | 153 | PHE  | CD1-CE1 | 6.02  | 1.51        | 1.39     |
| 1   | G     | 24  | ALA  | CA-CB   | -6.02 | 1.39        | 1.52     |
| 1   | K     | 159 | ASN  | CB-CG   | 6.01  | 1.64        | 1.51     |
| 1   | C     | 153 | PHE  | CE1-CZ  | 5.99  | 1.48        | 1.37     |
| 1   | A     | 95  | PHE  | CE1-CZ  | 5.99  | 1.48        | 1.37     |
| 1   | C     | 127 | TYR  | CD1-CE1 | 5.98  | 1.48        | 1.39     |
| 1   | I     | 177 | TYR  | CD1-CE1 | 5.97  | 1.48        | 1.39     |
| 1   | A     | 26  | GLN  | CB-CG   | -5.96 | 1.36        | 1.52     |
| 1   | I     | 159 | ASN  | CB-CG   | 5.93  | 1.64        | 1.51     |
| 1   | I     | 183 | VAL  | CB-CG2  | 5.93  | 1.65        | 1.52     |
| 1   | H     | 64  | ALA  | CA-CB   | -5.92 | 1.40        | 1.52     |
| 1   | B     | 194 | ALA  | CA-CB   | 5.92  | 1.64        | 1.52     |
| 1   | D     | 134 | PHE  | CE1-CZ  | 5.92  | 1.48        | 1.37     |
| 1   | I     | 4   | LYS  | CB-CG   | 5.92  | 1.68        | 1.52     |
| 1   | H     | 56  | TYR  | CD2-CE2 | 5.92  | 1.48        | 1.39     |
| 1   | A     | 140 | GLU  | CD-OE1  | 5.92  | 1.32        | 1.25     |
| 1   | A     | 169 | PRO  | CA-C    | 5.92  | 1.64        | 1.52     |
| 1   | I     | 4   | LYS  | N-CA    | 5.90  | 1.58        | 1.46     |
| 1   | G     | 171 | PHE  | CD1-CE1 | 5.89  | 1.51        | 1.39     |
| 1   | A     | 134 | PHE  | CB-CG   | 5.88  | 1.61        | 1.51     |
| 1   | A     | 176 | TYR  | CE2-CZ  | 5.88  | 1.46        | 1.38     |
| 1   | A     | 191 | VAL  | CA-CB   | -5.88 | 1.42        | 1.54     |
| 1   | I     | 114 | ARG  | CG-CD   | 5.87  | 1.66        | 1.51     |
| 1   | D     | 210 | GLN  | CG-CD   | 5.86  | 1.64        | 1.51     |
| 1   | D     | 216 | GLN  | CG-CD   | 5.85  | 1.64        | 1.51     |
| 1   | H     | 176 | TYR  | CD1-CE1 | 5.85  | 1.48        | 1.39     |
| 1   | D     | 111 | ASP  | CB-CG   | -5.85 | 1.39        | 1.51     |
| 1   | B     | 109 | TYR  | CD1-CE1 | 5.85  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 28  | VAL  | CB-CG1  | 5.85  | 1.65        | 1.52     |
| 1   | D     | 105 | LEU  | CG-CD1  | 5.84  | 1.73        | 1.51     |
| 1   | H     | 144 | PHE  | C-O     | 5.82  | 1.34        | 1.23     |
| 1   | B     | 190 | GLN  | CB-CG   | -5.82 | 1.36        | 1.52     |
| 1   | F     | 109 | TYR  | CD2-CE2 | -5.81 | 1.30        | 1.39     |
| 1   | E     | 170 | VAL  | CB-CG2  | 5.80  | 1.65        | 1.52     |
| 1   | A     | 95  | PHE  | CG-CD2  | 5.80  | 1.47        | 1.38     |
| 1   | F     | 22  | PHE  | CE2-CZ  | 5.79  | 1.48        | 1.37     |
| 1   | D     | 177 | TYR  | CG-CD2  | 5.78  | 1.46        | 1.39     |
| 1   | B     | 200 | HIS  | C-O     | -5.78 | 1.12        | 1.23     |
| 1   | G     | 167 | PHE  | CG-CD2  | 5.78  | 1.47        | 1.38     |
| 1   | D     | 133 | TYR  | CG-CD1  | 5.75  | 1.46        | 1.39     |
| 1   | K     | 189 | ILE  | CA-CB   | 5.75  | 1.68        | 1.54     |
| 1   | H     | 167 | PHE  | CD1-CE1 | 5.75  | 1.50        | 1.39     |
| 1   | D     | 211 | TYR  | C-O     | -5.74 | 1.12        | 1.23     |
| 1   | A     | 167 | PHE  | CB-CG   | 5.73  | 1.61        | 1.51     |
| 1   | H     | 79  | ASP  | CB-CG   | 5.72  | 1.63        | 1.51     |
| 1   | J     | 16  | TRP  | CG-CD1  | 5.72  | 1.44        | 1.36     |
| 1   | C     | 102 | PHE  | CD1-CE1 | 5.71  | 1.50        | 1.39     |
| 1   | C     | 83  | VAL  | CB-CG1  | -5.71 | 1.40        | 1.52     |
| 1   | D     | 145 | VAL  | CB-CG2  | -5.70 | 1.40        | 1.52     |
| 1   | I     | 140 | GLU  | CG-CD   | 5.70  | 1.60        | 1.51     |
| 1   | A     | 59  | PHE  | CD1-CE1 | 5.70  | 1.50        | 1.39     |
| 1   | D     | 114 | ARG  | CG-CD   | 5.69  | 1.66        | 1.51     |
| 1   | I     | 194 | ALA  | C-O     | 5.68  | 1.34        | 1.23     |
| 1   | A     | 95  | PHE  | CG-CD1  | 5.66  | 1.47        | 1.38     |
| 1   | I     | 15  | GLN  | CB-CG   | 5.66  | 1.67        | 1.52     |
| 1   | C     | 127 | TYR  | CE2-CZ  | 5.66  | 1.46        | 1.38     |
| 1   | D     | 170 | VAL  | CA-CB   | -5.62 | 1.43        | 1.54     |
| 1   | H     | 150 | TRP  | CE3-CZ3 | 5.62  | 1.48        | 1.38     |
| 1   | A     | 196 | CYS  | CB-SG   | -5.62 | 1.72        | 1.81     |
| 1   | I     | 195 | VAL  | CB-CG1  | 5.61  | 1.64        | 1.52     |
| 1   | D     | 171 | PHE  | C-O     | 5.60  | 1.33        | 1.23     |
| 1   | D     | 109 | TYR  | CD2-CE2 | 5.60  | 1.47        | 1.39     |
| 1   | H     | 219 | ALA  | N-CA    | 5.59  | 1.57        | 1.46     |
| 1   | K     | 12  | ASP  | CB-CG   | 5.59  | 1.63        | 1.51     |
| 1   | C     | 65  | ARG  | CG-CD   | -5.59 | 1.38        | 1.51     |
| 1   | L     | 176 | TYR  | CD1-CE1 | 5.58  | 1.47        | 1.39     |
| 1   | K     | 98  | GLN  | CB-CG   | 5.58  | 1.67        | 1.52     |
| 1   | H     | 55  | PHE  | CD2-CE2 | 5.57  | 1.50        | 1.39     |
| 1   | A     | 65  | ARG  | NE-CZ   | 5.56  | 1.40        | 1.33     |
| 1   | B     | 127 | TYR  | CZ-OH   | 5.56  | 1.47        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | J     | 48  | VAL  | CB-CG2  | -5.56 | 1.41        | 1.52     |
| 1   | B     | 58  | ALA  | CA-CB   | 5.55  | 1.64        | 1.52     |
| 1   | L     | 94  | VAL  | CA-CB   | 5.55  | 1.66        | 1.54     |
| 1   | G     | 171 | PHE  | CE2-CZ  | 5.55  | 1.47        | 1.37     |
| 1   | I     | 4   | LYS  | CG-CD   | 5.55  | 1.71        | 1.52     |
| 1   | D     | 183 | VAL  | CB-CG2  | 5.54  | 1.64        | 1.52     |
| 1   | F     | 8   | TYR  | CD1-CE1 | -5.53 | 1.31        | 1.39     |
| 1   | H     | 74  | ARG  | CZ-NH1  | 5.53  | 1.40        | 1.33     |
| 1   | F     | 170 | VAL  | C-O     | 5.53  | 1.33        | 1.23     |
| 1   | G     | 162 | ASN  | CB-CG   | 5.52  | 1.63        | 1.51     |
| 1   | B     | 140 | GLU  | CG-CD   | 5.52  | 1.60        | 1.51     |
| 1   | E     | 102 | PHE  | CD1-CE1 | 5.52  | 1.50        | 1.39     |
| 1   | G     | 156 | PHE  | CE1-CZ  | -5.51 | 1.26        | 1.37     |
| 1   | I     | 104 | SER  | CB-OG   | -5.49 | 1.35        | 1.42     |
| 1   | L     | 55  | PHE  | CB-CG   | -5.49 | 1.42        | 1.51     |
| 1   | K     | 81  | GLU  | CG-CD   | 5.48  | 1.60        | 1.51     |
| 1   | F     | 95  | PHE  | CE2-CZ  | 5.48  | 1.47        | 1.37     |
| 1   | I     | 133 | TYR  | CB-CG   | -5.47 | 1.43        | 1.51     |
| 1   | A     | 156 | PHE  | CD1-CE1 | 5.46  | 1.50        | 1.39     |
| 1   | G     | 95  | PHE  | C-O     | -5.46 | 1.12        | 1.23     |
| 1   | I     | 88  | VAL  | CB-CG2  | -5.46 | 1.41        | 1.52     |
| 1   | A     | 143 | PHE  | CD2-CE2 | -5.45 | 1.28        | 1.39     |
| 1   | H     | 186 | PRO  | C-O     | 5.45  | 1.34        | 1.23     |
| 1   | A     | 23  | GLU  | CD-OE2  | 5.44  | 1.31        | 1.25     |
| 1   | C     | 58  | ALA  | CA-CB   | 5.44  | 1.63        | 1.52     |
| 1   | G     | 28  | VAL  | CB-CG1  | 5.44  | 1.64        | 1.52     |
| 1   | E     | 92  | TYR  | CD2-CE2 | 5.44  | 1.47        | 1.39     |
| 1   | J     | 28  | VAL  | CB-CG2  | 5.43  | 1.64        | 1.52     |
| 1   | E     | 106 | TRP  | CE3-CZ3 | 5.42  | 1.47        | 1.38     |
| 1   | A     | 211 | TYR  | CG-CD1  | 5.42  | 1.46        | 1.39     |
| 1   | J     | 74  | ARG  | CB-CG   | 5.39  | 1.67        | 1.52     |
| 1   | B     | 25  | PHE  | CE2-CZ  | -5.39 | 1.27        | 1.37     |
| 1   | D     | 88  | VAL  | CA-CB   | -5.39 | 1.43        | 1.54     |
| 1   | D     | 133 | TYR  | CE1-CZ  | 5.39  | 1.45        | 1.38     |
| 1   | K     | 28  | VAL  | CB-CG2  | 5.39  | 1.64        | 1.52     |
| 1   | A     | 134 | PHE  | CD1-CE1 | 5.37  | 1.50        | 1.39     |
| 1   | C     | 138 | PHE  | CD1-CE1 | 5.35  | 1.50        | 1.39     |
| 1   | L     | 156 | PHE  | CD2-CE2 | -5.35 | 1.28        | 1.39     |
| 1   | H     | 109 | TYR  | CD1-CE1 | -5.35 | 1.31        | 1.39     |
| 1   | A     | 59  | PHE  | CE2-CZ  | 5.35  | 1.47        | 1.37     |
| 1   | H     | 68  | ASN  | CB-CG   | 5.35  | 1.63        | 1.51     |
| 1   | H     | 95  | PHE  | CE2-CZ  | 5.35  | 1.47        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 84  | ILE  | CB-CG2  | 5.34  | 1.69        | 1.52     |
| 1   | I     | 48  | VAL  | CB-CG1  | 5.34  | 1.64        | 1.52     |
| 1   | L     | 176 | TYR  | CE1-CZ  | 5.34  | 1.45        | 1.38     |
| 1   | E     | 176 | TYR  | CD1-CE1 | 5.33  | 1.47        | 1.39     |
| 1   | C     | 102 | PHE  | CE2-CZ  | 5.33  | 1.47        | 1.37     |
| 1   | A     | 160 | VAL  | CB-CG2  | -5.32 | 1.41        | 1.52     |
| 1   | C     | 95  | PHE  | CG-CD1  | 5.31  | 1.46        | 1.38     |
| 1   | L     | 145 | VAL  | CB-CG2  | -5.29 | 1.41        | 1.52     |
| 1   | C     | 95  | PHE  | CG-CD2  | 5.29  | 1.46        | 1.38     |
| 1   | I     | 55  | PHE  | CG-CD2  | 5.29  | 1.46        | 1.38     |
| 1   | C     | 75  | MET  | C-O     | 5.27  | 1.33        | 1.23     |
| 1   | D     | 100 | GLU  | CD-OE2  | 5.27  | 1.31        | 1.25     |
| 1   | I     | 115 | GLN  | CG-CD   | 5.26  | 1.63        | 1.51     |
| 1   | A     | 33  | TYR  | CE2-CZ  | 5.25  | 1.45        | 1.38     |
| 1   | F     | 28  | VAL  | CB-CG2  | 5.25  | 1.63        | 1.52     |
| 1   | A     | 54  | LYS  | CG-CD   | 5.24  | 1.70        | 1.52     |
| 1   | C     | 177 | TYR  | CG-CD2  | 5.24  | 1.46        | 1.39     |
| 1   | B     | 156 | PHE  | CD2-CE2 | 5.24  | 1.49        | 1.39     |
| 1   | J     | 144 | PHE  | CE2-CZ  | 5.24  | 1.47        | 1.37     |
| 1   | A     | 138 | PHE  | CD1-CE1 | 5.24  | 1.49        | 1.39     |
| 1   | G     | 152 | SER  | CA-CB   | 5.23  | 1.60        | 1.52     |
| 1   | H     | 127 | TYR  | CD1-CE1 | 5.23  | 1.47        | 1.39     |
| 1   | I     | 90  | PRO  | CG-CD   | 5.22  | 1.67        | 1.50     |
| 1   | F     | 154 | THR  | N-CA    | -5.22 | 1.35        | 1.46     |
| 1   | C     | 44  | PHE  | CE2-CZ  | -5.22 | 1.27        | 1.37     |
| 1   | K     | 144 | PHE  | CD2-CE2 | 5.21  | 1.49        | 1.39     |
| 1   | C     | 133 | TYR  | CE2-CZ  | 5.20  | 1.45        | 1.38     |
| 1   | H     | 56  | TYR  | CD1-CE1 | 5.20  | 1.47        | 1.39     |
| 1   | D     | 143 | PHE  | CE2-CZ  | 5.20  | 1.47        | 1.37     |
| 1   | A     | 34  | ASN  | CG-ND2  | 5.19  | 1.45        | 1.32     |
| 1   | G     | 33  | TYR  | CG-CD1  | 5.19  | 1.45        | 1.39     |
| 1   | A     | 29  | ALA  | N-CA    | -5.19 | 1.35        | 1.46     |
| 1   | L     | 133 | TYR  | CE2-CZ  | 5.19  | 1.45        | 1.38     |
| 1   | A     | 175 | LYS  | CB-CG   | 5.18  | 1.66        | 1.52     |
| 1   | E     | 69  | ALA  | CA-CB   | 5.18  | 1.63        | 1.52     |
| 1   | A     | 81  | GLU  | CD-OE2  | 5.17  | 1.31        | 1.25     |
| 1   | D     | 55  | PHE  | CE1-CZ  | 5.17  | 1.47        | 1.37     |
| 1   | F     | 33  | TYR  | C-O     | 5.16  | 1.33        | 1.23     |
| 1   | A     | 132 | ALA  | CA-CB   | 5.16  | 1.63        | 1.52     |
| 1   | G     | 176 | TYR  | CG-CD1  | 5.16  | 1.45        | 1.39     |
| 1   | J     | 8   | TYR  | CE2-CZ  | 5.15  | 1.45        | 1.38     |
| 1   | D     | 95  | PHE  | CE2-CZ  | 5.15  | 1.47        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 108 | GLU  | CD-OE2  | 5.15  | 1.31        | 1.25     |
| 1   | L     | 143 | PHE  | CG-CD1  | 5.15  | 1.46        | 1.38     |
| 1   | D     | 124 | VAL  | CB-CG1  | 5.14  | 1.63        | 1.52     |
| 1   | L     | 25  | PHE  | CE1-CZ  | 5.14  | 1.47        | 1.37     |
| 1   | L     | 59  | PHE  | CD1-CE1 | 5.14  | 1.49        | 1.39     |
| 1   | C     | 161 | ALA  | CA-CB   | -5.14 | 1.41        | 1.52     |
| 1   | K     | 23  | GLU  | CD-OE2  | 5.13  | 1.31        | 1.25     |
| 1   | E     | 149 | PRO  | CA-C    | -5.12 | 1.42        | 1.52     |
| 1   | D     | 83  | VAL  | CA-CB   | -5.12 | 1.44        | 1.54     |
| 1   | E     | 180 | GLY  | C-O     | 5.12  | 1.31        | 1.23     |
| 1   | C     | 170 | VAL  | C-O     | 5.11  | 1.33        | 1.23     |
| 1   | D     | 211 | TYR  | CZ-OH   | -5.11 | 1.29        | 1.37     |
| 1   | C     | 56  | TYR  | CB-CG   | 5.10  | 1.59        | 1.51     |
| 1   | F     | 109 | TYR  | CD1-CE1 | -5.10 | 1.31        | 1.39     |
| 1   | B     | 46  | LYS  | CB-CG   | 5.10  | 1.66        | 1.52     |
| 1   | A     | 47  | THR  | C-O     | 5.09  | 1.33        | 1.23     |
| 1   | J     | 35  | GLN  | C-O     | 5.08  | 1.33        | 1.23     |
| 1   | F     | 167 | PHE  | CE1-CZ  | 5.08  | 1.47        | 1.37     |
| 1   | D     | 49  | LYS  | CE-NZ   | 5.08  | 1.61        | 1.49     |
| 1   | E     | 177 | TYR  | CE1-CZ  | 5.08  | 1.45        | 1.38     |
| 1   | A     | 102 | PHE  | CD2-CE2 | -5.08 | 1.29        | 1.39     |
| 1   | L     | 35  | GLN  | CB-CG   | -5.07 | 1.38        | 1.52     |
| 1   | A     | 134 | PHE  | CE1-CZ  | 5.07  | 1.47        | 1.37     |
| 1   | E     | 95  | PHE  | CG-CD2  | 5.07  | 1.46        | 1.38     |
| 1   | D     | 88  | VAL  | CB-CG1  | 5.06  | 1.63        | 1.52     |
| 1   | G     | 196 | CYS  | CB-SG   | -5.06 | 1.73        | 1.81     |
| 1   | D     | 28  | VAL  | CB-CG2  | 5.06  | 1.63        | 1.52     |
| 1   | H     | 167 | PHE  | CE2-CZ  | 5.06  | 1.47        | 1.37     |
| 1   | J     | 33  | TYR  | CE2-CZ  | 5.05  | 1.45        | 1.38     |
| 1   | H     | 171 | PHE  | CE2-CZ  | 5.05  | 1.47        | 1.37     |
| 1   | A     | 28  | VAL  | CB-CG2  | 5.04  | 1.63        | 1.52     |
| 1   | F     | 74  | ARG  | CZ-NH1  | 5.04  | 1.39        | 1.33     |
| 1   | F     | 159 | ASN  | CB-CG   | 5.04  | 1.62        | 1.51     |
| 1   | A     | 52  | LYS  | CD-CE   | 5.04  | 1.63        | 1.51     |
| 1   | F     | 16  | TRP  | CB-CG   | 5.04  | 1.59        | 1.50     |
| 1   | D     | 151 | VAL  | CA-CB   | 5.03  | 1.65        | 1.54     |
| 1   | A     | 23  | GLU  | CD-OE1  | 5.03  | 1.31        | 1.25     |
| 1   | L     | 143 | PHE  | CG-CD2  | 5.01  | 1.46        | 1.38     |
| 1   | H     | 62  | ILE  | CA-C    | 5.01  | 1.66        | 1.52     |
| 1   | A     | 167 | PHE  | CD2-CE2 | 5.00  | 1.49        | 1.39     |
| 1   | B     | 72  | GLU  | CD-OE2  | 5.00  | 1.31        | 1.25     |
| 1   | J     | 13  | ILE  | CA-CB   | 5.00  | 1.66        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | C     | 98  | GLN  | CB-CG | 5.00 | 1.66        | 1.52     |

All (315) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 111 | ASP  | CB-CG-OD2 | 13.02 | 130.02      | 118.30   |
| 1   | A     | 65  | ARG  | NE-CZ-NH1 | 11.59 | 126.09      | 120.30   |
| 1   | C     | 157 | ASP  | CB-CG-OD2 | 11.45 | 128.60      | 118.30   |
| 1   | C     | 18  | ARG  | NE-CZ-NH1 | 11.39 | 126.00      | 120.30   |
| 1   | I     | 181 | ASP  | CB-CG-OD2 | 11.01 | 128.21      | 118.30   |
| 1   | A     | 197 | ASP  | CB-CG-OD1 | 10.86 | 128.07      | 118.30   |
| 1   | B     | 112 | ASP  | CB-CG-OD1 | 10.58 | 127.82      | 118.30   |
| 1   | J     | 111 | ASP  | CB-CG-OD1 | 10.52 | 127.77      | 118.30   |
| 1   | J     | 40  | ASP  | CB-CG-OD2 | 10.32 | 127.59      | 118.30   |
| 1   | B     | 111 | ASP  | CB-CG-OD2 | 10.26 | 127.53      | 118.30   |
| 1   | J     | 86  | ASP  | CB-CG-OD2 | 10.22 | 127.50      | 118.30   |
| 1   | F     | 40  | ASP  | CB-CG-OD2 | 10.10 | 127.39      | 118.30   |
| 1   | B     | 18  | ARG  | NE-CZ-NH2 | -9.95 | 115.33      | 120.30   |
| 1   | D     | 157 | ASP  | CB-CG-OD2 | 9.80  | 127.12      | 118.30   |
| 1   | C     | 86  | ASP  | CB-CG-OD2 | 9.77  | 127.09      | 118.30   |
| 1   | C     | 18  | ARG  | NE-CZ-NH2 | -9.76 | 115.42      | 120.30   |
| 1   | H     | 86  | ASP  | CB-CG-OD2 | 9.56  | 126.90      | 118.30   |
| 1   | J     | 197 | ASP  | CB-CG-OD2 | 9.41  | 126.77      | 118.30   |
| 1   | J     | 157 | ASP  | CB-CG-OD1 | -9.39 | 109.85      | 118.30   |
| 1   | D     | 40  | ASP  | CB-CG-OD2 | 9.39  | 126.75      | 118.30   |
| 1   | I     | 67  | MET  | CG-SD-CE  | -9.27 | 85.37       | 100.20   |
| 1   | H     | 213 | ASP  | CB-CG-OD2 | 9.22  | 126.60      | 118.30   |
| 1   | I     | 163 | MET  | CG-SD-CE  | 9.21  | 114.93      | 100.20   |
| 1   | B     | 111 | ASP  | CB-CG-OD1 | -9.19 | 110.03      | 118.30   |
| 1   | B     | 123 | ASP  | CB-CG-OD2 | 9.17  | 126.55      | 118.30   |
| 1   | F     | 213 | ASP  | CB-CG-OD2 | 9.08  | 126.47      | 118.30   |
| 1   | L     | 111 | ASP  | CB-CG-OD2 | 9.05  | 126.44      | 118.30   |
| 1   | H     | 5   | ILE  | C-N-CA    | 8.99  | 144.17      | 121.70   |
| 1   | G     | 45  | LEU  | CB-CG-CD2 | 8.98  | 126.27      | 111.00   |
| 1   | K     | 40  | ASP  | CB-CG-OD2 | 8.98  | 126.38      | 118.30   |
| 1   | E     | 86  | ASP  | CB-CG-OD2 | 8.96  | 126.36      | 118.30   |
| 1   | A     | 217 | GLY  | C-N-CA    | -8.92 | 103.56      | 122.30   |
| 1   | K     | 86  | ASP  | CB-CG-OD2 | 8.70  | 126.13      | 118.30   |
| 1   | H     | 111 | ASP  | CB-CG-OD1 | 8.68  | 126.11      | 118.30   |
| 1   | H     | 39  | LEU  | CB-CG-CD2 | 8.68  | 125.75      | 111.00   |
| 1   | L     | 181 | ASP  | CB-CG-OD2 | 8.62  | 126.06      | 118.30   |
| 1   | J     | 157 | ASP  | CB-CG-OD2 | 8.59  | 126.03      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | L     | 79  | ASP  | CB-CG-OD2  | 8.52  | 125.97      | 118.30   |
| 1   | G     | 111 | ASP  | CB-CG-OD1  | -8.52 | 110.64      | 118.30   |
| 1   | G     | 157 | ASP  | CB-CG-OD2  | 8.43  | 125.89      | 118.30   |
| 1   | A     | 32  | THR  | N-CA-CB    | -8.42 | 94.30       | 110.30   |
| 1   | B     | 187 | LEU  | CB-CG-CD2  | 8.36  | 125.22      | 111.00   |
| 1   | D     | 65  | ARG  | NE-CZ-NH2  | -8.36 | 116.12      | 120.30   |
| 1   | F     | 86  | ASP  | CB-CG-OD2  | 8.33  | 125.80      | 118.30   |
| 1   | G     | 181 | ASP  | CB-CG-OD2  | 8.27  | 125.74      | 118.30   |
| 1   | F     | 12  | ASP  | CB-CG-OD2  | 8.19  | 125.67      | 118.30   |
| 1   | C     | 203 | ARG  | NE-CZ-NH1  | -8.11 | 116.24      | 120.30   |
| 1   | G     | 40  | ASP  | CB-CG-OD2  | 8.06  | 125.56      | 118.30   |
| 1   | H     | 112 | ASP  | CB-CG-OD1  | 8.01  | 125.51      | 118.30   |
| 1   | F     | 181 | ASP  | CB-CG-OD2  | 7.97  | 125.47      | 118.30   |
| 1   | H     | 66  | LEU  | CB-CG-CD2  | -7.95 | 97.49       | 111.00   |
| 1   | H     | 52  | LYS  | CA-C-N     | -7.94 | 99.73       | 117.20   |
| 1   | F     | 12  | ASP  | CB-CG-OD1  | -7.88 | 111.21      | 118.30   |
| 1   | H     | 39  | LEU  | CA-CB-CG   | 7.87  | 133.40      | 115.30   |
| 1   | I     | 164 | ASP  | CB-CG-OD2  | 7.85  | 125.37      | 118.30   |
| 1   | G     | 12  | ASP  | CB-CG-OD1  | 7.78  | 125.30      | 118.30   |
| 1   | J     | 74  | ARG  | NE-CZ-NH1  | -7.71 | 116.45      | 120.30   |
| 1   | H     | 157 | ASP  | CB-CG-OD1  | -7.67 | 111.40      | 118.30   |
| 1   | H     | 6   | THR  | N-CA-C     | 7.66  | 131.67      | 111.00   |
| 1   | B     | 28  | VAL  | N-CA-CB    | 7.65  | 128.33      | 111.50   |
| 1   | J     | 157 | ASP  | CB-CA-C    | -7.63 | 95.14       | 110.40   |
| 1   | C     | 181 | ASP  | CB-CG-OD2  | 7.56  | 125.10      | 118.30   |
| 1   | A     | 18  | ARG  | NE-CZ-NH1  | 7.56  | 124.08      | 120.30   |
| 1   | I     | 79  | ASP  | CB-CG-OD2  | 7.55  | 125.10      | 118.30   |
| 1   | D     | 158 | LEU  | CB-CG-CD2  | -7.51 | 98.22       | 111.00   |
| 1   | J     | 32  | THR  | OG1-CB-CG2 | -7.50 | 92.74       | 110.00   |
| 1   | F     | 151 | VAL  | CG1-CB-CG2 | -7.49 | 98.91       | 110.90   |
| 1   | A     | 12  | ASP  | CB-CG-OD2  | 7.46  | 125.02      | 118.30   |
| 1   | I     | 28  | VAL  | CG1-CB-CG2 | 7.46  | 122.84      | 110.90   |
| 1   | J     | 12  | ASP  | CB-CG-OD2  | 7.33  | 124.90      | 118.30   |
| 1   | G     | 111 | ASP  | CB-CG-OD2  | 7.33  | 124.89      | 118.30   |
| 1   | J     | 128 | GLY  | N-CA-C     | -7.31 | 94.82       | 113.10   |
| 1   | G     | 32  | THR  | N-CA-CB    | -7.30 | 96.43       | 110.30   |
| 1   | I     | 28  | VAL  | CB-CA-C    | 7.25  | 125.17      | 111.40   |
| 1   | C     | 157 | ASP  | CB-CG-OD1  | -7.24 | 111.79      | 118.30   |
| 1   | E     | 154 | THR  | N-CA-CB    | -7.18 | 96.66       | 110.30   |
| 1   | D     | 181 | ASP  | CB-CG-OD2  | 7.17  | 124.76      | 118.30   |
| 1   | H     | 87  | SER  | CB-CA-C    | -7.17 | 96.49       | 110.10   |
| 1   | J     | 6   | THR  | C-N-CA     | -7.14 | 107.30      | 122.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 97  | GLU  | CB-CA-C    | -7.08 | 96.25       | 110.40   |
| 1   | H     | 12  | ASP  | CB-CG-OD2  | 7.08  | 124.67      | 118.30   |
| 1   | A     | 111 | ASP  | CB-CG-OD2  | 7.05  | 124.64      | 118.30   |
| 1   | D     | 12  | ASP  | CB-CG-OD2  | 7.05  | 124.64      | 118.30   |
| 1   | F     | 123 | ASP  | CB-CG-OD2  | 7.04  | 124.64      | 118.30   |
| 1   | L     | 164 | ASP  | CB-CG-OD2  | 7.03  | 124.62      | 118.30   |
| 1   | C     | 86  | ASP  | CB-CG-OD1  | -6.95 | 112.05      | 118.30   |
| 1   | A     | 39  | LEU  | CB-CG-CD2  | 6.90  | 122.73      | 111.00   |
| 1   | H     | 8   | TYR  | CB-CG-CD2  | 6.84  | 125.11      | 121.00   |
| 1   | C     | 87  | SER  | CB-CA-C    | -6.81 | 97.17       | 110.10   |
| 1   | H     | 6   | THR  | N-CA-CB    | -6.78 | 97.41       | 110.30   |
| 1   | J     | 67  | MET  | CG-SD-CE   | 6.77  | 111.03      | 100.20   |
| 1   | H     | 83  | VAL  | N-CA-CB    | -6.77 | 96.61       | 111.50   |
| 1   | L     | 187 | LEU  | CA-CB-CG   | -6.76 | 99.76       | 115.30   |
| 1   | J     | 65  | ARG  | NE-CZ-NH1  | -6.75 | 116.93      | 120.30   |
| 1   | B     | 40  | ASP  | CB-CG-OD2  | 6.75  | 124.37      | 118.30   |
| 1   | A     | 197 | ASP  | OD1-CG-OD2 | -6.74 | 110.49      | 123.30   |
| 1   | A     | 49  | LYS  | CD-CE-NZ   | -6.74 | 96.20       | 111.70   |
| 1   | C     | 213 | ASP  | CB-CG-OD2  | 6.73  | 124.36      | 118.30   |
| 1   | A     | 97  | GLU  | CA-CB-CG   | 6.73  | 128.20      | 113.40   |
| 1   | G     | 112 | ASP  | CB-CG-OD2  | 6.70  | 124.33      | 118.30   |
| 1   | E     | 187 | LEU  | CB-CG-CD2  | 6.70  | 122.39      | 111.00   |
| 1   | E     | 40  | ASP  | CB-CG-OD2  | 6.69  | 124.33      | 118.30   |
| 1   | I     | 12  | ASP  | CB-CG-OD2  | 6.67  | 124.30      | 118.30   |
| 1   | H     | 219 | ALA  | N-CA-CB    | 6.64  | 119.39      | 110.10   |
| 1   | E     | 187 | LEU  | CA-CB-CG   | -6.62 | 100.08      | 115.30   |
| 1   | A     | 181 | ASP  | CB-CG-OD2  | 6.61  | 124.25      | 118.30   |
| 1   | J     | 18  | ARG  | CG-CD-NE   | 6.60  | 125.65      | 111.80   |
| 1   | H     | 5   | ILE  | CA-C-N     | -6.59 | 102.71      | 117.20   |
| 1   | I     | 40  | ASP  | CB-CG-OD2  | 6.57  | 124.22      | 118.30   |
| 1   | A     | 203 | ARG  | NE-CZ-NH2  | -6.56 | 117.02      | 120.30   |
| 1   | C     | 39  | LEU  | CB-CG-CD2  | 6.56  | 122.15      | 111.00   |
| 1   | F     | 121 | SER  | N-CA-CB    | 6.55  | 120.33      | 110.50   |
| 1   | B     | 51  | ASN  | C-N-CA     | -6.53 | 105.38      | 121.70   |
| 1   | D     | 213 | ASP  | CB-CG-OD2  | 6.51  | 124.16      | 118.30   |
| 1   | C     | 176 | TYR  | CB-CG-CD2  | -6.51 | 117.10      | 121.00   |
| 1   | B     | 74  | ARG  | NE-CZ-NH2  | -6.50 | 117.05      | 120.30   |
| 1   | E     | 32  | THR  | N-CA-CB    | -6.49 | 97.97       | 110.30   |
| 1   | G     | 51  | ASN  | N-CA-C     | -6.46 | 93.56       | 111.00   |
| 1   | L     | 39  | LEU  | CA-CB-CG   | 6.45  | 130.12      | 115.30   |
| 1   | B     | 181 | ASP  | CB-CG-OD2  | 6.44  | 124.10      | 118.30   |
| 1   | D     | 54  | LYS  | CD-CE-NZ   | 6.43  | 126.48      | 111.70   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 123 | ASP  | CB-CG-OD2 | 6.42  | 124.08      | 118.30   |
| 1   | C     | 32  | THR  | N-CA-CB   | -6.38 | 98.17       | 110.30   |
| 1   | B     | 105 | LEU  | CB-CG-CD2 | -6.38 | 100.15      | 111.00   |
| 1   | A     | 213 | ASP  | CB-CG-OD2 | 6.37  | 124.03      | 118.30   |
| 1   | G     | 197 | ASP  | CB-CG-OD1 | 6.37  | 124.03      | 118.30   |
| 1   | D     | 32  | THR  | N-CA-CB   | -6.36 | 98.21       | 110.30   |
| 1   | H     | 52  | LYS  | C-N-CA    | 6.36  | 137.60      | 121.70   |
| 1   | D     | 51  | ASN  | C-N-CA    | -6.36 | 105.81      | 121.70   |
| 1   | A     | 217 | GLY  | O-C-N     | -6.34 | 112.42      | 123.20   |
| 1   | F     | 18  | ARG  | NE-CZ-NH2 | -6.29 | 117.15      | 120.30   |
| 1   | A     | 86  | ASP  | CB-CG-OD2 | 6.29  | 123.96      | 118.30   |
| 1   | A     | 87  | SER  | CB-CA-C   | -6.29 | 98.15       | 110.10   |
| 1   | B     | 77  | MET  | CG-SD-CE  | -6.29 | 90.14       | 100.20   |
| 1   | G     | 63  | LEU  | CB-CG-CD1 | 6.28  | 121.68      | 111.00   |
| 1   | I     | 123 | ASP  | CB-CG-OD2 | 6.27  | 123.94      | 118.30   |
| 1   | C     | 12  | ASP  | CB-CG-OD2 | 6.26  | 123.94      | 118.30   |
| 1   | K     | 187 | LEU  | CA-CB-CG  | -6.25 | 100.92      | 115.30   |
| 1   | D     | 52  | LYS  | CB-CA-C   | 6.24  | 122.89      | 110.40   |
| 1   | B     | 86  | ASP  | CB-CG-OD2 | 6.24  | 123.92      | 118.30   |
| 1   | B     | 12  | ASP  | CB-CG-OD2 | 6.24  | 123.91      | 118.30   |
| 1   | G     | 45  | LEU  | CA-CB-CG  | 6.23  | 129.63      | 115.30   |
| 1   | D     | 111 | ASP  | N-CA-CB   | -6.23 | 99.39       | 110.60   |
| 1   | A     | 205 | LEU  | CB-CG-CD1 | -6.23 | 100.41      | 111.00   |
| 1   | A     | 79  | ASP  | CB-CG-OD2 | 6.22  | 123.90      | 118.30   |
| 1   | B     | 39  | LEU  | CB-CA-C   | -6.22 | 98.38       | 110.20   |
| 1   | G     | 145 | VAL  | CB-CA-C   | -6.21 | 99.61       | 111.40   |
| 1   | G     | 146 | SER  | CB-CA-C   | -6.19 | 98.34       | 110.10   |
| 1   | L     | 187 | LEU  | CB-CG-CD1 | 6.19  | 121.52      | 111.00   |
| 1   | I     | 105 | LEU  | CB-CG-CD1 | -6.17 | 100.52      | 111.00   |
| 1   | F     | 94  | VAL  | N-CA-C    | -6.16 | 94.36       | 111.00   |
| 1   | F     | 117 | LEU  | CB-CG-CD2 | 6.16  | 121.47      | 111.00   |
| 1   | F     | 163 | MET  | CG-SD-CE  | -6.16 | 90.34       | 100.20   |
| 1   | D     | 74  | ARG  | NE-CZ-NH2 | -6.16 | 117.22      | 120.30   |
| 1   | A     | 75  | MET  | CG-SD-CE  | 6.16  | 110.06      | 100.20   |
| 1   | C     | 154 | THR  | N-CA-CB   | -6.16 | 98.60       | 110.30   |
| 1   | H     | 114 | ARG  | NE-CZ-NH2 | 6.16  | 123.38      | 120.30   |
| 1   | G     | 19  | LYS  | CB-CA-C   | -6.14 | 98.11       | 110.40   |
| 1   | A     | 27  | SER  | CB-CA-C   | -6.09 | 98.52       | 110.10   |
| 1   | B     | 154 | THR  | CA-CB-CG2 | 6.09  | 120.92      | 112.40   |
| 1   | C     | 162 | ASN  | CB-CA-C   | -6.09 | 98.23       | 110.40   |
| 1   | B     | 19  | LYS  | CD-CE-NZ  | -6.08 | 97.72       | 111.70   |
| 1   | G     | 196 | CYS  | CA-CB-SG  | -6.07 | 103.07      | 114.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 136 | LYS  | CB-CA-C    | -6.06 | 98.28       | 110.40   |
| 1   | L     | 169 | PRO  | N-CD-CG    | -6.06 | 94.11       | 103.20   |
| 1   | J     | 213 | ASP  | CB-CG-OD1  | 6.05  | 123.75      | 118.30   |
| 1   | B     | 18  | ARG  | NE-CZ-NH1  | 6.05  | 123.33      | 120.30   |
| 1   | F     | 39  | LEU  | CB-CG-CD2  | 6.05  | 121.29      | 111.00   |
| 1   | C     | 40  | ASP  | CB-CG-OD2  | 6.04  | 123.73      | 118.30   |
| 1   | D     | 77  | MET  | CG-SD-CE   | -6.04 | 90.54       | 100.20   |
| 1   | J     | 152 | SER  | N-CA-CB    | -6.03 | 101.45      | 110.50   |
| 1   | G     | 50  | LYS  | CD-CE-NZ   | -6.03 | 97.83       | 111.70   |
| 1   | A     | 62  | ILE  | CG1-CB-CG2 | -6.03 | 98.14       | 111.40   |
| 1   | A     | 105 | LEU  | CB-CG-CD2  | -6.03 | 100.75      | 111.00   |
| 1   | I     | 135 | PRO  | N-CD-CG    | -6.02 | 94.16       | 103.20   |
| 1   | J     | 131 | LEU  | CA-CB-CG   | 6.02  | 129.15      | 115.30   |
| 1   | D     | 86  | ASP  | CB-CG-OD2  | 6.02  | 123.72      | 118.30   |
| 1   | A     | 40  | ASP  | CB-CG-OD2  | 6.02  | 123.72      | 118.30   |
| 1   | F     | 74  | ARG  | NE-CZ-NH2  | -6.01 | 117.30      | 120.30   |
| 1   | J     | 79  | ASP  | CB-CG-OD2  | 6.01  | 123.71      | 118.30   |
| 1   | J     | 123 | ASP  | CB-CG-OD1  | 6.00  | 123.70      | 118.30   |
| 1   | E     | 114 | ARG  | NE-CZ-NH1  | 5.99  | 123.29      | 120.30   |
| 1   | K     | 37  | VAL  | N-CA-C     | -5.99 | 94.84       | 111.00   |
| 1   | A     | 154 | THR  | N-CA-CB    | -5.96 | 98.98       | 110.30   |
| 1   | C     | 78  | LYS  | CD-CE-NZ   | -5.95 | 98.01       | 111.70   |
| 1   | F     | 65  | ARG  | NE-CZ-NH2  | -5.93 | 117.33      | 120.30   |
| 1   | G     | 217 | GLY  | N-CA-C     | -5.92 | 98.30       | 113.10   |
| 1   | B     | 123 | ASP  | CB-CG-OD1  | -5.90 | 112.99      | 118.30   |
| 1   | B     | 28  | VAL  | CA-CB-CG2  | 5.89  | 119.74      | 110.90   |
| 1   | F     | 158 | LEU  | CB-CG-CD1  | -5.89 | 100.99      | 111.00   |
| 1   | L     | 123 | ASP  | CB-CG-OD2  | 5.88  | 123.59      | 118.30   |
| 1   | J     | 181 | ASP  | CB-CG-OD2  | 5.87  | 123.58      | 118.30   |
| 1   | A     | 187 | LEU  | CB-CG-CD2  | 5.85  | 120.94      | 111.00   |
| 1   | F     | 186 | PRO  | N-CD-CG    | -5.84 | 94.43       | 103.20   |
| 1   | C     | 83  | VAL  | CG1-CB-CG2 | 5.82  | 120.22      | 110.90   |
| 1   | C     | 158 | LEU  | CB-CG-CD2  | 5.82  | 120.89      | 111.00   |
| 1   | K     | 187 | LEU  | CB-CG-CD2  | 5.81  | 120.88      | 111.00   |
| 1   | A     | 175 | LYS  | CD-CE-NZ   | -5.80 | 98.35       | 111.70   |
| 1   | L     | 203 | ARG  | NE-CZ-NH1  | -5.79 | 117.40      | 120.30   |
| 1   | L     | 74  | ARG  | NE-CZ-NH1  | 5.77  | 123.18      | 120.30   |
| 1   | B     | 32  | THR  | N-CA-CB    | -5.75 | 99.37       | 110.30   |
| 1   | K     | 12  | ASP  | CB-CG-OD1  | 5.75  | 123.47      | 118.30   |
| 1   | C     | 117 | LEU  | CA-CB-CG   | 5.75  | 128.52      | 115.30   |
| 1   | C     | 74  | ARG  | NE-CZ-NH2  | -5.72 | 117.44      | 120.30   |
| 1   | C     | 152 | SER  | N-CA-C     | -5.72 | 95.55       | 111.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 158 | LEU  | CB-CG-CD2  | 5.72  | 120.73      | 111.00   |
| 1   | K     | 208 | LEU  | CB-CG-CD2  | -5.72 | 101.27      | 111.00   |
| 1   | C     | 178 | THR  | CA-CB-CG2  | -5.72 | 104.39      | 112.40   |
| 1   | D     | 111 | ASP  | CB-CA-C    | -5.72 | 98.97       | 110.40   |
| 1   | E     | 123 | ASP  | CB-CG-OD2  | 5.69  | 123.42      | 118.30   |
| 1   | B     | 47  | THR  | OG1-CB-CG2 | -5.68 | 96.93       | 110.00   |
| 1   | A     | 187 | LEU  | CB-CG-CD1  | -5.63 | 101.44      | 111.00   |
| 1   | A     | 54  | LYS  | CD-CE-NZ   | 5.62  | 124.63      | 111.70   |
| 1   | D     | 51  | ASN  | O-C-N      | -5.62 | 113.70      | 122.70   |
| 1   | G     | 51  | ASN  | C-N-CA     | -5.61 | 107.68      | 121.70   |
| 1   | B     | 90  | PRO  | N-CD-CG    | -5.60 | 94.81       | 103.20   |
| 1   | I     | 143 | PHE  | N-CA-C     | -5.58 | 95.92       | 111.00   |
| 1   | L     | 176 | TYR  | CB-CG-CD1  | 5.58  | 124.35      | 121.00   |
| 1   | C     | 77  | MET  | CG-SD-CE   | -5.58 | 91.28       | 100.20   |
| 1   | A     | 37  | VAL  | CG1-CB-CG2 | 5.58  | 119.82      | 110.90   |
| 1   | J     | 178 | THR  | OG1-CB-CG2 | -5.56 | 97.21       | 110.00   |
| 1   | A     | 65  | ARG  | NH1-CZ-NH2 | -5.56 | 113.29      | 119.40   |
| 1   | C     | 203 | ARG  | NE-CZ-NH2  | 5.54  | 123.07      | 120.30   |
| 1   | L     | 173 | MET  | CB-CG-SD   | -5.54 | 95.78       | 112.40   |
| 1   | F     | 94  | VAL  | CG1-CB-CG2 | -5.54 | 102.04      | 110.90   |
| 1   | I     | 5   | ILE  | N-CA-C     | 5.53  | 125.92      | 111.00   |
| 1   | B     | 136 | LYS  | CD-CE-NZ   | -5.51 | 99.02       | 111.70   |
| 1   | D     | 49  | LYS  | CD-CE-NZ   | 5.50  | 124.36      | 111.70   |
| 1   | G     | 79  | ASP  | CB-CG-OD1  | 5.50  | 123.25      | 118.30   |
| 1   | I     | 9   | THR  | OG1-CB-CG2 | -5.49 | 97.37       | 110.00   |
| 1   | E     | 189 | ILE  | CG1-CB-CG2 | -5.49 | 99.32       | 111.40   |
| 1   | B     | 117 | LEU  | CA-CB-CG   | 5.48  | 127.90      | 115.30   |
| 1   | C     | 127 | TYR  | CD1-CE1-CZ | -5.48 | 114.87      | 119.80   |
| 1   | A     | 13  | ILE  | CG1-CB-CG2 | -5.47 | 99.36       | 111.40   |
| 1   | K     | 32  | THR  | N-CA-CB    | -5.44 | 99.96       | 110.30   |
| 1   | B     | 28  | VAL  | CG1-CB-CG2 | 5.44  | 119.60      | 110.90   |
| 1   | D     | 79  | ASP  | CB-CG-OD1  | 5.43  | 123.19      | 118.30   |
| 1   | H     | 52  | LYS  | O-C-N      | 5.43  | 131.38      | 122.70   |
| 1   | E     | 211 | TYR  | CB-CG-CD1  | -5.41 | 117.75      | 121.00   |
| 1   | E     | 183 | VAL  | CB-CA-C    | -5.41 | 101.12      | 111.40   |
| 1   | D     | 208 | LEU  | CB-CG-CD2  | 5.40  | 120.18      | 111.00   |
| 1   | H     | 65  | ARG  | NE-CZ-NH2  | 5.36  | 122.98      | 120.30   |
| 1   | H     | 143 | PHE  | N-CA-C     | -5.36 | 96.52       | 111.00   |
| 1   | B     | 117 | LEU  | CB-CG-CD2  | 5.35  | 120.10      | 111.00   |
| 1   | I     | 178 | THR  | OG1-CB-CG2 | -5.35 | 97.70       | 110.00   |
| 1   | G     | 98  | GLN  | CA-CB-CG   | 5.34  | 125.15      | 113.40   |
| 1   | D     | 160 | VAL  | CB-CA-C    | 5.33  | 121.54      | 111.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 89  | HIS  | CB-CA-C    | 5.33  | 121.06      | 110.40   |
| 1   | C     | 27  | SER  | CB-CA-C    | -5.32 | 99.99       | 110.10   |
| 1   | I     | 74  | ARG  | NE-CZ-NH2  | 5.32  | 122.96      | 120.30   |
| 1   | G     | 178 | THR  | OG1-CB-CG2 | -5.31 | 97.78       | 110.00   |
| 1   | L     | 211 | TYR  | CB-CG-CD1  | 5.31  | 124.19      | 121.00   |
| 1   | D     | 89  | HIS  | CB-CA-C    | 5.31  | 121.01      | 110.40   |
| 1   | F     | 117 | LEU  | CA-CB-CG   | 5.30  | 127.50      | 115.30   |
| 1   | G     | 158 | LEU  | CA-CB-CG   | 5.30  | 127.49      | 115.30   |
| 1   | A     | 87  | SER  | CA-CB-OG   | -5.29 | 96.90       | 111.20   |
| 1   | J     | 39  | LEU  | CA-CB-CG   | 5.29  | 127.47      | 115.30   |
| 1   | C     | 111 | ASP  | N-CA-CB    | -5.28 | 101.10      | 110.60   |
| 1   | F     | 187 | LEU  | CA-CB-CG   | -5.28 | 103.16      | 115.30   |
| 1   | C     | 118 | HIS  | N-CA-CB    | 5.27  | 120.09      | 110.60   |
| 1   | H     | 77  | MET  | N-CA-C     | -5.27 | 96.76       | 111.00   |
| 1   | I     | 111 | ASP  | CB-CG-OD2  | 5.27  | 123.05      | 118.30   |
| 1   | A     | 111 | ASP  | OD1-CG-OD2 | -5.26 | 113.30      | 123.30   |
| 1   | G     | 160 | VAL  | CG1-CB-CG2 | 5.25  | 119.30      | 110.90   |
| 1   | H     | 5   | ILE  | O-C-N      | 5.25  | 131.10      | 122.70   |
| 1   | B     | 150 | TRP  | C-N-CA     | -5.25 | 108.58      | 121.70   |
| 1   | D     | 36  | THR  | OG1-CB-CG2 | -5.25 | 97.93       | 110.00   |
| 1   | I     | 32  | THR  | N-CA-CB    | -5.23 | 100.36      | 110.30   |
| 1   | G     | 37  | VAL  | CG1-CB-CG2 | -5.23 | 102.53      | 110.90   |
| 1   | L     | 57  | PRO  | N-CD-CG    | -5.23 | 95.35       | 103.20   |
| 1   | B     | 154 | THR  | N-CA-CB    | -5.22 | 100.38      | 110.30   |
| 1   | H     | 218 | GLY  | C-N-CA     | -5.21 | 108.66      | 121.70   |
| 1   | I     | 16  | TRP  | CA-CB-CG   | 5.20  | 123.58      | 113.70   |
| 1   | B     | 77  | MET  | CA-CB-CG   | -5.20 | 104.46      | 113.30   |
| 1   | G     | 35  | GLN  | CA-CB-CG   | 5.20  | 124.84      | 113.40   |
| 1   | K     | 208 | LEU  | CB-CG-CD1  | 5.20  | 119.83      | 111.00   |
| 1   | D     | 90  | PRO  | N-CD-CG    | -5.20 | 95.41       | 103.20   |
| 1   | H     | 181 | ASP  | CB-CG-OD2  | 5.19  | 122.97      | 118.30   |
| 1   | C     | 142 | MET  | CG-SD-CE   | 5.19  | 108.50      | 100.20   |
| 1   | J     | 204 | MET  | CG-SD-CE   | -5.19 | 91.90       | 100.20   |
| 1   | F     | 46  | LYS  | CD-CE-NZ   | -5.18 | 99.78       | 111.70   |
| 1   | A     | 18  | ARG  | NE-CZ-NH2  | -5.18 | 117.71      | 120.30   |
| 1   | E     | 164 | ASP  | CB-CG-OD2  | 5.18  | 122.96      | 118.30   |
| 1   | I     | 4   | LYS  | N-CA-C     | 5.17  | 124.97      | 111.00   |
| 1   | I     | 154 | THR  | N-CA-CB    | -5.17 | 100.48      | 110.30   |
| 1   | L     | 211 | TYR  | CB-CG-CD2  | -5.16 | 117.90      | 121.00   |
| 1   | E     | 63  | LEU  | CB-CG-CD1  | -5.16 | 102.23      | 111.00   |
| 1   | F     | 91  | CYS  | CB-CA-C    | 5.16  | 120.72      | 110.40   |
| 1   | J     | 86  | ASP  | CB-CG-OD1  | -5.15 | 113.67      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 157 | ASP  | CB-CG-OD1  | 5.14  | 122.93      | 118.30   |
| 1   | L     | 40  | ASP  | CB-CG-OD2  | 5.14  | 122.93      | 118.30   |
| 1   | A     | 170 | VAL  | CA-CB-CG2  | -5.14 | 103.19      | 110.90   |
| 1   | C     | 29  | ALA  | N-CA-C     | 5.13  | 124.86      | 111.00   |
| 1   | E     | 65  | ARG  | N-CA-CB    | 5.11  | 119.79      | 110.60   |
| 1   | H     | 86  | ASP  | CB-CG-OD1  | -5.10 | 113.71      | 118.30   |
| 1   | A     | 190 | GLN  | C-N-CA     | -5.10 | 108.95      | 121.70   |
| 1   | F     | 83  | VAL  | N-CA-CB    | -5.08 | 100.31      | 111.50   |
| 1   | L     | 112 | ASP  | CB-CG-OD1  | 5.08  | 122.87      | 118.30   |
| 1   | L     | 118 | HIS  | N-CA-C     | -5.07 | 97.31       | 111.00   |
| 1   | B     | 45  | LEU  | CB-CG-CD1  | 5.07  | 119.61      | 111.00   |
| 1   | C     | 9   | THR  | CA-CB-CG2  | 5.06  | 119.48      | 112.40   |
| 1   | F     | 123 | ASP  | CB-CG-OD1  | -5.05 | 113.75      | 118.30   |
| 1   | F     | 18  | ARG  | NE-CZ-NH1  | 5.05  | 122.82      | 120.30   |
| 1   | C     | 66  | LEU  | CB-CG-CD2  | -5.05 | 102.42      | 111.00   |
| 1   | A     | 123 | ASP  | CB-CG-OD1  | 5.04  | 122.83      | 118.30   |
| 1   | J     | 142 | MET  | CB-CA-C    | -5.03 | 100.34      | 110.40   |
| 1   | D     | 114 | ARG  | NE-CZ-NH1  | 5.02  | 122.81      | 120.30   |
| 1   | C     | 187 | LEU  | CB-CG-CD2  | 5.02  | 119.53      | 111.00   |
| 1   | C     | 95  | PHE  | CB-CA-C    | 5.02  | 120.43      | 110.40   |
| 1   | B     | 184 | LEU  | CA-CB-CG   | 5.01  | 126.83      | 115.30   |
| 1   | G     | 105 | LEU  | CA-CB-CG   | 5.01  | 126.83      | 115.30   |
| 1   | F     | 169 | PRO  | N-CD-CG    | -5.01 | 95.68       | 103.20   |
| 1   | H     | 18  | ARG  | NE-CZ-NH1  | 5.01  | 122.81      | 120.30   |
| 1   | B     | 65  | ARG  | NE-CZ-NH1  | -5.01 | 117.80      | 120.30   |
| 1   | F     | 62  | ILE  | CG1-CB-CG2 | 5.01  | 122.41      | 111.40   |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 168 | ALA  | Mainchain |
| 1   | C     | 28  | VAL  | Peptide   |
| 1   | C     | 52  | LYS  | Peptide   |
| 1   | G     | 217 | GLY  | Peptide   |
| 1   | I     | 4   | LYS  | Peptide   |
| 1   | J     | 127 | TYR  | Peptide   |
| 1   | J     | 13  | ILE  | Peptide   |
| 1   | J     | 153 | PHE  | Peptide   |
| 1   | K     | 50  | LYS  | Peptide   |
| 1   | L     | 128 | GLY  | Peptide   |

## 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     | 1763  | 0        | 1647     | 72      | 0            |
| 1   | B     | 1789  | 0        | 1684     | 58      | 0            |
| 1   | C     | 1763  | 0        | 1647     | 83      | 0            |
| 1   | D     | 1763  | 0        | 1647     | 79      | 0            |
| 1   | E     | 1785  | 0        | 1681     | 61      | 0            |
| 1   | F     | 1759  | 0        | 1644     | 56      | 0            |
| 1   | G     | 1763  | 0        | 1647     | 83      | 0            |
| 1   | H     | 1785  | 0        | 1675     | 72      | 0            |
| 1   | I     | 1776  | 0        | 1668     | 104     | 0            |
| 1   | J     | 1755  | 0        | 1641     | 115     | 0            |
| 1   | K     | 1763  | 0        | 1657     | 92      | 0            |
| 1   | L     | 1746  | 0        | 1633     | 94      | 0            |
| 2   | A     | 19    | 0        | 0        | 1       | 0            |
| 2   | B     | 22    | 0        | 0        | 1       | 0            |
| 2   | C     | 19    | 0        | 0        | 1       | 0            |
| 2   | D     | 21    | 0        | 0        | 2       | 0            |
| 2   | E     | 15    | 0        | 0        | 1       | 0            |
| 2   | F     | 16    | 0        | 0        | 1       | 0            |
| 2   | G     | 20    | 0        | 0        | 3       | 0            |
| 2   | H     | 36    | 0        | 0        | 3       | 0            |
| 2   | I     | 17    | 0        | 0        | 0       | 0            |
| 2   | J     | 11    | 0        | 0        | 5       | 0            |
| 2   | K     | 4     | 0        | 0        | 1       | 0            |
| 2   | L     | 8     | 0        | 0        | 0       | 0            |
| All | All   | 21418 | 0        | 19871    | 881     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (881) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:C:13:ILE:CG1 | 1:C:13:ILE:CD1  | 1.83                     | 1.56              |
| 1:I:6:THR:CG2  | 1:I:6:THR:CB    | 1.74                     | 1.55              |
| 1:I:139:ILE:N  | 1:I:142:MET:HE3 | 1.19                     | 1.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:139:ILE:H    | 1:I:142:MET:CE   | 1.36                     | 1.37              |
| 1:I:171:PHE:CZ   | 1:I:204:MET:HE3  | 1.61                     | 1.35              |
| 1:I:171:PHE:HZ   | 1:I:204:MET:CE   | 1.41                     | 1.34              |
| 1:I:171:PHE:CZ   | 1:I:204:MET:CE   | 2.12                     | 1.31              |
| 1:A:67:MET:CE    | 1:A:171:PHE:HE1  | 1.46                     | 1.26              |
| 1:C:145:VAL:CG1  | 1:C:173:MET:CE   | 2.18                     | 1.21              |
| 1:E:59:PHE:HD2   | 1:E:173:MET:CE   | 1.57                     | 1.17              |
| 1:G:32:THR:HG22  | 1:I:159:ASN:HB3  | 1.26                     | 1.17              |
| 1:H:67:MET:HE3   | 1:H:73:PHE:HB3   | 1.18                     | 1.15              |
| 1:I:6:THR:HG21   | 1:I:141:ASN:HD21 | 1.11                     | 1.15              |
| 1:B:158:LEU:CD1  | 1:B:160:VAL:HG23 | 1.77                     | 1.13              |
| 1:C:145:VAL:HG12 | 1:C:173:MET:HE3  | 1.32                     | 1.12              |
| 1:C:145:VAL:CG1  | 1:C:173:MET:HE2  | 1.80                     | 1.11              |
| 1:K:154:THR:HG23 | 1:L:154:THR:O    | 1.50                     | 1.11              |
| 1:J:154:THR:HG22 | 1:K:154:THR:O    | 1.47                     | 1.11              |
| 1:A:67:MET:CE    | 1:A:171:PHE:CE1  | 2.34                     | 1.11              |
| 1:A:67:MET:HE2   | 1:A:171:PHE:CE1  | 1.87                     | 1.08              |
| 1:J:159:ASN:HB3  | 1:K:32:THR:HG22  | 1.34                     | 1.06              |
| 1:C:67:MET:CE    | 1:C:73:PHE:CG    | 2.39                     | 1.06              |
| 1:A:67:MET:HE2   | 1:A:171:PHE:HE1  | 0.96                     | 1.05              |
| 1:K:8:TYR:CZ     | 1:K:78:LYS:HD3   | 1.91                     | 1.05              |
| 1:L:129:GLU:OE2  | 1:L:129:GLU:HA   | 1.36                     | 1.05              |
| 1:E:59:PHE:HD2   | 1:E:173:MET:HE1  | 1.20                     | 1.04              |
| 1:I:138:PHE:HA   | 1:I:142:MET:HE1  | 1.41                     | 1.03              |
| 1:I:67:MET:HE1   | 1:I:169:PRO:HG2  | 1.07                     | 1.03              |
| 1:C:67:MET:HE1   | 1:C:73:PHE:CG    | 1.95                     | 1.02              |
| 1:I:171:PHE:HZ   | 1:I:204:MET:HE3  | 0.92                     | 1.02              |
| 1:C:67:MET:HE3   | 1:C:73:PHE:CB    | 1.90                     | 1.02              |
| 1:E:59:PHE:CD2   | 1:E:173:MET:CE   | 2.44                     | 1.01              |
| 1:H:67:MET:CE    | 1:H:73:PHE:HB3   | 1.90                     | 1.01              |
| 1:I:67:MET:CE    | 1:I:169:PRO:HG2  | 1.89                     | 1.01              |
| 1:J:159:ASN:HD22 | 1:L:159:ASN:HD21 | 1.02                     | 1.00              |
| 1:A:159:ASN:HB3  | 1:B:32:THR:HG22  | 1.39                     | 0.98              |
| 1:A:154:THR:HG23 | 1:B:154:THR:O    | 1.61                     | 0.98              |
| 1:J:67:MET:HA    | 1:J:67:MET:HE2   | 1.41                     | 0.97              |
| 1:A:154:THR:O    | 1:C:154:THR:HG23 | 1.65                     | 0.96              |
| 1:D:67:MET:CE    | 1:D:169:PRO:HG2  | 1.95                     | 0.96              |
| 1:L:67:MET:HE3   | 1:L:73:PHE:HB3   | 1.43                     | 0.96              |
| 1:C:67:MET:CE    | 1:C:73:PHE:HB3   | 1.95                     | 0.95              |
| 1:H:32:THR:HG21  | 2:H:224:HOH:O    | 1.65                     | 0.95              |
| 1:B:158:LEU:HD11 | 1:B:160:VAL:HG23 | 1.45                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:159:ASN:ND2  | 1:L:159:ASN:HD21 | 1.65                     | 0.95              |
| 1:L:106:TRP:CD1  | 1:L:142:MET:HE3  | 2.02                     | 0.94              |
| 1:I:171:PHE:CZ   | 1:I:204:MET:HE1  | 2.02                     | 0.94              |
| 1:A:123:ASP:OD1  | 1:A:136:LYS:NZ   | 2.01                     | 0.93              |
| 1:C:67:MET:CE    | 1:C:73:PHE:CB    | 2.45                     | 0.93              |
| 1:I:112:ASP:OD2  | 1:I:115:GLN:HG2  | 1.68                     | 0.93              |
| 1:B:149:PRO:O    | 1:B:175:LYS:HG3  | 1.67                     | 0.93              |
| 1:C:145:VAL:HG11 | 1:C:173:MET:CE   | 1.98                     | 0.93              |
| 1:A:56:TYR:HE1   | 1:A:173:MET:HE3  | 1.31                     | 0.92              |
| 1:B:67:MET:CE    | 1:B:169:PRO:HG2  | 1.99                     | 0.92              |
| 1:H:67:MET:HE3   | 1:H:73:PHE:CB    | 1.99                     | 0.92              |
| 1:J:67:MET:CE    | 1:J:67:MET:HA    | 1.98                     | 0.92              |
| 1:K:148:ASN:HD22 | 1:K:150:TRP:HE3  | 1.17                     | 0.92              |
| 1:A:56:TYR:CD1   | 1:A:173:MET:HE1  | 2.03                     | 0.92              |
| 1:C:56:TYR:HB3   | 1:C:57:PRO:HD3   | 1.51                     | 0.92              |
| 1:G:59:PHE:HD2   | 1:G:173:MET:CE   | 1.82                     | 0.92              |
| 1:F:110:HIS:HD2  | 1:F:119:ILE:HD11 | 1.34                     | 0.91              |
| 1:D:154:THR:O    | 1:F:154:THR:HG23 | 1.71                     | 0.91              |
| 1:G:32:THR:CG2   | 1:I:159:ASN:HB3  | 1.99                     | 0.91              |
| 1:E:59:PHE:CD2   | 1:E:173:MET:SD   | 2.65                     | 0.90              |
| 1:I:6:THR:HG21   | 1:I:141:ASN:ND2  | 1.84                     | 0.90              |
| 1:J:154:THR:CG2  | 1:K:154:THR:O    | 2.19                     | 0.90              |
| 1:D:163:MET:O    | 1:D:164:ASP:HB2  | 1.71                     | 0.90              |
| 1:A:67:MET:HE1   | 1:A:171:PHE:CE1  | 2.04                     | 0.90              |
| 1:H:192:HIS:HD1  | 1:H:194:ALA:H    | 1.14                     | 0.89              |
| 1:E:139:ILE:H    | 1:E:142:MET:HE3  | 1.35                     | 0.89              |
| 1:I:67:MET:HE1   | 1:I:169:PRO:CG   | 1.99                     | 0.89              |
| 1:L:7:GLY:HA3    | 1:L:86:ASP:OD1   | 1.70                     | 0.88              |
| 1:H:54:LYS:HD3   | 2:H:249:HOH:O    | 1.73                     | 0.88              |
| 1:L:67:MET:CE    | 1:L:169:PRO:HG2  | 2.04                     | 0.88              |
| 1:A:56:TYR:CE1   | 1:A:173:MET:HE3  | 2.09                     | 0.88              |
| 1:C:114:ARG:HH11 | 1:C:114:ARG:CG   | 1.86                     | 0.88              |
| 1:H:91:CYS:HB2   | 1:H:142:MET:HE2  | 1.55                     | 0.88              |
| 1:C:114:ARG:HH11 | 1:C:114:ARG:HG2  | 1.40                     | 0.86              |
| 1:C:216:GLN:HA   | 1:C:216:GLN:HE21 | 1.40                     | 0.86              |
| 1:G:59:PHE:CD2   | 1:G:173:MET:CE   | 2.59                     | 0.85              |
| 1:D:67:MET:HE3   | 1:D:73:PHE:HB3   | 1.59                     | 0.85              |
| 1:J:106:TRP:CD1  | 1:J:142:MET:HE3  | 2.12                     | 0.84              |
| 1:J:154:THR:O    | 1:L:154:THR:HG23 | 1.78                     | 0.84              |
| 1:K:47:THR:O     | 1:K:49:LYS:N     | 2.11                     | 0.84              |
| 1:G:59:PHE:HD2   | 1:G:173:MET:HE1  | 1.43                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:171:PHE:CE2  | 1:I:204:MET:CE   | 2.60                     | 0.83              |
| 1:J:30:GLN:NE2   | 1:J:163:MET:O    | 2.11                     | 0.83              |
| 1:K:171:PHE:CZ   | 1:K:204:MET:CE   | 2.63                     | 0.82              |
| 1:E:59:PHE:CD2   | 1:E:173:MET:HE1  | 2.07                     | 0.82              |
| 2:A:220:HOH:O    | 1:C:159:ASN:HB2  | 1.79                     | 0.82              |
| 1:D:67:MET:HE1   | 1:D:169:PRO:HG2  | 1.60                     | 0.82              |
| 1:A:56:TYR:HD1   | 1:A:173:MET:HE1  | 1.43                     | 0.82              |
| 1:D:8:TYR:N      | 1:D:8:TYR:CD2    | 2.44                     | 0.82              |
| 1:F:106:TRP:CD1  | 1:F:142:MET:CE   | 2.62                     | 0.81              |
| 1:A:56:TYR:CE1   | 1:A:173:MET:CE   | 2.64                     | 0.81              |
| 1:C:49:LYS:O     | 1:C:51:ASN:N     | 2.13                     | 0.81              |
| 1:C:145:VAL:CG1  | 1:C:173:MET:HE3  | 1.95                     | 0.81              |
| 1:G:154:THR:HG23 | 1:H:154:THR:O    | 1.82                     | 0.80              |
| 1:J:159:ASN:HD21 | 1:K:159:ASN:ND2  | 1.80                     | 0.80              |
| 1:D:67:MET:CE    | 1:D:73:PHE:HB3   | 2.11                     | 0.80              |
| 1:F:110:HIS:CD2  | 1:F:119:ILE:HD11 | 2.17                     | 0.80              |
| 1:L:91:CYS:HB2   | 1:L:142:MET:HE2  | 1.63                     | 0.79              |
| 1:K:154:THR:CG2  | 1:L:154:THR:O    | 2.28                     | 0.79              |
| 1:L:192:HIS:HD1  | 1:L:194:ALA:H    | 1.30                     | 0.79              |
| 1:C:145:VAL:HG11 | 1:C:173:MET:HE2  | 1.56                     | 0.79              |
| 1:A:192:HIS:HD1  | 1:A:194:ALA:H    | 1.29                     | 0.79              |
| 1:G:171:PHE:HZ   | 1:G:204:MET:HE3  | 1.47                     | 0.79              |
| 1:I:139:ILE:N    | 1:I:142:MET:CE   | 2.13                     | 0.79              |
| 1:J:138:PHE:CD2  | 1:J:138:PHE:O    | 2.36                     | 0.79              |
| 1:J:89:HIS:CE1   | 1:J:108:GLU:HG3  | 2.18                     | 0.79              |
| 1:G:171:PHE:CZ   | 1:G:204:MET:HE3  | 2.18                     | 0.78              |
| 1:K:171:PHE:CZ   | 1:K:204:MET:HE3  | 2.19                     | 0.78              |
| 1:K:25:PHE:O     | 1:K:30:GLN:HG3   | 1.84                     | 0.78              |
| 1:G:50:LYS:C     | 1:G:51:ASN:O     | 2.12                     | 0.78              |
| 1:E:106:TRP:CE2  | 1:E:136:LYS:HD2  | 2.18                     | 0.78              |
| 1:D:154:THR:HG23 | 1:E:154:THR:O    | 1.84                     | 0.77              |
| 1:J:192:HIS:HD1  | 1:J:194:ALA:H    | 1.33                     | 0.77              |
| 1:F:100:GLU:OE1  | 1:J:6:THR:HG22   | 1.85                     | 0.77              |
| 1:B:67:MET:HE1   | 1:B:169:PRO:HG2  | 1.63                     | 0.77              |
| 1:F:192:HIS:HD1  | 1:F:194:ALA:H    | 1.29                     | 0.77              |
| 1:C:145:VAL:HG13 | 1:C:173:MET:HE2  | 1.65                     | 0.77              |
| 1:L:106:TRP:CD1  | 1:L:142:MET:CE   | 2.68                     | 0.77              |
| 1:E:67:MET:HE3   | 1:E:171:PHE:CE1  | 2.20                     | 0.77              |
| 1:E:34:ASN:ND2   | 1:E:190:GLN:HB3  | 2.00                     | 0.77              |
| 1:K:8:TYR:CE2    | 1:K:78:LYS:HD3   | 2.19                     | 0.77              |
| 1:G:91:CYS:SG    | 1:G:142:MET:HE2  | 2.25                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:192:HIS:HD1  | 1:G:194:ALA:H    | 1.33                     | 0.76              |
| 1:I:171:PHE:CE2  | 1:I:204:MET:HE3  | 2.17                     | 0.76              |
| 1:C:112:ASP:HB3  | 1:C:115:GLN:HG3  | 1.68                     | 0.75              |
| 1:A:154:THR:CG2  | 1:B:154:THR:O    | 2.35                     | 0.75              |
| 1:E:67:MET:CE    | 1:E:171:PHE:CE1  | 2.70                     | 0.75              |
| 1:D:159:ASN:HB3  | 1:E:32:THR:HG22  | 1.68                     | 0.75              |
| 1:L:67:MET:HE1   | 1:L:169:PRO:HG2  | 1.67                     | 0.75              |
| 1:J:10:THR:HG23  | 1:J:10:THR:O     | 1.86                     | 0.75              |
| 1:G:15:GLN:HA    | 1:G:15:GLN:HE21  | 1.51                     | 0.74              |
| 1:G:171:PHE:CZ   | 1:G:204:MET:CE   | 2.70                     | 0.74              |
| 1:J:6:THR:O      | 1:J:6:THR:HG23   | 1.84                     | 0.74              |
| 1:K:59:PHE:CD2   | 1:K:173:MET:SD   | 2.80                     | 0.74              |
| 1:J:40:ASP:HA    | 1:J:184:LEU:HD23 | 1.67                     | 0.74              |
| 1:G:13:ILE:O     | 1:G:19:LYS:HG3   | 1.86                     | 0.74              |
| 1:K:10:THR:OG1   | 1:K:83:VAL:HG23  | 1.87                     | 0.74              |
| 1:B:154:THR:HG23 | 1:C:154:THR:O    | 1.88                     | 0.74              |
| 1:L:106:TRP:HB3  | 1:L:142:MET:HE2  | 1.70                     | 0.74              |
| 1:A:56:TYR:CD1   | 1:A:173:MET:CE   | 2.71                     | 0.73              |
| 1:E:139:ILE:O    | 1:E:142:MET:SD   | 2.46                     | 0.73              |
| 1:F:106:TRP:O    | 1:F:136:LYS:NZ   | 2.22                     | 0.73              |
| 1:J:190:GLN:C    | 1:J:190:GLN:HE21 | 1.91                     | 0.73              |
| 1:C:67:MET:HE3   | 1:C:73:PHE:CG    | 2.19                     | 0.73              |
| 1:E:59:PHE:HD2   | 1:E:173:MET:SD   | 2.06                     | 0.72              |
| 1:J:106:TRP:CD1  | 1:J:142:MET:CE   | 2.72                     | 0.72              |
| 1:D:163:MET:O    | 1:D:164:ASP:CB   | 2.36                     | 0.72              |
| 1:J:123:ASP:OD1  | 1:J:136:LYS:HE2  | 1.88                     | 0.72              |
| 1:J:159:ASN:CB   | 1:K:32:THR:HG22  | 2.18                     | 0.72              |
| 1:D:75:MET:HE3   | 2:D:235:HOH:O    | 1.88                     | 0.72              |
| 1:J:35:GLN:HG3   | 1:L:156:PHE:HD1  | 1.54                     | 0.72              |
| 1:C:67:MET:HE2   | 1:C:73:PHE:HB3   | 1.70                     | 0.72              |
| 1:L:129:GLU:OE2  | 1:L:129:GLU:CA   | 2.26                     | 0.72              |
| 1:B:155:SER:HB2  | 1:C:155:SER:HB2  | 1.71                     | 0.71              |
| 1:J:35:GLN:HG3   | 1:L:156:PHE:CD1  | 2.24                     | 0.71              |
| 1:K:45:LEU:HD22  | 1:K:49:LYS:HD2   | 1.71                     | 0.71              |
| 1:K:106:TRP:CD1  | 1:K:142:MET:CE   | 2.74                     | 0.71              |
| 1:L:59:PHE:CD2   | 1:L:173:MET:HE1  | 2.26                     | 0.71              |
| 1:H:47:THR:O     | 1:H:51:ASN:ND2   | 2.24                     | 0.71              |
| 1:I:171:PHE:CE2  | 1:I:204:MET:HE1  | 2.22                     | 0.71              |
| 1:G:159:ASN:ND2  | 1:I:159:ASN:ND2  | 2.39                     | 0.70              |
| 1:D:65:ARG:CD    | 1:J:111:ASP:OD2  | 2.39                     | 0.70              |
| 1:E:3:LYS:O      | 1:E:4:LYS:HG2    | 1.90                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:154:THR:O    | 1:C:154:THR:CG2  | 2.39                     | 0.70              |
| 1:K:72:GLU:HA    | 1:K:75:MET:HE2   | 1.72                     | 0.70              |
| 1:C:145:VAL:HG12 | 1:C:173:MET:CE   | 1.94                     | 0.70              |
| 1:G:171:PHE:HZ   | 1:G:204:MET:CE   | 2.03                     | 0.70              |
| 1:I:59:PHE:CD2   | 1:I:173:MET:SD   | 2.84                     | 0.70              |
| 1:L:59:PHE:HD2   | 1:L:173:MET:HE1  | 1.57                     | 0.70              |
| 1:B:34:ASN:CG    | 1:B:157:ASP:HB2  | 2.12                     | 0.70              |
| 1:B:204:MET:HE1  | 1:B:205:LEU:HD23 | 1.73                     | 0.69              |
| 1:H:149:PRO:O    | 1:H:175:LYS:HD3  | 1.91                     | 0.69              |
| 1:A:34:ASN:HB2   | 1:A:157:ASP:OD2  | 1.93                     | 0.69              |
| 1:D:65:ARG:HD3   | 1:J:111:ASP:OD2  | 1.92                     | 0.69              |
| 1:H:159:ASN:HB3  | 1:I:32:THR:HG22  | 1.74                     | 0.69              |
| 1:F:190:GLN:C    | 1:F:190:GLN:HE21 | 1.96                     | 0.69              |
| 1:G:59:PHE:CD2   | 1:G:173:MET:HE1  | 2.24                     | 0.69              |
| 1:G:154:THR:O    | 1:I:154:THR:HG23 | 1.93                     | 0.69              |
| 1:C:67:MET:HE1   | 1:C:73:PHE:CD2   | 2.28                     | 0.69              |
| 1:A:204:MET:HE2  | 1:A:205:LEU:HG   | 1.73                     | 0.69              |
| 1:E:132:ALA:O    | 1:E:135:PRO:HD3  | 1.92                     | 0.68              |
| 1:E:67:MET:CE    | 1:E:171:PHE:HE1  | 2.06                     | 0.68              |
| 1:I:59:PHE:HD2   | 1:I:173:MET:HE1  | 1.58                     | 0.68              |
| 1:J:159:ASN:ND2  | 1:K:159:ASN:ND2  | 2.40                     | 0.68              |
| 1:I:138:PHE:CA   | 1:I:142:MET:HE1  | 2.21                     | 0.68              |
| 1:L:8:TYR:HB2    | 1:L:83:VAL:HG13  | 1.74                     | 0.68              |
| 1:C:13:ILE:H     | 1:C:13:ILE:HD12  | 1.58                     | 0.68              |
| 1:D:34:ASN:ND2   | 1:D:158:LEU:H    | 1.92                     | 0.68              |
| 1:E:159:ASN:HB3  | 1:F:32:THR:HG22  | 1.76                     | 0.68              |
| 1:C:57:PRO:HG3   | 1:C:120:TYR:CE2  | 2.29                     | 0.68              |
| 1:J:35:GLN:HA    | 1:L:155:SER:O    | 1.94                     | 0.68              |
| 1:H:67:MET:CE    | 1:H:169:PRO:HG2  | 2.24                     | 0.68              |
| 1:I:145:VAL:HG11 | 1:I:173:MET:CE   | 2.24                     | 0.67              |
| 1:J:44:PHE:HB2   | 1:J:212:CYS:O    | 1.95                     | 0.67              |
| 1:C:67:MET:HE3   | 1:C:73:PHE:HB3   | 1.59                     | 0.67              |
| 1:C:192:HIS:HD1  | 1:C:194:ALA:H    | 1.40                     | 0.67              |
| 1:F:34:ASN:ND2   | 1:F:190:GLN:HB2  | 2.08                     | 0.67              |
| 1:H:91:CYS:HB2   | 1:H:142:MET:CE   | 2.24                     | 0.67              |
| 1:J:171:PHE:CZ   | 1:J:204:MET:HE3  | 2.29                     | 0.67              |
| 1:F:110:HIS:HD2  | 1:F:119:ILE:CD1  | 2.06                     | 0.67              |
| 1:A:32:THR:HG22  | 1:C:159:ASN:HB3  | 1.77                     | 0.67              |
| 1:F:92:TYR:HA    | 1:F:145:VAL:O    | 1.94                     | 0.67              |
| 1:L:214:GLU:O    | 1:L:215:TRP:C    | 2.33                     | 0.67              |
| 1:F:214:GLU:O    | 1:F:215:TRP:C    | 2.32                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:171:PHE:HZ   | 1:J:204:MET:HE3  | 1.60                     | 0.66              |
| 1:B:34:ASN:ND2   | 1:B:190:GLN:HB3  | 2.11                     | 0.66              |
| 1:H:113:PHE:H    | 1:H:219:ALA:HB3  | 1.59                     | 0.66              |
| 1:H:67:MET:HE1   | 1:H:73:PHE:CD2   | 2.30                     | 0.66              |
| 1:B:156:PHE:O    | 1:B:157:ASP:HB3  | 1.95                     | 0.66              |
| 1:E:3:LYS:O      | 1:E:4:LYS:CG     | 2.42                     | 0.66              |
| 1:J:65:ARG:HD3   | 2:J:229:HOH:O    | 1.95                     | 0.66              |
| 1:F:30:GLN:HE22  | 1:F:164:ASP:HA   | 1.60                     | 0.66              |
| 1:I:6:THR:CG2    | 1:I:6:THR:CA     | 2.69                     | 0.66              |
| 1:F:120:TYR:O    | 1:F:124:VAL:HG23 | 1.95                     | 0.66              |
| 1:I:145:VAL:HG11 | 1:I:173:MET:HE3  | 1.77                     | 0.66              |
| 1:J:16:TRP:CE2   | 1:J:18:ARG:HB2   | 2.30                     | 0.66              |
| 1:G:30:GLN:HB3   | 1:I:161:ALA:HB3  | 1.78                     | 0.65              |
| 1:H:56:TYR:HD1   | 1:H:173:MET:HE1  | 1.61                     | 0.65              |
| 1:J:10:THR:CG2   | 1:J:10:THR:O     | 2.44                     | 0.65              |
| 1:I:7:GLY:CA     | 1:I:86:ASP:OD1   | 2.44                     | 0.65              |
| 1:J:176:TYR:HB3  | 1:J:185:MET:HB2  | 1.77                     | 0.65              |
| 1:H:67:MET:HE1   | 1:H:169:PRO:HG2  | 1.78                     | 0.65              |
| 1:F:106:TRP:CD1  | 1:F:142:MET:HE3  | 2.31                     | 0.65              |
| 1:I:7:GLY:C      | 1:I:86:ASP:OD1   | 2.36                     | 0.65              |
| 1:D:32:THR:HG21  | 2:D:220:HOH:O    | 1.96                     | 0.64              |
| 1:C:110:HIS:CD2  | 1:C:119:ILE:HD13 | 2.32                     | 0.64              |
| 1:K:67:MET:HE2   | 1:K:67:MET:HA    | 1.79                     | 0.64              |
| 1:H:56:TYR:CD1   | 1:H:173:MET:HE1  | 2.32                     | 0.64              |
| 1:J:13:ILE:HG22  | 1:J:19:LYS:HD2   | 1.80                     | 0.64              |
| 1:A:56:TYR:O     | 1:A:60:ILE:HG13  | 1.99                     | 0.63              |
| 1:L:123:ASP:OD1  | 1:L:136:LYS:HE3  | 1.97                     | 0.63              |
| 1:L:59:PHE:HD2   | 1:L:173:MET:CE   | 2.10                     | 0.63              |
| 1:A:204:MET:HE1  | 1:A:205:LEU:CD2  | 2.29                     | 0.63              |
| 1:A:56:TYR:N     | 1:A:57:PRO:HD2   | 2.13                     | 0.63              |
| 1:I:139:ILE:HG13 | 1:I:142:MET:CE   | 2.28                     | 0.63              |
| 1:G:154:THR:O    | 1:I:154:THR:CG2  | 2.47                     | 0.63              |
| 1:G:159:ASN:HD22 | 1:I:159:ASN:CG   | 2.01                     | 0.63              |
| 1:J:106:TRP:HB3  | 1:J:142:MET:HE2  | 1.81                     | 0.63              |
| 1:E:106:TRP:CZ2  | 1:E:136:LYS:HD2  | 2.33                     | 0.63              |
| 1:F:40:ASP:HA    | 1:F:184:LEU:HD23 | 1.81                     | 0.63              |
| 1:H:22:PHE:CE2   | 1:H:82:LEU:HD22  | 2.34                     | 0.63              |
| 1:H:91:CYS:SG    | 1:H:142:MET:HE1  | 2.38                     | 0.63              |
| 1:K:57:PRO:HG3   | 1:K:120:TYR:CE2  | 2.34                     | 0.63              |
| 1:K:159:ASN:HB3  | 1:L:32:THR:HG23  | 1.80                     | 0.62              |
| 1:K:56:TYR:HB3   | 1:K:57:PRO:HD3   | 1.80                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:148:ASN:ND2  | 1:K:150:TRP:HE3  | 1.92                     | 0.62              |
| 1:D:34:ASN:HD21  | 1:D:158:LEU:H    | 1.46                     | 0.62              |
| 1:E:139:ILE:H    | 1:E:142:MET:CE   | 2.10                     | 0.62              |
| 1:I:190:GLN:HE21 | 1:I:190:GLN:C    | 2.01                     | 0.62              |
| 1:C:114:ARG:CG   | 1:C:114:ARG:NH1  | 2.51                     | 0.62              |
| 1:J:10:THR:HB    | 2:J:225:HOH:O    | 2.00                     | 0.62              |
| 1:L:115:GLN:O    | 1:L:118:HIS:O    | 2.17                     | 0.62              |
| 1:F:179:GLN:O    | 1:F:180:GLY:C    | 2.38                     | 0.62              |
| 1:H:57:PRO:HG3   | 1:H:120:TYR:CE2  | 2.35                     | 0.62              |
| 1:I:7:GLY:HA3    | 1:I:86:ASP:OD1   | 1.99                     | 0.61              |
| 1:A:34:ASN:OD1   | 1:A:157:ASP:OD2  | 2.18                     | 0.61              |
| 1:E:67:MET:HE3   | 1:E:171:PHE:HE1  | 1.62                     | 0.61              |
| 1:A:39:LEU:O     | 1:A:184:LEU:HA   | 2.00                     | 0.61              |
| 1:J:49:LYS:O     | 1:J:51:ASN:O     | 2.18                     | 0.61              |
| 1:L:66:LEU:CD2   | 1:L:211:TYR:CE2  | 2.83                     | 0.61              |
| 1:K:117:LEU:HD22 | 1:K:117:LEU:O    | 2.00                     | 0.61              |
| 1:L:66:LEU:HD23  | 1:L:211:TYR:CE2  | 2.36                     | 0.61              |
| 1:A:34:ASN:CB    | 1:A:157:ASP:OD2  | 2.49                     | 0.61              |
| 1:D:59:PHE:CD2   | 1:D:173:MET:SD   | 2.94                     | 0.61              |
| 1:H:58:ALA:HA    | 1:H:113:PHE:CE1  | 2.36                     | 0.61              |
| 1:K:34:ASN:ND2   | 1:K:190:GLN:HB2  | 2.15                     | 0.61              |
| 1:A:34:ASN:CG    | 1:A:157:ASP:OD2  | 2.39                     | 0.61              |
| 1:J:158:LEU:HD13 | 1:J:160:VAL:HG23 | 1.81                     | 0.61              |
| 1:I:138:PHE:HA   | 1:I:142:MET:CE   | 2.23                     | 0.61              |
| 1:K:171:PHE:HZ   | 1:K:204:MET:SD   | 2.23                     | 0.60              |
| 1:A:83:VAL:CG1   | 1:A:84:ILE:N     | 2.64                     | 0.60              |
| 1:L:26:GLN:HA    | 1:L:26:GLN:NE2   | 2.16                     | 0.60              |
| 1:H:65:ARG:HH22  | 1:H:219:ALA:HB1  | 1.66                     | 0.60              |
| 1:K:171:PHE:CE2  | 1:K:204:MET:HE1  | 2.36                     | 0.60              |
| 1:I:148:ASN:O    | 1:I:174:GLY:HA2  | 2.01                     | 0.60              |
| 1:I:112:ASP:OD2  | 1:I:115:GLN:CG   | 2.48                     | 0.60              |
| 1:B:67:MET:HE3   | 1:B:169:PRO:HG2  | 1.84                     | 0.60              |
| 1:G:154:THR:CG2  | 1:H:154:THR:O    | 2.47                     | 0.60              |
| 1:A:83:VAL:HG13  | 1:A:84:ILE:N     | 2.17                     | 0.60              |
| 1:L:59:PHE:CD2   | 1:L:173:MET:CE   | 2.84                     | 0.60              |
| 1:I:67:MET:CE    | 1:I:169:PRO:CG   | 2.71                     | 0.59              |
| 1:C:13:ILE:H     | 1:C:13:ILE:CD1   | 2.15                     | 0.59              |
| 1:L:127:TYR:O    | 1:L:129:GLU:N    | 2.34                     | 0.59              |
| 1:F:139:ILE:HG13 | 1:F:142:MET:HG3  | 1.84                     | 0.59              |
| 1:C:110:HIS:CD2  | 1:C:119:ILE:CD1  | 2.86                     | 0.59              |
| 1:G:59:PHE:CE2   | 1:G:63:LEU:HD11  | 2.37                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:8:TYR:C      | 1:H:8:TYR:CD1    | 2.75                     | 0.59              |
| 1:D:57:PRO:HG3   | 1:D:120:TYR:CE2  | 2.38                     | 0.58              |
| 1:E:154:THR:CG2  | 1:F:154:THR:O    | 2.51                     | 0.58              |
| 1:A:67:MET:HE3   | 1:A:169:PRO:HB2  | 1.84                     | 0.58              |
| 1:D:35:GLN:OE1   | 1:F:151:VAL:HG11 | 2.03                     | 0.58              |
| 1:H:22:PHE:CZ    | 1:H:82:LEU:HD22  | 2.38                     | 0.58              |
| 1:L:106:TRP:HB3  | 1:L:142:MET:CE   | 2.33                     | 0.58              |
| 1:E:8:TYR:CE2    | 1:E:78:LYS:HE2   | 2.38                     | 0.58              |
| 1:H:139:ILE:HD12 | 1:H:141:ASN:OD1  | 2.03                     | 0.58              |
| 1:I:138:PHE:C    | 1:I:142:MET:HE3  | 2.14                     | 0.58              |
| 1:D:8:TYR:HD1    | 1:D:83:VAL:HG22  | 1.69                     | 0.58              |
| 1:F:110:HIS:CD2  | 1:F:119:ILE:CD1  | 2.84                     | 0.58              |
| 1:H:25:PHE:HB2   | 1:H:194:ALA:HA   | 1.85                     | 0.58              |
| 1:A:187:LEU:CD2  | 1:A:208:LEU:HD21 | 2.34                     | 0.58              |
| 1:F:57:PRO:HG3   | 1:F:120:TYR:CE2  | 2.39                     | 0.58              |
| 1:L:106:TRP:HD1  | 1:L:142:MET:CE   | 2.14                     | 0.58              |
| 1:C:9:THR:HG22   | 2:C:228:HOH:O    | 2.03                     | 0.58              |
| 1:B:67:MET:CE    | 1:B:169:PRO:CG   | 2.79                     | 0.58              |
| 1:C:49:LYS:C     | 1:C:51:ASN:N     | 2.56                     | 0.58              |
| 1:H:127:TYR:CE2  | 1:H:136:LYS:HG2  | 2.38                     | 0.58              |
| 1:A:204:MET:CE   | 1:A:205:LEU:HD23 | 2.33                     | 0.57              |
| 1:E:192:HIS:HD1  | 1:E:194:ALA:H    | 1.52                     | 0.57              |
| 1:G:113:PHE:HD2  | 1:G:218:GLY:HA3  | 1.67                     | 0.57              |
| 1:K:47:THR:O     | 1:K:48:VAL:C     | 2.42                     | 0.57              |
| 1:B:158:LEU:HD12 | 1:B:160:VAL:HG23 | 1.82                     | 0.57              |
| 1:I:38:GLN:NE2   | 1:I:177:TYR:OH   | 2.37                     | 0.57              |
| 1:A:204:MET:CE   | 1:A:205:LEU:HG   | 2.35                     | 0.57              |
| 1:G:159:ASN:ND2  | 1:H:159:ASN:ND2  | 2.53                     | 0.57              |
| 1:J:149:PRO:O    | 1:J:175:LYS:HB2  | 2.04                     | 0.57              |
| 1:C:56:TYR:HB3   | 1:C:57:PRO:CD    | 2.30                     | 0.57              |
| 1:K:106:TRP:CD1  | 1:K:142:MET:HE1  | 2.39                     | 0.57              |
| 1:A:204:MET:HE1  | 1:A:205:LEU:HD23 | 1.87                     | 0.57              |
| 1:G:72:GLU:N     | 1:G:72:GLU:OE2   | 2.30                     | 0.57              |
| 1:K:171:PHE:HZ   | 1:K:204:MET:CE   | 2.15                     | 0.57              |
| 1:K:192:HIS:HD1  | 1:K:194:ALA:H    | 1.53                     | 0.57              |
| 1:J:138:PHE:CG   | 1:J:138:PHE:O    | 2.57                     | 0.57              |
| 1:H:4:LYS:HB2    | 1:H:89:HIS:HE2   | 1.70                     | 0.56              |
| 1:I:149:PRO:HD2  | 1:I:150:TRP:CZ3  | 2.39                     | 0.56              |
| 1:G:53:HIS:HE1   | 1:G:114:ARG:NH1  | 2.02                     | 0.56              |
| 1:G:14:SER:HA    | 1:G:19:LYS:HE2   | 1.87                     | 0.56              |
| 1:C:49:LYS:O     | 1:C:50:LYS:C     | 2.43                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:92:TYR:HA    | 1:E:145:VAL:O    | 2.05                     | 0.56              |
| 1:G:155:SER:O    | 1:H:35:GLN:HA    | 2.05                     | 0.56              |
| 1:F:157:ASP:OD2  | 1:F:157:ASP:N    | 2.37                     | 0.56              |
| 1:I:59:PHE:HD2   | 1:I:173:MET:CE   | 2.18                     | 0.56              |
| 1:I:59:PHE:HD2   | 1:I:173:MET:SD   | 2.27                     | 0.56              |
| 1:D:67:MET:CE    | 1:D:169:PRO:CG   | 2.79                     | 0.56              |
| 1:H:48:VAL:HG13  | 1:H:53:HIS:O     | 2.06                     | 0.56              |
| 1:C:114:ARG:HG3  | 1:C:114:ARG:NH1  | 2.19                     | 0.56              |
| 1:D:56:TYR:HB3   | 1:D:57:PRO:HD3   | 1.86                     | 0.56              |
| 1:K:171:PHE:CE2  | 1:K:204:MET:CE   | 2.89                     | 0.56              |
| 1:L:179:GLN:HE21 | 1:L:184:LEU:HD12 | 1.70                     | 0.56              |
| 1:L:30:GLN:HE22  | 1:L:164:ASP:HA   | 1.71                     | 0.56              |
| 1:B:67:MET:HE1   | 1:B:169:PRO:CG   | 2.35                     | 0.56              |
| 1:G:59:PHE:HD2   | 1:G:173:MET:HE2  | 1.69                     | 0.56              |
| 1:L:45:LEU:HD23  | 1:L:45:LEU:C     | 2.25                     | 0.56              |
| 1:A:89:HIS:O     | 1:A:142:MET:HA   | 2.06                     | 0.56              |
| 1:D:8:TYR:CD1    | 1:D:83:VAL:HG22  | 2.40                     | 0.56              |
| 1:G:159:ASN:ND2  | 1:I:159:ASN:HD21 | 2.04                     | 0.56              |
| 1:L:118:HIS:O    | 1:L:119:ILE:HB   | 2.06                     | 0.56              |
| 1:L:37:VAL:HG13  | 1:L:38:GLN:N     | 2.21                     | 0.56              |
| 1:I:118:HIS:CE1  | 1:I:122:GLN:NE2  | 2.73                     | 0.55              |
| 1:I:77:MET:HE1   | 1:I:82:LEU:HB2   | 1.87                     | 0.55              |
| 1:J:67:MET:HE1   | 1:J:73:PHE:CG    | 2.41                     | 0.55              |
| 1:D:65:ARG:HD2   | 1:J:111:ASP:OD2  | 2.06                     | 0.55              |
| 1:I:118:HIS:ND1  | 1:I:122:GLN:NE2  | 2.53                     | 0.55              |
| 1:J:106:TRP:HD1  | 1:J:142:MET:CE   | 2.19                     | 0.55              |
| 1:J:25:PHE:O     | 1:J:30:GLN:HG3   | 2.06                     | 0.55              |
| 1:K:74:ARG:HD2   | 1:K:88:VAL:HG13  | 1.89                     | 0.55              |
| 1:E:25:PHE:O     | 1:E:30:GLN:HG3   | 2.07                     | 0.55              |
| 1:L:26:GLN:HA    | 1:L:26:GLN:HE21  | 1.70                     | 0.55              |
| 1:L:77:MET:HG3   | 1:L:165:ASN:OD1  | 2.07                     | 0.55              |
| 1:H:45:LEU:HD13  | 1:H:49:LYS:NZ    | 2.22                     | 0.55              |
| 1:J:57:PRO:HA    | 1:J:60:ILE:HB    | 1.88                     | 0.55              |
| 1:K:34:ASN:OD1   | 1:K:157:ASP:HB3  | 2.07                     | 0.55              |
| 1:C:49:LYS:C     | 1:C:51:ASN:H     | 2.10                     | 0.55              |
| 1:A:115:GLN:O    | 1:A:119:ILE:HD12 | 2.07                     | 0.55              |
| 1:B:156:PHE:C    | 1:B:156:PHE:CD2  | 2.80                     | 0.55              |
| 1:I:34:ASN:ND2   | 1:I:158:LEU:H    | 2.04                     | 0.55              |
| 1:D:203:ARG:O    | 1:D:207:GLU:HG3  | 2.07                     | 0.55              |
| 1:H:65:ARG:HH22  | 1:H:219:ALA:CB   | 2.20                     | 0.55              |
| 1:H:38:GLN:NE2   | 1:H:177:TYR:OH   | 2.40                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:138:PHE:CA   | 1:I:142:MET:CE   | 2.84                     | 0.54              |
| 1:K:90:PRO:HD2   | 1:K:107:SER:O    | 2.07                     | 0.54              |
| 1:B:204:MET:CE   | 1:B:205:LEU:HD23 | 2.37                     | 0.54              |
| 1:D:110:HIS:HD2  | 1:D:112:ASP:H    | 1.54                     | 0.54              |
| 1:J:29:ALA:O     | 1:J:30:GLN:C     | 2.45                     | 0.54              |
| 1:K:106:TRP:CD1  | 1:K:142:MET:HE3  | 2.43                     | 0.54              |
| 1:G:72:GLU:HG3   | 1:G:200:HIS:HB3  | 1.89                     | 0.54              |
| 1:I:34:ASN:HD21  | 1:I:158:LEU:H    | 1.55                     | 0.54              |
| 1:I:75:MET:HA    | 1:I:83:VAL:O     | 2.08                     | 0.54              |
| 1:J:67:MET:HE1   | 1:J:73:PHE:CD1   | 2.42                     | 0.54              |
| 1:G:159:ASN:HB3  | 1:H:32:THR:HG22  | 1.90                     | 0.54              |
| 1:C:148:ASN:O    | 1:C:174:GLY:HA2  | 2.08                     | 0.54              |
| 1:D:25:PHE:O     | 1:D:30:GLN:HG3   | 2.08                     | 0.54              |
| 1:I:118:HIS:CE1  | 1:I:122:GLN:HE21 | 2.25                     | 0.54              |
| 1:K:159:ASN:HB3  | 1:L:32:THR:CG2   | 2.38                     | 0.54              |
| 1:G:159:ASN:HD22 | 1:I:159:ASN:ND2  | 2.06                     | 0.54              |
| 1:G:91:CYS:HB2   | 1:G:142:MET:HE2  | 1.90                     | 0.54              |
| 1:G:93:THR:HG23  | 1:G:146:SER:HB3  | 1.90                     | 0.54              |
| 1:J:27:SER:OG    | 1:J:28:VAL:HG22  | 2.08                     | 0.54              |
| 1:F:11:VAL:HG21  | 1:F:82:LEU:HD23  | 1.89                     | 0.54              |
| 1:K:106:TRP:CG   | 1:K:142:MET:CE   | 2.91                     | 0.54              |
| 1:C:67:MET:HE3   | 1:C:67:MET:HA    | 1.90                     | 0.54              |
| 1:K:56:TYR:HB3   | 1:K:57:PRO:CD    | 2.37                     | 0.54              |
| 1:L:66:LEU:HD21  | 1:L:211:TYR:CD2  | 2.43                     | 0.54              |
| 1:G:59:PHE:HE2   | 1:G:63:LEU:HD11  | 1.72                     | 0.53              |
| 1:H:4:LYS:HB2    | 1:H:89:HIS:NE2   | 2.23                     | 0.53              |
| 1:I:6:THR:CG2    | 1:I:141:ASN:HD21 | 2.01                     | 0.53              |
| 1:J:159:ASN:HB3  | 1:K:32:THR:CG2   | 2.24                     | 0.53              |
| 1:J:62:ILE:HD11  | 1:J:215:TRP:CD1  | 2.43                     | 0.53              |
| 1:B:78:LYS:O     | 1:B:81:GLU:N     | 2.39                     | 0.53              |
| 1:J:171:PHE:CZ   | 1:J:204:MET:CE   | 2.91                     | 0.53              |
| 1:D:190:GLN:O    | 1:D:190:GLN:HG3  | 2.06                     | 0.53              |
| 1:E:148:ASN:N    | 1:E:149:PRO:HD3  | 2.22                     | 0.53              |
| 1:G:59:PHE:CD2   | 1:G:173:MET:SD   | 3.02                     | 0.53              |
| 1:J:40:ASP:HA    | 1:J:184:LEU:CD2  | 2.38                     | 0.53              |
| 1:A:187:LEU:CD2  | 1:A:208:LEU:CD2  | 2.85                     | 0.53              |
| 1:F:177:TYR:OH   | 2:F:233:HOH:O    | 2.19                     | 0.53              |
| 1:E:44:PHE:O     | 1:E:48:VAL:HG23  | 2.09                     | 0.53              |
| 1:E:154:THR:HG23 | 1:F:154:THR:O    | 2.08                     | 0.53              |
| 1:K:171:PHE:CZ   | 1:K:204:MET:SD   | 3.01                     | 0.53              |
| 1:C:190:GLN:C    | 1:C:190:GLN:HE21 | 2.12                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:93:THR:CG2   | 1:G:146:SER:HB3  | 2.39                     | 0.53              |
| 1:G:98:GLN:HB2   | 1:G:99:THR:HG23  | 1.90                     | 0.53              |
| 1:J:123:ASP:OD1  | 1:J:136:LYS:CE   | 2.56                     | 0.53              |
| 1:H:26:GLN:HE21  | 1:H:26:GLN:HA    | 1.74                     | 0.53              |
| 1:H:5:ILE:HA     | 1:H:6:THR:HG23   | 1.90                     | 0.53              |
| 1:J:27:SER:OG    | 1:J:28:VAL:N     | 2.40                     | 0.53              |
| 1:J:30:GLN:NE2   | 2:J:226:HOH:O    | 2.41                     | 0.53              |
| 1:D:110:HIS:HD2  | 1:D:111:ASP:N    | 2.06                     | 0.53              |
| 1:G:139:ILE:HG13 | 1:G:142:MET:CG   | 2.38                     | 0.53              |
| 1:J:99:THR:HB    | 1:K:17:HIS:HD2   | 1.73                     | 0.53              |
| 1:K:154:THR:HG22 | 1:L:36:THR:HB    | 1.90                     | 0.53              |
| 1:C:216:GLN:HA   | 1:C:216:GLN:NE2  | 2.17                     | 0.52              |
| 1:A:56:TYR:N     | 1:A:57:PRO:CD    | 2.71                     | 0.52              |
| 1:G:12:ASP:OD2   | 1:G:15:GLN:HG2   | 2.10                     | 0.52              |
| 1:H:56:TYR:HB3   | 1:H:57:PRO:HD3   | 1.91                     | 0.52              |
| 1:I:143:PHE:HB2  | 1:I:169:PRO:HD2  | 1.92                     | 0.52              |
| 1:E:156:PHE:C    | 1:E:156:PHE:CD2  | 2.82                     | 0.52              |
| 1:L:57:PRO:HG2   | 1:L:58:ALA:N     | 2.23                     | 0.52              |
| 1:L:67:MET:HE1   | 1:L:73:PHE:CD2   | 2.44                     | 0.52              |
| 1:E:187:LEU:HG   | 1:E:188:ALA:N    | 2.21                     | 0.52              |
| 1:H:30:GLN:NE2   | 1:H:163:MET:HG3  | 2.25                     | 0.52              |
| 1:G:187:LEU:CD2  | 1:G:208:LEU:HD21 | 2.40                     | 0.52              |
| 1:G:75:MET:HA    | 1:G:83:VAL:O     | 2.08                     | 0.52              |
| 1:J:130:ASN:HB3  | 1:J:135:PRO:HG3  | 1.92                     | 0.52              |
| 1:K:106:TRP:HB3  | 1:K:142:MET:HE1  | 1.92                     | 0.52              |
| 1:L:35:GLN:O     | 1:L:188:ALA:HA   | 2.09                     | 0.52              |
| 1:B:154:THR:HG21 | 1:C:38:GLN:OE1   | 2.10                     | 0.52              |
| 1:C:67:MET:HE3   | 1:C:73:PHE:HB2   | 1.88                     | 0.52              |
| 1:D:214:GLU:OE2  | 1:J:115:GLN:HG3  | 2.10                     | 0.52              |
| 1:B:187:LEU:HG   | 1:B:188:ALA:N    | 2.18                     | 0.52              |
| 1:C:47:THR:O     | 1:C:48:VAL:C     | 2.48                     | 0.52              |
| 1:J:59:PHE:HD2   | 1:J:173:MET:HE1  | 1.74                     | 0.52              |
| 1:K:34:ASN:HD21  | 1:K:190:GLN:HB2  | 1.75                     | 0.52              |
| 1:C:67:MET:HE1   | 1:C:73:PHE:CD1   | 2.44                     | 0.52              |
| 1:D:16:TRP:CE2   | 1:D:18:ARG:HB2   | 2.45                     | 0.52              |
| 1:G:133:TYR:O    | 1:G:135:PRO:HD3  | 2.10                     | 0.52              |
| 1:L:171:PHE:HA   | 1:L:188:ALA:O    | 2.10                     | 0.51              |
| 1:A:129:GLU:HA   | 1:A:129:GLU:OE1  | 2.10                     | 0.51              |
| 1:A:56:TYR:HB3   | 1:A:57:PRO:HD3   | 1.92                     | 0.51              |
| 1:C:29:ALA:O     | 1:C:30:GLN:C     | 2.45                     | 0.51              |
| 1:D:110:HIS:CD2  | 1:D:112:ASP:H    | 2.29                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:189:ILE:O    | 1:D:189:ILE:HG23 | 2.10                     | 0.51              |
| 1:C:113:PHE:CD2  | 1:C:215:TRP:HZ2  | 2.29                     | 0.51              |
| 1:D:73:PHE:HB3   | 1:D:169:PRO:HG2  | 1.91                     | 0.51              |
| 1:E:90:PRO:HD2   | 1:E:107:SER:O    | 2.10                     | 0.51              |
| 1:I:30:GLN:NE2   | 1:I:192:HIS:NE2  | 2.47                     | 0.51              |
| 1:J:145:VAL:CG1  | 1:J:173:MET:HE3  | 2.41                     | 0.51              |
| 1:L:106:TRP:CG   | 1:L:142:MET:HE3  | 2.43                     | 0.51              |
| 1:D:27:SER:O     | 1:D:28:VAL:C     | 2.45                     | 0.51              |
| 1:A:204:MET:CE   | 1:A:205:LEU:CD2  | 2.88                     | 0.51              |
| 1:B:78:LYS:O     | 1:B:80:GLY:N     | 2.43                     | 0.51              |
| 1:G:45:LEU:HD12  | 1:G:183:VAL:HG11 | 1.92                     | 0.51              |
| 1:F:89:HIS:ND1   | 1:F:109:TYR:HB3  | 2.25                     | 0.51              |
| 1:I:30:GLN:NE2   | 1:I:163:MET:HG3  | 2.26                     | 0.51              |
| 1:I:49:LYS:O     | 1:I:51:ASN:O     | 2.29                     | 0.51              |
| 1:K:59:PHE:HD2   | 1:K:173:MET:CE   | 2.24                     | 0.51              |
| 1:D:148:ASN:ND2  | 1:D:150:TRP:HE3  | 2.09                     | 0.51              |
| 1:I:25:PHE:O     | 1:I:30:GLN:HG3   | 2.10                     | 0.51              |
| 1:K:171:PHE:CZ   | 1:K:189:ILE:HD13 | 2.46                     | 0.51              |
| 1:B:5:ILE:N      | 1:B:5:ILE:CD1    | 2.74                     | 0.51              |
| 1:D:8:TYR:CD1    | 1:D:83:VAL:CG2   | 2.94                     | 0.51              |
| 1:G:34:ASN:ND2   | 2:G:232:HOH:O    | 2.44                     | 0.51              |
| 1:H:59:PHE:CD2   | 1:H:173:MET:SD   | 3.04                     | 0.51              |
| 1:A:77:MET:HG3   | 1:A:165:ASN:OD1  | 2.11                     | 0.50              |
| 1:F:106:TRP:CD1  | 1:F:142:MET:HE2  | 2.45                     | 0.50              |
| 1:F:151:VAL:CG1  | 1:F:153:PHE:HB3  | 2.40                     | 0.50              |
| 1:G:127:TYR:CE2  | 1:G:136:LYS:HG2  | 2.46                     | 0.50              |
| 1:I:110:HIS:HB3  | 1:I:115:GLN:OE1  | 2.11                     | 0.50              |
| 1:K:172:THR:HB   | 1:K:188:ALA:HB3  | 1.93                     | 0.50              |
| 1:C:62:ILE:HG21  | 1:C:208:LEU:HD12 | 1.94                     | 0.50              |
| 1:E:26:GLN:HA    | 1:E:26:GLN:HE21  | 1.76                     | 0.50              |
| 1:E:67:MET:CE    | 1:E:171:PHE:CZ   | 2.93                     | 0.50              |
| 1:I:40:ASP:HB3   | 1:I:209:GLN:OE1  | 2.12                     | 0.50              |
| 1:J:163:MET:SD   | 1:L:161:ALA:HB2  | 2.51                     | 0.50              |
| 1:K:139:ILE:HG13 | 1:K:142:MET:HG2  | 1.93                     | 0.50              |
| 1:G:159:ASN:ND2  | 1:H:159:ASN:HD21 | 2.10                     | 0.50              |
| 1:G:59:PHE:CD2   | 1:G:173:MET:HE2  | 2.42                     | 0.50              |
| 1:D:114:ARG:CG   | 1:D:114:ARG:HH11 | 2.25                     | 0.50              |
| 1:J:56:TYR:CZ    | 1:J:147:ALA:HB2  | 2.46                     | 0.50              |
| 1:L:179:GLN:HE21 | 1:L:184:LEU:CD1  | 2.24                     | 0.50              |
| 1:D:113:PHE:O    | 1:D:117:LEU:HB2  | 2.12                     | 0.50              |
| 1:D:159:ASN:OD1  | 1:E:159:ASN:ND2  | 2.45                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:91:CYS:CB   | 1:G:142:MET:HE2  | 2.42                     | 0.50              |
| 1:C:204:MET:CE  | 1:C:205:LEU:HD23 | 2.41                     | 0.50              |
| 1:D:56:TYR:HB3  | 1:D:57:PRO:CD    | 2.41                     | 0.50              |
| 1:F:68:ASN:OD1  | 1:F:87:SER:HA    | 2.10                     | 0.50              |
| 1:J:159:ASN:ND2 | 1:K:159:ASN:HD22 | 2.10                     | 0.50              |
| 1:B:34:ASN:CB   | 1:B:157:ASP:HB2  | 2.41                     | 0.50              |
| 1:I:67:MET:HE1  | 1:I:73:PHE:HB3   | 1.93                     | 0.50              |
| 1:J:34:ASN:ND2  | 1:J:190:GLN:HB2  | 2.27                     | 0.50              |
| 1:L:84:ILE:HG22 | 1:L:85:TRP:O     | 2.12                     | 0.50              |
| 1:C:110:HIS:HD2 | 1:C:119:ILE:HD13 | 1.76                     | 0.50              |
| 1:D:30:GLN:HE22 | 1:D:164:ASP:HA   | 1.77                     | 0.50              |
| 1:G:18:ARG:O    | 1:G:19:LYS:C     | 2.50                     | 0.50              |
| 1:D:148:ASN:ND2 | 1:D:150:TRP:CE3  | 2.81                     | 0.49              |
| 1:K:10:THR:O    | 1:K:10:THR:CG2   | 2.60                     | 0.49              |
| 1:L:153:PHE:O   | 1:L:186:PRO:HB3  | 2.11                     | 0.49              |
| 1:F:39:LEU:HD13 | 1:F:41:ILE:CG2   | 2.42                     | 0.49              |
| 1:G:91:CYS:SG   | 1:G:142:MET:CE   | 2.96                     | 0.49              |
| 1:J:106:TRP:HB3 | 1:J:142:MET:CE   | 2.42                     | 0.49              |
| 1:L:123:ASP:OD1 | 1:L:136:LYS:CE   | 2.60                     | 0.49              |
| 1:K:8:TYR:OH    | 1:K:78:LYS:HD3   | 2.12                     | 0.49              |
| 1:D:110:HIS:CD2 | 1:D:111:ASP:N    | 2.81                     | 0.49              |
| 1:D:38:GLN:NE2  | 1:D:177:TYR:OH   | 2.44                     | 0.49              |
| 1:A:13:ILE:HG22 | 1:A:19:LYS:HG3   | 1.95                     | 0.49              |
| 1:J:106:TRP:O   | 1:J:136:LYS:HE3  | 2.12                     | 0.49              |
| 1:J:34:ASN:O    | 1:L:157:ASP:N    | 2.45                     | 0.49              |
| 1:E:56:TYR:HB3  | 1:E:57:PRO:CD    | 2.42                     | 0.49              |
| 1:G:26:GLN:NE2  | 2:G:225:HOH:O    | 2.37                     | 0.49              |
| 1:H:5:ILE:O     | 1:H:5:ILE:HG22   | 2.12                     | 0.49              |
| 1:K:22:PHE:CE1  | 1:K:26:GLN:HG3   | 2.47                     | 0.49              |
| 1:B:99:THR:O    | 1:B:100:GLU:HB2  | 2.12                     | 0.49              |
| 2:B:240:HOH:O   | 1:C:17:HIS:HD2   | 1.94                     | 0.49              |
| 1:D:25:PHE:HB2  | 1:D:194:ALA:HA   | 1.95                     | 0.49              |
| 1:D:67:MET:HE1  | 1:D:169:PRO:CG   | 2.40                     | 0.49              |
| 1:I:14:SER:HA   | 1:I:19:LYS:HD2   | 1.95                     | 0.49              |
| 1:J:179:GLN:O   | 1:J:179:GLN:CG   | 2.60                     | 0.49              |
| 1:L:103:SER:HB3 | 1:L:132:ALA:O    | 2.12                     | 0.49              |
| 1:L:8:TYR:HB2   | 1:L:83:VAL:CG1   | 2.41                     | 0.49              |
| 1:B:67:MET:HE2  | 1:B:169:PRO:HB2  | 1.94                     | 0.49              |
| 1:D:38:GLN:NE2  | 1:D:177:TYR:HE2  | 2.09                     | 0.49              |
| 1:E:67:MET:HE2  | 1:E:171:PHE:CE1  | 2.48                     | 0.49              |
| 1:G:127:TYR:CE2 | 1:G:136:LYS:CG   | 2.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:67:MET:CE    | 1:J:73:PHE:CG    | 2.96                     | 0.49              |
| 1:K:171:PHE:CE2  | 1:K:189:ILE:HD13 | 2.47                     | 0.49              |
| 1:B:191:VAL:HG21 | 1:B:201:VAL:HG21 | 1.95                     | 0.49              |
| 1:A:90:PRO:HD2   | 1:A:107:SER:O    | 2.12                     | 0.49              |
| 1:D:38:GLN:NE2   | 1:D:177:TYR:CE2  | 2.81                     | 0.49              |
| 1:G:92:TYR:HA    | 1:G:145:VAL:O    | 2.13                     | 0.48              |
| 1:I:145:VAL:CG1  | 1:I:173:MET:CE   | 2.91                     | 0.48              |
| 1:K:44:PHE:HB2   | 1:K:212:CYS:HB3  | 1.94                     | 0.48              |
| 1:D:36:THR:HB    | 1:F:155:SER:HB3  | 1.94                     | 0.48              |
| 1:L:178:THR:O    | 1:L:179:GLN:HB3  | 2.14                     | 0.48              |
| 1:I:150:TRP:HB2  | 1:I:151:VAL:HG23 | 1.95                     | 0.48              |
| 1:J:10:THR:CB    | 2:J:225:HOH:O    | 2.59                     | 0.48              |
| 1:J:44:PHE:O     | 1:J:48:VAL:HG23  | 2.13                     | 0.48              |
| 1:B:215:TRP:CZ2  | 1:B:217:GLY:HA2  | 2.49                     | 0.48              |
| 1:D:87:SER:O     | 1:D:141:ASN:ND2  | 2.43                     | 0.48              |
| 1:E:134:PHE:O    | 1:E:135:PRO:C    | 2.50                     | 0.48              |
| 1:H:25:PHE:O     | 1:H:30:GLN:HG3   | 2.13                     | 0.48              |
| 1:I:110:HIS:CD2  | 1:I:119:ILE:HD12 | 2.48                     | 0.48              |
| 1:I:139:ILE:HG13 | 1:I:142:MET:HE2  | 1.95                     | 0.48              |
| 1:J:159:ASN:ND2  | 1:L:159:ASN:ND2  | 2.48                     | 0.48              |
| 1:I:148:ASN:HD22 | 1:I:150:TRP:HE3  | 1.60                     | 0.48              |
| 1:K:138:PHE:CD2  | 1:K:138:PHE:N    | 2.81                     | 0.48              |
| 1:F:151:VAL:HG12 | 1:F:153:PHE:HD2  | 1.79                     | 0.48              |
| 1:K:11:VAL:HG23  | 1:K:82:LEU:O     | 2.14                     | 0.48              |
| 1:E:30:GLN:HE22  | 1:E:164:ASP:HA   | 1.79                     | 0.48              |
| 1:F:123:ASP:OD1  | 1:F:136:LYS:CE   | 2.62                     | 0.48              |
| 1:A:187:LEU:HD22 | 1:A:208:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:157:ASP:HB2  | 1:C:157:ASP:OD2  | 2.14                     | 0.48              |
| 1:G:35:GLN:O     | 1:G:188:ALA:HA   | 2.14                     | 0.48              |
| 1:I:67:MET:CE    | 1:I:73:PHE:HB3   | 2.44                     | 0.48              |
| 1:K:10:THR:HG22  | 1:K:10:THR:O     | 2.13                     | 0.48              |
| 1:J:63:LEU:HD13  | 1:J:171:PHE:CD1  | 2.49                     | 0.47              |
| 1:K:67:MET:HG3   | 1:K:143:PHE:CG   | 2.48                     | 0.47              |
| 1:L:89:HIS:ND1   | 1:L:109:TYR:N    | 2.49                     | 0.47              |
| 1:D:136:LYS:O    | 1:D:137:GLY:C    | 2.51                     | 0.47              |
| 1:G:22:PHE:O     | 1:G:23:GLU:C     | 2.50                     | 0.47              |
| 1:K:72:GLU:HA    | 1:K:75:MET:CE    | 2.41                     | 0.47              |
| 1:L:66:LEU:HD23  | 1:L:211:TYR:HE2  | 1.79                     | 0.47              |
| 1:G:154:THR:HG22 | 1:H:36:THR:HB    | 1.97                     | 0.47              |
| 1:G:161:ALA:HB2  | 1:H:163:MET:SD   | 2.54                     | 0.47              |
| 1:J:57:PRO:O     | 1:J:58:ALA:C     | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:77:MET:HE3   | 1:E:165:ASN:OD1  | 2.15                     | 0.47              |
| 1:J:159:ASN:CG   | 1:K:159:ASN:HD22 | 2.17                     | 0.47              |
| 1:K:92:TYR:HA    | 1:K:145:VAL:O    | 2.13                     | 0.47              |
| 1:A:123:ASP:OD1  | 1:A:136:LYS:CE   | 2.62                     | 0.47              |
| 1:B:109:TYR:O    | 1:B:110:HIS:CG   | 2.68                     | 0.47              |
| 1:B:151:VAL:CG1  | 1:B:152:SER:N    | 2.78                     | 0.47              |
| 1:F:204:MET:HE2  | 1:F:205:LEU:HA   | 1.96                     | 0.47              |
| 1:J:57:PRO:HB3   | 1:J:120:TYR:CE2  | 2.49                     | 0.47              |
| 1:A:192:HIS:HD1  | 1:A:194:ALA:N    | 2.05                     | 0.47              |
| 1:A:29:ALA:O     | 1:A:30:GLN:C     | 2.52                     | 0.47              |
| 1:C:120:TYR:CZ   | 1:C:124:VAL:HG21 | 2.49                     | 0.47              |
| 1:I:109:TYR:O    | 1:I:110:HIS:CD2  | 2.68                     | 0.47              |
| 1:I:92:TYR:HA    | 1:I:145:VAL:O    | 2.14                     | 0.47              |
| 1:I:59:PHE:CD2   | 1:I:173:MET:HE1  | 2.45                     | 0.47              |
| 1:A:184:LEU:HD23 | 1:A:184:LEU:HA   | 1.63                     | 0.47              |
| 1:B:5:ILE:N      | 1:B:5:ILE:HD13   | 2.29                     | 0.47              |
| 1:D:67:MET:HE3   | 1:D:169:PRO:HG2  | 1.92                     | 0.47              |
| 1:I:139:ILE:HG13 | 1:I:142:MET:HE3  | 1.92                     | 0.47              |
| 1:G:30:GLN:HB3   | 1:I:161:ALA:CB   | 2.43                     | 0.47              |
| 1:J:85:TRP:CD2   | 1:J:141:ASN:HB3  | 2.50                     | 0.47              |
| 1:J:67:MET:CE    | 1:J:67:MET:CA    | 2.84                     | 0.47              |
| 1:L:67:MET:CE    | 1:L:169:PRO:CG   | 2.85                     | 0.47              |
| 1:K:190:GLN:C    | 1:K:190:GLN:HE21 | 2.17                     | 0.47              |
| 1:K:77:MET:HE2   | 1:K:82:LEU:HD13  | 1.97                     | 0.47              |
| 1:D:59:PHE:HD2   | 1:D:173:MET:CE   | 2.28                     | 0.47              |
| 1:B:67:MET:HG3   | 1:B:143:PHE:CG   | 2.50                     | 0.46              |
| 1:D:59:PHE:CE2   | 1:D:63:LEU:HD11  | 2.50                     | 0.46              |
| 1:K:157:ASP:OD2  | 1:L:157:ASP:OD2  | 2.33                     | 0.46              |
| 1:A:26:GLN:O     | 1:A:26:GLN:HG3   | 2.15                     | 0.46              |
| 1:B:151:VAL:HG12 | 1:B:152:SER:N    | 2.29                     | 0.46              |
| 1:J:189:ILE:HG23 | 1:J:189:ILE:O    | 2.14                     | 0.46              |
| 1:J:18:ARG:HE    | 1:J:197:ASP:CG   | 2.19                     | 0.46              |
| 1:K:8:TYR:CD1    | 1:K:8:TYR:O      | 2.68                     | 0.46              |
| 1:B:171:PHE:HA   | 1:B:188:ALA:O    | 2.15                     | 0.46              |
| 1:E:153:PHE:O    | 1:E:186:PRO:HB3  | 2.16                     | 0.46              |
| 1:J:45:LEU:HD23  | 1:J:45:LEU:HA    | 1.77                     | 0.46              |
| 1:K:165:ASN:HA   | 1:K:167:PHE:CZ   | 2.50                     | 0.46              |
| 1:B:39:LEU:O     | 1:B:185:MET:N    | 2.44                     | 0.46              |
| 1:E:56:TYR:HB3   | 1:E:57:PRO:HD3   | 1.97                     | 0.46              |
| 1:F:202:GLY:O    | 1:F:203:ARG:C    | 2.54                     | 0.46              |
| 1:J:64:ALA:O     | 1:J:68:ASN:ND2   | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:204:MET:CE   | 1:B:205:LEU:HA   | 2.45                     | 0.46              |
| 1:E:105:LEU:HD21 | 1:E:127:TYR:HB2  | 1.97                     | 0.46              |
| 1:E:59:PHE:CE2   | 1:E:173:MET:SD   | 3.08                     | 0.46              |
| 1:J:122:GLN:O    | 1:J:126:CYS:HB3  | 2.16                     | 0.46              |
| 1:J:145:VAL:HG11 | 1:J:173:MET:HE3  | 1.97                     | 0.46              |
| 1:L:67:MET:HB3   | 1:L:88:VAL:HG21  | 1.97                     | 0.46              |
| 1:A:204:MET:HE2  | 1:A:205:LEU:N    | 2.31                     | 0.46              |
| 1:B:155:SER:O    | 1:C:35:GLN:HA    | 2.16                     | 0.46              |
| 1:D:51:ASN:H     | 1:D:51:ASN:ND2   | 2.12                     | 0.46              |
| 1:E:67:MET:HE2   | 1:E:171:PHE:HE1  | 1.79                     | 0.46              |
| 1:J:106:TRP:CG   | 1:J:142:MET:HE3  | 2.49                     | 0.46              |
| 1:A:139:ILE:HG12 | 1:A:142:MET:HE3  | 1.98                     | 0.46              |
| 1:I:145:VAL:CG1  | 1:I:173:MET:HE2  | 2.46                     | 0.46              |
| 1:K:154:THR:HG21 | 1:L:38:GLN:OE1   | 2.16                     | 0.46              |
| 1:K:34:ASN:HB3   | 1:K:157:ASP:OD1  | 2.16                     | 0.46              |
| 1:E:26:GLN:HA    | 1:E:26:GLN:NE2   | 2.30                     | 0.46              |
| 1:G:113:PHE:CG   | 1:G:113:PHE:O    | 2.68                     | 0.46              |
| 1:B:105:LEU:HA   | 1:B:105:LEU:HD23 | 1.61                     | 0.45              |
| 1:E:59:PHE:CD2   | 1:E:173:MET:HE2  | 2.45                     | 0.45              |
| 1:I:67:MET:HG3   | 1:I:143:PHE:CG   | 2.51                     | 0.45              |
| 1:J:124:VAL:O    | 1:J:128:GLY:CA   | 2.65                     | 0.45              |
| 1:J:90:PRO:HD2   | 1:J:107:SER:O    | 2.16                     | 0.45              |
| 1:C:51:ASN:HB3   | 1:C:52:LYS:H     | 1.57                     | 0.45              |
| 1:H:26:GLN:NE2   | 1:H:26:GLN:HA    | 2.30                     | 0.45              |
| 1:F:26:GLN:HA    | 1:F:26:GLN:NE2   | 2.31                     | 0.45              |
| 1:J:159:ASN:HD22 | 1:L:159:ASN:ND2  | 1.87                     | 0.45              |
| 1:A:175:LYS:HZ3  | 1:A:175:LYS:HG3  | 1.40                     | 0.45              |
| 1:A:40:ASP:HA    | 1:A:184:LEU:HD23 | 1.98                     | 0.45              |
| 1:A:35:GLN:O     | 1:A:188:ALA:HA   | 2.17                     | 0.45              |
| 1:B:158:LEU:HD13 | 1:B:160:VAL:HG23 | 1.87                     | 0.45              |
| 1:B:19:LYS:HE3   | 1:B:23:GLU:OE2   | 2.17                     | 0.45              |
| 1:H:192:HIS:HD1  | 1:H:194:ALA:N    | 1.97                     | 0.45              |
| 1:I:6:THR:CG2    | 1:I:6:THR:OG1    | 2.52                     | 0.45              |
| 1:J:63:LEU:HD13  | 1:J:171:PHE:CG   | 2.51                     | 0.45              |
| 1:K:59:PHE:CE2   | 1:K:173:MET:SD   | 3.09                     | 0.45              |
| 1:L:74:ARG:HB2   | 1:L:84:ILE:HG23  | 1.97                     | 0.45              |
| 1:I:171:PHE:HA   | 1:I:188:ALA:O    | 2.16                     | 0.45              |
| 1:L:182:LYS:HZ2  | 1:L:182:LYS:HG2  | 1.62                     | 0.45              |
| 1:A:145:VAL:CG1  | 1:A:173:MET:HE2  | 2.46                     | 0.45              |
| 1:H:205:LEU:O    | 1:H:208:LEU:HB3  | 2.17                     | 0.45              |
| 1:J:89:HIS:CE1   | 1:J:108:GLU:CG   | 2.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:106:TRP:HD1  | 1:L:142:MET:HE1  | 1.82                     | 0.45              |
| 1:C:56:TYR:CE1   | 1:C:173:MET:HE1  | 2.52                     | 0.45              |
| 1:D:36:THR:HG22  | 1:F:154:THR:HG22 | 1.99                     | 0.45              |
| 1:G:36:THR:HB    | 1:I:155:SER:HB3  | 1.98                     | 0.45              |
| 1:L:149:PRO:HD2  | 1:L:150:TRP:CZ3  | 2.52                     | 0.45              |
| 1:L:144:PHE:HB2  | 1:L:170:VAL:HG22 | 1.99                     | 0.45              |
| 1:C:96:HIS:CE1   | 1:C:128:GLY:O    | 2.70                     | 0.45              |
| 1:C:56:TYR:HE1   | 1:C:173:MET:CE   | 2.29                     | 0.45              |
| 1:F:26:GLN:HA    | 1:F:26:GLN:HE21  | 1.81                     | 0.45              |
| 1:H:101:THR:HB   | 2:H:231:HOH:O    | 2.16                     | 0.45              |
| 1:K:49:LYS:C     | 1:K:51:ASN:O     | 2.55                     | 0.45              |
| 1:A:13:ILE:H     | 1:A:13:ILE:HD12  | 1.82                     | 0.45              |
| 1:B:204:MET:HE2  | 1:B:205:LEU:HG   | 1.99                     | 0.45              |
| 1:C:67:MET:CE    | 1:C:73:PHE:CD1   | 2.99                     | 0.45              |
| 1:D:77:MET:HB2   | 1:D:165:ASN:HB3  | 1.99                     | 0.45              |
| 1:F:204:MET:HE2  | 1:F:205:LEU:CA   | 2.47                     | 0.45              |
| 1:J:93:THR:HA    | 1:J:103:SER:O    | 2.16                     | 0.45              |
| 1:K:205:LEU:HD23 | 1:K:205:LEU:HA   | 1.85                     | 0.45              |
| 1:J:159:ASN:HD21 | 1:K:159:ASN:HD21 | 1.60                     | 0.45              |
| 1:J:6:THR:O      | 1:J:6:THR:CG2    | 2.53                     | 0.45              |
| 1:A:149:PRO:O    | 1:A:175:LYS:HB2  | 2.18                     | 0.44              |
| 1:B:78:LYS:O     | 1:B:79:ASP:C     | 2.55                     | 0.44              |
| 1:G:30:GLN:NE2   | 2:G:225:HOH:O    | 2.50                     | 0.44              |
| 1:H:113:PHE:N    | 1:H:219:ALA:HB3  | 2.30                     | 0.44              |
| 1:J:25:PHE:HB2   | 1:J:194:ALA:HA   | 1.99                     | 0.44              |
| 1:J:98:GLN:N     | 1:J:98:GLN:HE21  | 2.16                     | 0.44              |
| 1:I:57:PRO:HB3   | 1:I:120:TYR:CD2  | 2.52                     | 0.44              |
| 1:J:203:ARG:HG2  | 1:J:207:GLU:OE2  | 2.17                     | 0.44              |
| 1:J:75:MET:HA    | 1:J:83:VAL:O     | 2.17                     | 0.44              |
| 1:C:30:GLN:HE22  | 1:C:164:ASP:HA   | 1.83                     | 0.44              |
| 1:D:67:MET:HE1   | 1:D:73:PHE:HB3   | 1.92                     | 0.44              |
| 1:E:6:THR:HG21   | 1:E:89:HIS:HE2   | 1.82                     | 0.44              |
| 1:H:132:ALA:O    | 1:H:135:PRO:HD3  | 2.16                     | 0.44              |
| 1:H:35:GLN:NE2   | 1:H:201:VAL:HG11 | 2.32                     | 0.44              |
| 1:K:187:LEU:HG   | 1:K:188:ALA:N    | 2.30                     | 0.44              |
| 1:D:159:ASN:ND2  | 1:F:159:ASN:CG   | 2.70                     | 0.44              |
| 1:G:171:PHE:HA   | 1:G:188:ALA:O    | 2.17                     | 0.44              |
| 1:H:155:SER:HB3  | 1:I:36:THR:HB    | 1.98                     | 0.44              |
| 1:G:106:TRP:HB3  | 1:G:142:MET:HE3  | 2.00                     | 0.44              |
| 1:I:94:VAL:N     | 1:I:103:SER:O    | 2.38                     | 0.44              |
| 1:J:124:VAL:O    | 1:J:128:GLY:HA2  | 2.18                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:59:PHE:O    | 1:J:60:ILE:C     | 2.55                     | 0.44              |
| 1:E:139:ILE:N   | 1:E:142:MET:HE3  | 2.18                     | 0.44              |
| 1:F:59:PHE:O    | 1:F:60:ILE:C     | 2.55                     | 0.44              |
| 1:H:57:PRO:HG3  | 1:H:120:TYR:CZ   | 2.53                     | 0.44              |
| 1:H:67:MET:CE   | 1:H:73:PHE:CB    | 2.73                     | 0.44              |
| 1:L:130:ASN:HB2 | 1:L:135:PRO:HB3  | 2.00                     | 0.44              |
| 1:L:25:PHE:HB2  | 1:L:194:ALA:HA   | 2.00                     | 0.44              |
| 1:A:159:ASN:OD1 | 1:B:159:ASN:ND2  | 2.47                     | 0.44              |
| 1:A:30:GLN:HE22 | 1:A:164:ASP:HA   | 1.82                     | 0.44              |
| 1:C:63:LEU:HD23 | 1:C:208:LEU:HD13 | 1.99                     | 0.44              |
| 1:G:38:GLN:NE2  | 1:G:177:TYR:OH   | 2.50                     | 0.44              |
| 1:H:34:ASN:ND2  | 1:H:158:LEU:H    | 2.15                     | 0.44              |
| 1:D:163:MET:HG2 | 1:D:163:MET:H    | 1.61                     | 0.44              |
| 1:D:185:MET:HA  | 1:D:186:PRO:HD3  | 1.75                     | 0.44              |
| 1:D:20:GLU:OE1  | 1:F:133:TYR:N    | 2.42                     | 0.44              |
| 1:I:149:PRO:HD2 | 1:I:150:TRP:CE3  | 2.52                     | 0.44              |
| 1:I:77:MET:CE   | 1:I:82:LEU:HB2   | 2.47                     | 0.44              |
| 1:K:66:LEU:HD23 | 1:K:66:LEU:HA    | 1.71                     | 0.44              |
| 1:K:72:GLU:HG2  | 1:K:73:PHE:H     | 1.83                     | 0.44              |
| 1:E:4:LYS:HB3   | 1:E:4:LYS:HE3    | 1.30                     | 0.44              |
| 1:K:59:PHE:O    | 1:K:60:ILE:C     | 2.56                     | 0.44              |
| 1:G:159:ASN:CG  | 1:H:159:ASN:ND2  | 2.72                     | 0.43              |
| 1:G:85:TRP:CH2  | 1:G:140:GLU:HG3  | 2.53                     | 0.43              |
| 1:I:192:HIS:HD1 | 1:I:194:ALA:H    | 1.64                     | 0.43              |
| 1:G:29:ALA:O    | 1:G:30:GLN:C     | 2.56                     | 0.43              |
| 1:L:92:TYR:HA   | 1:L:145:VAL:O    | 2.18                     | 0.43              |
| 1:B:66:LEU:O    | 1:B:67:MET:C     | 2.50                     | 0.43              |
| 1:D:85:TRP:CZ2  | 1:D:140:GLU:HB3  | 2.53                     | 0.43              |
| 1:D:85:TRP:CG   | 1:D:141:ASN:HB3  | 2.53                     | 0.43              |
| 1:H:156:PHE:CD2 | 1:H:157:ASP:N    | 2.85                     | 0.43              |
| 1:J:32:THR:HG22 | 1:J:163:MET:SD   | 2.59                     | 0.43              |
| 1:C:203:ARG:O   | 1:C:207:GLU:HG3  | 2.18                     | 0.43              |
| 1:E:77:MET:HE3  | 1:E:77:MET:HB2   | 1.52                     | 0.43              |
| 1:G:15:GLN:HA   | 1:G:15:GLN:NE2   | 2.25                     | 0.43              |
| 1:H:210:GLN:O   | 1:H:211:TYR:C    | 2.57                     | 0.43              |
| 1:I:91:CYS:HA   | 1:I:105:LEU:O    | 2.19                     | 0.43              |
| 1:D:168:ALA:HA  | 1:D:169:PRO:HD3  | 1.79                     | 0.43              |
| 1:G:30:GLN:HG2  | 1:G:163:MET:SD   | 2.58                     | 0.43              |
| 1:H:168:ALA:HA  | 1:H:169:PRO:HD3  | 1.88                     | 0.43              |
| 1:I:4:LYS:HB3   | 1:I:5:ILE:HD13   | 2.01                     | 0.43              |
| 1:I:6:THR:CG2   | 1:I:6:THR:N      | 2.81                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:59:PHE:CD2   | 1:J:173:MET:HE1  | 2.53                     | 0.43              |
| 1:L:92:TYR:CD1   | 1:L:92:TYR:O     | 2.72                     | 0.43              |
| 1:G:50:LYS:HA    | 1:G:50:LYS:HD2   | 1.68                     | 0.43              |
| 1:B:47:THR:HG21  | 1:B:215:TRP:O    | 2.19                     | 0.43              |
| 1:C:38:GLN:HE22  | 1:C:186:PRO:HG3  | 1.83                     | 0.43              |
| 1:H:45:LEU:HD23  | 1:H:45:LEU:HA    | 1.91                     | 0.43              |
| 1:H:67:MET:CE    | 1:H:73:PHE:CG    | 3.02                     | 0.43              |
| 1:J:18:ARG:NH2   | 1:J:193:HIS:O    | 2.52                     | 0.43              |
| 1:J:22:PHE:O     | 1:J:26:GLN:N     | 2.47                     | 0.43              |
| 1:L:57:PRO:HG2   | 1:L:58:ALA:H     | 1.81                     | 0.43              |
| 1:C:27:SER:OG    | 1:C:28:VAL:N     | 2.45                     | 0.43              |
| 1:C:56:TYR:N     | 1:C:57:PRO:CD    | 2.81                     | 0.43              |
| 1:C:70:HIS:HB3   | 1:C:72:GLU:OE1   | 2.19                     | 0.43              |
| 1:D:159:ASN:ND2  | 1:F:159:ASN:ND2  | 2.67                     | 0.43              |
| 1:H:25:PHE:CZ    | 1:H:193:HIS:CE1  | 3.06                     | 0.43              |
| 1:D:187:LEU:HD22 | 1:D:208:LEU:CD2  | 2.48                     | 0.43              |
| 1:F:38:GLN:NE2   | 1:F:177:TYR:OH   | 2.51                     | 0.43              |
| 1:H:63:LEU:O     | 1:H:67:MET:HG2   | 2.18                     | 0.43              |
| 1:J:171:PHE:CE2  | 1:J:204:MET:CE   | 3.01                     | 0.43              |
| 1:K:67:MET:HG3   | 1:K:143:PHE:CD2  | 2.54                     | 0.43              |
| 1:L:56:TYR:HB3   | 1:L:57:PRO:CD    | 2.49                     | 0.43              |
| 1:B:112:ASP:HB3  | 1:B:115:GLN:HB2  | 1.99                     | 0.43              |
| 1:G:40:ASP:HA    | 1:G:184:LEU:HD23 | 2.01                     | 0.43              |
| 1:L:206:ASN:O    | 1:L:210:GLN:HB2  | 2.19                     | 0.43              |
| 1:L:66:LEU:HD21  | 1:L:211:TYR:CE2  | 2.51                     | 0.43              |
| 1:C:105:LEU:HA   | 1:C:105:LEU:HD23 | 1.89                     | 0.42              |
| 1:H:25:PHE:HB2   | 1:H:194:ALA:CA   | 2.48                     | 0.42              |
| 1:J:57:PRO:HB3   | 1:J:120:TYR:CD2  | 2.54                     | 0.42              |
| 1:L:67:MET:HE1   | 1:L:169:PRO:CG   | 2.42                     | 0.42              |
| 1:C:19:LYS:HE2   | 1:C:23:GLU:OE2   | 2.19                     | 0.42              |
| 1:C:25:PHE:O     | 1:C:30:GLN:HG3   | 2.18                     | 0.42              |
| 1:D:93:THR:HA    | 1:D:103:SER:O    | 2.19                     | 0.42              |
| 1:L:47:THR:HA    | 1:L:50:LYS:HD3   | 2.01                     | 0.42              |
| 1:C:66:LEU:HD11  | 1:C:208:LEU:HA   | 2.01                     | 0.42              |
| 1:C:89:HIS:O     | 1:C:142:MET:HA   | 2.19                     | 0.42              |
| 1:D:59:PHE:CD2   | 1:D:173:MET:CE   | 3.02                     | 0.42              |
| 1:D:42:THR:OG1   | 1:D:182:LYS:HA   | 2.20                     | 0.42              |
| 1:E:147:ALA:C    | 1:E:149:PRO:HD3  | 2.39                     | 0.42              |
| 1:I:57:PRO:HB3   | 1:I:120:TYR:CE2  | 2.55                     | 0.42              |
| 1:J:59:PHE:HD2   | 1:J:173:MET:CE   | 2.32                     | 0.42              |
| 1:A:28:VAL:HG23  | 1:A:29:ALA:H     | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:133:TYR:CE2  | 1:D:134:PHE:HE1  | 2.37                     | 0.42              |
| 1:D:50:LYS:C     | 1:D:51:ASN:O     | 2.56                     | 0.42              |
| 1:G:25:PHE:HB2   | 1:G:194:ALA:HA   | 2.01                     | 0.42              |
| 1:H:34:ASN:HD21  | 1:H:158:LEU:H    | 1.67                     | 0.42              |
| 1:A:190:GLN:CG   | 1:A:190:GLN:O    | 2.66                     | 0.42              |
| 1:C:56:TYR:CE1   | 1:C:173:MET:CE   | 3.02                     | 0.42              |
| 1:D:29:ALA:O     | 1:D:30:GLN:C     | 2.57                     | 0.42              |
| 1:I:132:ALA:O    | 1:I:135:PRO:HD3  | 2.20                     | 0.42              |
| 1:I:6:THR:CG2    | 1:I:141:ASN:ND2  | 2.67                     | 0.42              |
| 1:K:176:TYR:HA   | 1:K:184:LEU:O    | 2.19                     | 0.42              |
| 1:K:73:PHE:CZ    | 1:K:204:MET:HB2  | 2.54                     | 0.42              |
| 1:L:158:LEU:HB3  | 1:L:190:GLN:HG3  | 2.02                     | 0.42              |
| 1:A:56:TYR:H     | 1:A:57:PRO:HD2   | 1.84                     | 0.42              |
| 1:F:56:TYR:HB3   | 1:F:57:PRO:HD3   | 2.01                     | 0.42              |
| 1:G:56:TYR:HB3   | 1:G:57:PRO:CD    | 2.49                     | 0.42              |
| 1:J:154:THR:O    | 1:L:154:THR:CG2  | 2.58                     | 0.42              |
| 1:J:34:ASN:HB2   | 1:L:157:ASP:HB2  | 2.01                     | 0.42              |
| 1:E:34:ASN:ND2   | 1:E:190:GLN:CB   | 2.77                     | 0.42              |
| 1:H:35:GLN:O     | 1:H:188:ALA:HA   | 2.19                     | 0.42              |
| 1:B:100:GLU:HG2  | 1:C:199:PHE:CE1  | 2.55                     | 0.42              |
| 1:L:197:ASP:O    | 1:L:201:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:106:TRP:HB3  | 1:A:142:MET:HE2  | 2.01                     | 0.42              |
| 1:E:120:TYR:CD2  | 1:E:120:TYR:C    | 2.93                     | 0.42              |
| 1:F:204:MET:HE2  | 1:F:205:LEU:N    | 2.35                     | 0.42              |
| 1:G:184:LEU:HD23 | 1:G:184:LEU:HA   | 1.71                     | 0.42              |
| 1:G:32:THR:HG22  | 1:I:159:ASN:CB   | 2.20                     | 0.42              |
| 1:K:122:GLN:HG3  | 1:K:122:GLN:O    | 2.19                     | 0.42              |
| 1:D:117:LEU:HD23 | 1:D:117:LEU:HA   | 1.96                     | 0.41              |
| 1:F:25:PHE:O     | 1:F:30:GLN:HA    | 2.19                     | 0.41              |
| 1:J:132:ALA:O    | 1:J:135:PRO:HD3  | 2.19                     | 0.41              |
| 1:L:22:PHE:O     | 1:L:26:GLN:HG2   | 2.19                     | 0.41              |
| 1:G:156:PHE:C    | 1:G:156:PHE:CD2  | 2.93                     | 0.41              |
| 1:I:145:VAL:HG11 | 1:I:173:MET:HE2  | 2.01                     | 0.41              |
| 1:L:105:LEU:HD21 | 1:L:127:TYR:HB2  | 2.02                     | 0.41              |
| 1:L:70:HIS:NE2   | 1:L:207:GLU:OE1  | 2.47                     | 0.41              |
| 1:K:57:PRO:HB3   | 1:K:120:TYR:CD2  | 2.56                     | 0.41              |
| 1:D:182:LYS:HZ3  | 1:D:182:LYS:HG3  | 1.46                     | 0.41              |
| 1:K:59:PHE:CD2   | 1:K:173:MET:CE   | 3.03                     | 0.41              |
| 1:L:205:LEU:HD23 | 1:L:205:LEU:HA   | 1.96                     | 0.41              |
| 1:D:114:ARG:CG   | 1:D:114:ARG:NH1  | 2.83                     | 0.41              |
| 1:D:85:TRP:CD2   | 1:D:141:ASN:HB3  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:165:ASN:HA   | 1:E:167:PHE:CE1  | 2.55                     | 0.41              |
| 1:F:153:PHE:O    | 1:F:186:PRO:HB3  | 2.21                     | 0.41              |
| 1:G:139:ILE:HG13 | 1:G:142:MET:HG3  | 2.02                     | 0.41              |
| 1:K:89:HIS:O     | 1:K:142:MET:HA   | 2.20                     | 0.41              |
| 1:A:90:PRO:O     | 1:A:106:TRP:HA   | 2.21                     | 0.41              |
| 1:B:82:LEU:HD12  | 1:B:82:LEU:HA    | 1.81                     | 0.41              |
| 1:B:91:CYS:HA    | 1:B:105:LEU:O    | 2.21                     | 0.41              |
| 1:E:41:ILE:HG13  | 1:E:183:VAL:O    | 2.19                     | 0.41              |
| 1:E:66:LEU:HD23  | 1:E:66:LEU:HA    | 1.89                     | 0.41              |
| 1:G:118:HIS:O    | 1:G:122:GLN:HG3  | 2.21                     | 0.41              |
| 1:I:120:TYR:O    | 1:I:123:ASP:HB2  | 2.21                     | 0.41              |
| 1:J:162:ASN:HB3  | 2:K:221:HOH:O    | 2.20                     | 0.41              |
| 1:K:92:TYR:N     | 1:K:92:TYR:CD2   | 2.88                     | 0.41              |
| 1:A:38:GLN:HE22  | 1:A:186:PRO:HG3  | 1.86                     | 0.41              |
| 1:C:25:PHE:HB2   | 1:C:194:ALA:HA   | 2.03                     | 0.41              |
| 1:F:151:VAL:HG12 | 1:F:151:VAL:O    | 2.21                     | 0.41              |
| 1:L:171:PHE:CZ   | 1:L:189:ILE:HD13 | 2.55                     | 0.41              |
| 1:B:154:THR:CG2  | 1:C:154:THR:O    | 2.65                     | 0.41              |
| 1:F:72:GLU:HG3   | 1:F:200:HIS:HB3  | 2.03                     | 0.41              |
| 1:H:154:THR:HG22 | 1:I:154:THR:O    | 2.21                     | 0.41              |
| 1:J:8:TYR:CD1    | 1:J:83:VAL:HG21  | 2.55                     | 0.41              |
| 1:L:118:HIS:O    | 1:L:119:ILE:CB   | 2.69                     | 0.41              |
| 1:I:59:PHE:CD2   | 1:I:173:MET:CE   | 3.03                     | 0.41              |
| 1:I:89:HIS:ND1   | 1:I:108:GLU:HA   | 2.36                     | 0.41              |
| 1:L:67:MET:HE3   | 1:L:73:PHE:CB    | 2.31                     | 0.41              |
| 1:C:67:MET:CE    | 1:C:73:PHE:CD2   | 2.94                     | 0.41              |
| 1:E:65:ARG:NH2   | 2:E:230:HOH:O    | 2.53                     | 0.41              |
| 1:K:57:PRO:HA    | 1:K:60:ILE:HD12  | 2.02                     | 0.41              |
| 1:B:204:MET:HE3  | 1:B:204:MET:O    | 2.21                     | 0.41              |
| 1:C:204:MET:HE2  | 1:C:205:LEU:HD23 | 2.02                     | 0.41              |
| 1:E:64:ALA:HB1   | 1:E:109:TYR:CD1  | 2.56                     | 0.41              |
| 1:F:204:MET:CE   | 1:F:205:LEU:HA   | 2.50                     | 0.41              |
| 1:I:26:GLN:HA    | 1:I:26:GLN:HE21  | 1.86                     | 0.41              |
| 1:A:27:SER:OG    | 1:A:28:VAL:HG22  | 2.20                     | 0.40              |
| 1:B:119:ILE:O    | 1:B:120:TYR:C    | 2.59                     | 0.40              |
| 1:B:18:ARG:NE    | 1:B:197:ASP:OD1  | 2.46                     | 0.40              |
| 1:E:38:GLN:NE2   | 1:E:177:TYR:OH   | 2.54                     | 0.40              |
| 1:G:56:TYR:HB3   | 1:G:57:PRO:HD3   | 2.03                     | 0.40              |
| 1:H:91:CYS:SG    | 1:H:142:MET:CE   | 3.07                     | 0.40              |
| 1:I:138:PHE:C    | 1:I:142:MET:CE   | 2.82                     | 0.40              |
| 1:G:159:ASN:HD21 | 1:I:159:ASN:HD21 | 1.68                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:109:TYR:O    | 1:B:110:HIS:CD2  | 2.74                     | 0.40              |
| 1:F:106:TRP:HB3  | 1:F:142:MET:HE2  | 2.03                     | 0.40              |
| 1:F:168:ALA:HA   | 1:F:169:PRO:HD3  | 1.93                     | 0.40              |
| 1:J:136:LYS:NZ   | 2:J:223:HOH:O    | 2.54                     | 0.40              |
| 1:K:168:ALA:HA   | 1:K:169:PRO:HD3  | 1.96                     | 0.40              |
| 1:L:134:PHE:O    | 1:L:136:LYS:N    | 2.55                     | 0.40              |
| 1:A:187:LEU:HD23 | 1:A:208:LEU:CD2  | 2.51                     | 0.40              |
| 1:B:25:PHE:HB2   | 1:B:194:ALA:HA   | 2.02                     | 0.40              |
| 1:J:67:MET:CE    | 1:J:73:PHE:CD1   | 3.04                     | 0.40              |
| 1:K:154:THR:HG22 | 1:L:36:THR:CB    | 2.52                     | 0.40              |
| 1:K:75:MET:HB2   | 1:K:195:VAL:HG11 | 2.03                     | 0.40              |
| 1:A:63:LEU:O     | 1:A:67:MET:HG2   | 2.21                     | 0.40              |
| 1:A:8:TYR:HB2    | 1:A:83:VAL:HG13  | 2.04                     | 0.40              |
| 1:B:204:MET:HE3  | 1:B:205:LEU:HA   | 2.02                     | 0.40              |
| 1:D:114:ARG:NH1  | 1:D:114:ARG:HG3  | 2.36                     | 0.40              |
| 1:F:123:ASP:OD1  | 1:F:136:LYS:HE3  | 2.21                     | 0.40              |
| 1:K:185:MET:HA   | 1:K:186:PRO:HD3  | 1.97                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 211/219 (96%) | 203 (96%) | 7 (3%)  | 1 (0%)   | 29          | 48 |
| 1   | B     | 214/219 (98%) | 204 (95%) | 8 (4%)  | 2 (1%)   | 17          | 31 |
| 1   | C     | 211/219 (96%) | 200 (95%) | 8 (4%)  | 3 (1%)   | 11          | 20 |
| 1   | D     | 211/219 (96%) | 196 (93%) | 12 (6%) | 3 (1%)   | 11          | 20 |
| 1   | E     | 213/219 (97%) | 199 (93%) | 12 (6%) | 2 (1%)   | 17          | 31 |
| 1   | F     | 210/219 (96%) | 195 (93%) | 14 (7%) | 1 (0%)   | 29          | 48 |
| 1   | G     | 211/219 (96%) | 196 (93%) | 14 (7%) | 1 (0%)   | 29          | 48 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | H     | 214/219 (98%)   | 204 (95%)  | 8 (4%)   | 2 (1%)   | 17          | 31 |
| 1   | I     | 212/219 (97%)   | 199 (94%)  | 11 (5%)  | 2 (1%)   | 17          | 31 |
| 1   | J     | 209/219 (95%)   | 191 (91%)  | 16 (8%)  | 2 (1%)   | 15          | 28 |
| 1   | K     | 210/219 (96%)   | 195 (93%)  | 10 (5%)  | 5 (2%)   | 6           | 9  |
| 1   | L     | 208/219 (95%)   | 188 (90%)  | 16 (8%)  | 4 (2%)   | 8           | 13 |
| All | All   | 2534/2628 (96%) | 2370 (94%) | 136 (5%) | 28 (1%)  | 14          | 26 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | VAL  |
| 1   | B     | 79  | ASP  |
| 1   | D     | 164 | ASP  |
| 1   | K     | 48  | VAL  |
| 1   | L     | 119 | ILE  |
| 1   | B     | 28  | VAL  |
| 1   | C     | 29  | ALA  |
| 1   | E     | 4   | LYS  |
| 1   | E     | 29  | ALA  |
| 1   | K     | 166 | PHE  |
| 1   | L     | 128 | GLY  |
| 1   | C     | 50  | LYS  |
| 1   | D     | 50  | LYS  |
| 1   | H     | 6   | THR  |
| 1   | H     | 52  | LYS  |
| 1   | K     | 29  | ALA  |
| 1   | I     | 29  | ALA  |
| 1   | K     | 47  | THR  |
| 1   | K     | 165 | ASN  |
| 1   | D     | 180 | GLY  |
| 1   | G     | 19  | LYS  |
| 1   | J     | 72  | GLU  |
| 1   | F     | 198 | GLY  |
| 1   | L     | 129 | GLU  |
| 1   | I     | 135 | PRO  |
| 1   | J     | 13  | ILE  |
| 1   | L     | 80  | GLY  |
| 1   | C     | 28  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 189/194 (97%)   | 160 (85%)  | 29 (15%)  | 2           | 5  |
| 1   | B     | 192/194 (99%)   | 163 (85%)  | 29 (15%)  | 3           | 5  |
| 1   | C     | 189/194 (97%)   | 163 (86%)  | 26 (14%)  | 3           | 6  |
| 1   | D     | 189/194 (97%)   | 162 (86%)  | 27 (14%)  | 3           | 6  |
| 1   | E     | 192/194 (99%)   | 161 (84%)  | 31 (16%)  | 2           | 4  |
| 1   | F     | 189/194 (97%)   | 161 (85%)  | 28 (15%)  | 3           | 5  |
| 1   | G     | 189/194 (97%)   | 164 (87%)  | 25 (13%)  | 4           | 7  |
| 1   | H     | 191/194 (98%)   | 171 (90%)  | 20 (10%)  | 7           | 13 |
| 1   | I     | 191/194 (98%)   | 163 (85%)  | 28 (15%)  | 3           | 5  |
| 1   | J     | 189/194 (97%)   | 158 (84%)  | 31 (16%)  | 2           | 4  |
| 1   | K     | 190/194 (98%)   | 150 (79%)  | 40 (21%)  | 1           | 2  |
| 1   | L     | 188/194 (97%)   | 154 (82%)  | 34 (18%)  | 1           | 3  |
| All | All   | 2278/2328 (98%) | 1930 (85%) | 348 (15%) | 2           | 5  |

All (348) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | GLN  |
| 1   | A     | 28  | VAL  |
| 1   | A     | 32  | THR  |
| 1   | A     | 37  | VAL  |
| 1   | A     | 39  | LEU  |
| 1   | A     | 45  | LEU  |
| 1   | A     | 52  | LYS  |
| 1   | A     | 54  | LYS  |
| 1   | A     | 81  | GLU  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 94  | VAL  |
| 1   | A     | 97  | GLU  |
| 1   | A     | 114 | ARG  |
| 1   | A     | 135 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 136 | LYS  |
| 1   | A     | 140 | GLU  |
| 1   | A     | 142 | MET  |
| 1   | A     | 146 | SER  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 154 | THR  |
| 1   | A     | 160 | VAL  |
| 1   | A     | 173 | MET  |
| 1   | A     | 175 | LYS  |
| 1   | A     | 182 | LYS  |
| 1   | A     | 189 | ILE  |
| 1   | A     | 190 | GLN  |
| 1   | A     | 196 | CYS  |
| 1   | A     | 204 | MET  |
| 1   | A     | 211 | TYR  |
| 1   | B     | 5   | ILE  |
| 1   | B     | 9   | THR  |
| 1   | B     | 10  | THR  |
| 1   | B     | 19  | LYS  |
| 1   | B     | 28  | VAL  |
| 1   | B     | 32  | THR  |
| 1   | B     | 37  | VAL  |
| 1   | B     | 39  | LEU  |
| 1   | B     | 45  | LEU  |
| 1   | B     | 49  | LYS  |
| 1   | B     | 50  | LYS  |
| 1   | B     | 83  | VAL  |
| 1   | B     | 87  | SER  |
| 1   | B     | 94  | VAL  |
| 1   | B     | 104 | SER  |
| 1   | B     | 111 | ASP  |
| 1   | B     | 114 | ARG  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 129 | GLU  |
| 1   | B     | 140 | GLU  |
| 1   | B     | 154 | THR  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 159 | ASN  |
| 1   | B     | 160 | VAL  |
| 1   | B     | 175 | LYS  |
| 1   | B     | 187 | LEU  |
| 1   | B     | 189 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 190 | GLN  |
| 1   | B     | 204 | MET  |
| 1   | C     | 6   | THR  |
| 1   | C     | 9   | THR  |
| 1   | C     | 13  | ILE  |
| 1   | C     | 23  | GLU  |
| 1   | C     | 27  | SER  |
| 1   | C     | 32  | THR  |
| 1   | C     | 39  | LEU  |
| 1   | C     | 45  | LEU  |
| 1   | C     | 50  | LYS  |
| 1   | C     | 54  | LYS  |
| 1   | C     | 62  | ILE  |
| 1   | C     | 111 | ASP  |
| 1   | C     | 114 | ARG  |
| 1   | C     | 115 | GLN  |
| 1   | C     | 117 | LEU  |
| 1   | C     | 126 | CYS  |
| 1   | C     | 139 | ILE  |
| 1   | C     | 154 | THR  |
| 1   | C     | 155 | SER  |
| 1   | C     | 158 | LEU  |
| 1   | C     | 162 | ASN  |
| 1   | C     | 179 | GLN  |
| 1   | C     | 182 | LYS  |
| 1   | C     | 190 | GLN  |
| 1   | C     | 204 | MET  |
| 1   | C     | 216 | GLN  |
| 1   | D     | 8   | TYR  |
| 1   | D     | 9   | THR  |
| 1   | D     | 13  | ILE  |
| 1   | D     | 15  | GLN  |
| 1   | D     | 19  | LYS  |
| 1   | D     | 28  | VAL  |
| 1   | D     | 32  | THR  |
| 1   | D     | 39  | LEU  |
| 1   | D     | 45  | LEU  |
| 1   | D     | 54  | LYS  |
| 1   | D     | 71  | PRO  |
| 1   | D     | 77  | MET  |
| 1   | D     | 81  | GLU  |
| 1   | D     | 83  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 111 | ASP  |
| 1   | D     | 114 | ARG  |
| 1   | D     | 117 | LEU  |
| 1   | D     | 148 | ASN  |
| 1   | D     | 152 | SER  |
| 1   | D     | 154 | THR  |
| 1   | D     | 155 | SER  |
| 1   | D     | 160 | VAL  |
| 1   | D     | 163 | MET  |
| 1   | D     | 164 | ASP  |
| 1   | D     | 189 | ILE  |
| 1   | D     | 190 | GLN  |
| 1   | D     | 193 | HIS  |
| 1   | E     | 3   | LYS  |
| 1   | E     | 4   | LYS  |
| 1   | E     | 5   | ILE  |
| 1   | E     | 6   | THR  |
| 1   | E     | 9   | THR  |
| 1   | E     | 10  | THR  |
| 1   | E     | 15  | GLN  |
| 1   | E     | 19  | LYS  |
| 1   | E     | 20  | GLU  |
| 1   | E     | 32  | THR  |
| 1   | E     | 37  | VAL  |
| 1   | E     | 39  | LEU  |
| 1   | E     | 45  | LEU  |
| 1   | E     | 54  | LYS  |
| 1   | E     | 81  | GLU  |
| 1   | E     | 83  | VAL  |
| 1   | E     | 98  | GLN  |
| 1   | E     | 108 | GLU  |
| 1   | E     | 114 | ARG  |
| 1   | E     | 115 | GLN  |
| 1   | E     | 117 | LEU  |
| 1   | E     | 120 | TYR  |
| 1   | E     | 129 | GLU  |
| 1   | E     | 136 | LYS  |
| 1   | E     | 138 | PHE  |
| 1   | E     | 142 | MET  |
| 1   | E     | 154 | THR  |
| 1   | E     | 158 | LEU  |
| 1   | E     | 187 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 189 | ILE  |
| 1   | E     | 190 | GLN  |
| 1   | F     | 9   | THR  |
| 1   | F     | 12  | ASP  |
| 1   | F     | 15  | GLN  |
| 1   | F     | 19  | LYS  |
| 1   | F     | 32  | THR  |
| 1   | F     | 37  | VAL  |
| 1   | F     | 39  | LEU  |
| 1   | F     | 45  | LEU  |
| 1   | F     | 50  | LYS  |
| 1   | F     | 52  | LYS  |
| 1   | F     | 54  | LYS  |
| 1   | F     | 62  | ILE  |
| 1   | F     | 77  | MET  |
| 1   | F     | 83  | VAL  |
| 1   | F     | 114 | ARG  |
| 1   | F     | 115 | GLN  |
| 1   | F     | 117 | LEU  |
| 1   | F     | 119 | ILE  |
| 1   | F     | 121 | SER  |
| 1   | F     | 136 | LYS  |
| 1   | F     | 148 | ASN  |
| 1   | F     | 151 | VAL  |
| 1   | F     | 157 | ASP  |
| 1   | F     | 189 | ILE  |
| 1   | F     | 190 | GLN  |
| 1   | F     | 204 | MET  |
| 1   | F     | 212 | CYS  |
| 1   | F     | 215 | TRP  |
| 1   | G     | 9   | THR  |
| 1   | G     | 12  | ASP  |
| 1   | G     | 15  | GLN  |
| 1   | G     | 32  | THR  |
| 1   | G     | 35  | GLN  |
| 1   | G     | 39  | LEU  |
| 1   | G     | 45  | LEU  |
| 1   | G     | 48  | VAL  |
| 1   | G     | 50  | LYS  |
| 1   | G     | 52  | LYS  |
| 1   | G     | 54  | LYS  |
| 1   | G     | 67  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 78  | LYS  |
| 1   | G     | 111 | ASP  |
| 1   | G     | 115 | GLN  |
| 1   | G     | 119 | ILE  |
| 1   | G     | 146 | SER  |
| 1   | G     | 148 | ASN  |
| 1   | G     | 151 | VAL  |
| 1   | G     | 154 | THR  |
| 1   | G     | 158 | LEU  |
| 1   | G     | 160 | VAL  |
| 1   | G     | 181 | ASP  |
| 1   | G     | 190 | GLN  |
| 1   | G     | 204 | MET  |
| 1   | H     | 4   | LYS  |
| 1   | H     | 23  | GLU  |
| 1   | H     | 32  | THR  |
| 1   | H     | 37  | VAL  |
| 1   | H     | 39  | LEU  |
| 1   | H     | 45  | LEU  |
| 1   | H     | 50  | LYS  |
| 1   | H     | 52  | LYS  |
| 1   | H     | 54  | LYS  |
| 1   | H     | 62  | ILE  |
| 1   | H     | 83  | VAL  |
| 1   | H     | 87  | SER  |
| 1   | H     | 122 | GLN  |
| 1   | H     | 129 | GLU  |
| 1   | H     | 157 | ASP  |
| 1   | H     | 158 | LEU  |
| 1   | H     | 160 | VAL  |
| 1   | H     | 181 | ASP  |
| 1   | H     | 190 | GLN  |
| 1   | H     | 212 | CYS  |
| 1   | I     | 4   | LYS  |
| 1   | I     | 10  | THR  |
| 1   | I     | 14  | SER  |
| 1   | I     | 28  | VAL  |
| 1   | I     | 32  | THR  |
| 1   | I     | 39  | LEU  |
| 1   | I     | 45  | LEU  |
| 1   | I     | 46  | LYS  |
| 1   | I     | 52  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 54  | LYS  |
| 1   | I     | 62  | ILE  |
| 1   | I     | 81  | GLU  |
| 1   | I     | 83  | VAL  |
| 1   | I     | 97  | GLU  |
| 1   | I     | 105 | LEU  |
| 1   | I     | 112 | ASP  |
| 1   | I     | 114 | ARG  |
| 1   | I     | 115 | GLN  |
| 1   | I     | 117 | LEU  |
| 1   | I     | 126 | CYS  |
| 1   | I     | 136 | LYS  |
| 1   | I     | 139 | ILE  |
| 1   | I     | 146 | SER  |
| 1   | I     | 154 | THR  |
| 1   | I     | 157 | ASP  |
| 1   | I     | 158 | LEU  |
| 1   | I     | 160 | VAL  |
| 1   | I     | 190 | GLN  |
| 1   | J     | 9   | THR  |
| 1   | J     | 18  | ARG  |
| 1   | J     | 28  | VAL  |
| 1   | J     | 32  | THR  |
| 1   | J     | 35  | GLN  |
| 1   | J     | 39  | LEU  |
| 1   | J     | 45  | LEU  |
| 1   | J     | 50  | LYS  |
| 1   | J     | 56  | TYR  |
| 1   | J     | 67  | MET  |
| 1   | J     | 78  | LYS  |
| 1   | J     | 83  | VAL  |
| 1   | J     | 87  | SER  |
| 1   | J     | 94  | VAL  |
| 1   | J     | 98  | GLN  |
| 1   | J     | 107 | SER  |
| 1   | J     | 111 | ASP  |
| 1   | J     | 117 | LEU  |
| 1   | J     | 122 | GLN  |
| 1   | J     | 129 | GLU  |
| 1   | J     | 131 | LEU  |
| 1   | J     | 138 | PHE  |
| 1   | J     | 152 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 157 | ASP  |
| 1   | J     | 158 | LEU  |
| 1   | J     | 175 | LYS  |
| 1   | J     | 178 | THR  |
| 1   | J     | 181 | ASP  |
| 1   | J     | 182 | LYS  |
| 1   | J     | 190 | GLN  |
| 1   | J     | 215 | TRP  |
| 1   | K     | 4   | LYS  |
| 1   | K     | 9   | THR  |
| 1   | K     | 10  | THR  |
| 1   | K     | 12  | ASP  |
| 1   | K     | 14  | SER  |
| 1   | K     | 15  | GLN  |
| 1   | K     | 17  | HIS  |
| 1   | K     | 28  | VAL  |
| 1   | K     | 32  | THR  |
| 1   | K     | 37  | VAL  |
| 1   | K     | 39  | LEU  |
| 1   | K     | 45  | LEU  |
| 1   | K     | 46  | LYS  |
| 1   | K     | 52  | LYS  |
| 1   | K     | 54  | LYS  |
| 1   | K     | 77  | MET  |
| 1   | K     | 78  | LYS  |
| 1   | K     | 83  | VAL  |
| 1   | K     | 103 | SER  |
| 1   | K     | 105 | LEU  |
| 1   | K     | 108 | GLU  |
| 1   | K     | 114 | ARG  |
| 1   | K     | 117 | LEU  |
| 1   | K     | 122 | GLN  |
| 1   | K     | 126 | CYS  |
| 1   | K     | 136 | LYS  |
| 1   | K     | 140 | GLU  |
| 1   | K     | 142 | MET  |
| 1   | K     | 146 | SER  |
| 1   | K     | 151 | VAL  |
| 1   | K     | 154 | THR  |
| 1   | K     | 158 | LEU  |
| 1   | K     | 160 | VAL  |
| 1   | K     | 179 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 181 | ASP  |
| 1   | K     | 187 | LEU  |
| 1   | K     | 190 | GLN  |
| 1   | K     | 203 | ARG  |
| 1   | K     | 204 | MET  |
| 1   | K     | 210 | GLN  |
| 1   | L     | 6   | THR  |
| 1   | L     | 10  | THR  |
| 1   | L     | 15  | GLN  |
| 1   | L     | 19  | LYS  |
| 1   | L     | 27  | SER  |
| 1   | L     | 39  | LEU  |
| 1   | L     | 50  | LYS  |
| 1   | L     | 52  | LYS  |
| 1   | L     | 54  | LYS  |
| 1   | L     | 56  | TYR  |
| 1   | L     | 77  | MET  |
| 1   | L     | 78  | LYS  |
| 1   | L     | 79  | ASP  |
| 1   | L     | 83  | VAL  |
| 1   | L     | 94  | VAL  |
| 1   | L     | 97  | GLU  |
| 1   | L     | 100 | GLU  |
| 1   | L     | 104 | SER  |
| 1   | L     | 105 | LEU  |
| 1   | L     | 111 | ASP  |
| 1   | L     | 114 | ARG  |
| 1   | L     | 117 | LEU  |
| 1   | L     | 122 | GLN  |
| 1   | L     | 129 | GLU  |
| 1   | L     | 136 | LYS  |
| 1   | L     | 146 | SER  |
| 1   | L     | 151 | VAL  |
| 1   | L     | 154 | THR  |
| 1   | L     | 158 | LEU  |
| 1   | L     | 182 | LYS  |
| 1   | L     | 190 | GLN  |
| 1   | L     | 204 | MET  |
| 1   | L     | 210 | GLN  |
| 1   | L     | 214 | GLU  |

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     | 26  | GLN  |
| 1   | A     | 30  | GLN  |
| 1   | A     | 38  | GLN  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 159 | ASN  |
| 1   | B     | 26  | GLN  |
| 1   | B     | 34  | ASN  |
| 1   | B     | 38  | GLN  |
| 1   | B     | 159 | ASN  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 30  | GLN  |
| 1   | C     | 51  | ASN  |
| 1   | C     | 110 | HIS  |
| 1   | C     | 159 | ASN  |
| 1   | C     | 190 | GLN  |
| 1   | C     | 216 | GLN  |
| 1   | D     | 26  | GLN  |
| 1   | D     | 30  | GLN  |
| 1   | D     | 34  | ASN  |
| 1   | D     | 38  | GLN  |
| 1   | D     | 110 | HIS  |
| 1   | D     | 148 | ASN  |
| 1   | D     | 159 | ASN  |
| 1   | D     | 190 | GLN  |
| 1   | E     | 26  | GLN  |
| 1   | E     | 30  | GLN  |
| 1   | E     | 34  | ASN  |
| 1   | E     | 159 | ASN  |
| 1   | E     | 190 | GLN  |
| 1   | F     | 26  | GLN  |
| 1   | F     | 30  | GLN  |
| 1   | F     | 34  | ASN  |
| 1   | F     | 38  | GLN  |
| 1   | F     | 110 | HIS  |
| 1   | F     | 148 | ASN  |
| 1   | F     | 159 | ASN  |
| 1   | F     | 190 | GLN  |
| 1   | G     | 15  | GLN  |
| 1   | G     | 26  | GLN  |
| 1   | G     | 30  | GLN  |
| 1   | G     | 38  | GLN  |
| 1   | G     | 53  | HIS  |
| 1   | G     | 148 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 159 | ASN  |
| 1   | G     | 190 | GLN  |
| 1   | H     | 26  | GLN  |
| 1   | H     | 30  | GLN  |
| 1   | H     | 34  | ASN  |
| 1   | H     | 38  | GLN  |
| 1   | H     | 159 | ASN  |
| 1   | I     | 26  | GLN  |
| 1   | I     | 30  | GLN  |
| 1   | I     | 34  | ASN  |
| 1   | I     | 38  | GLN  |
| 1   | I     | 51  | ASN  |
| 1   | I     | 122 | GLN  |
| 1   | I     | 141 | ASN  |
| 1   | I     | 148 | ASN  |
| 1   | I     | 159 | ASN  |
| 1   | I     | 190 | GLN  |
| 1   | J     | 30  | GLN  |
| 1   | J     | 34  | ASN  |
| 1   | J     | 98  | GLN  |
| 1   | J     | 148 | ASN  |
| 1   | J     | 159 | ASN  |
| 1   | J     | 190 | GLN  |
| 1   | K     | 17  | HIS  |
| 1   | K     | 30  | GLN  |
| 1   | K     | 38  | GLN  |
| 1   | K     | 122 | GLN  |
| 1   | K     | 159 | ASN  |
| 1   | K     | 179 | GLN  |
| 1   | K     | 190 | GLN  |
| 1   | L     | 26  | GLN  |
| 1   | L     | 30  | GLN  |

### 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     | 213/219 (97%)   | -0.07  | 1 (0%) 91 91   | 21, 34, 50, 57        | 0     |
| 1   | B     | 216/219 (98%)   | -0.10  | 1 (0%) 91 91   | 23, 39, 59, 71        | 0     |
| 1   | C     | 213/219 (97%)   | 0.04   | 3 (1%) 75 77   | 24, 38, 62, 76        | 0     |
| 1   | D     | 213/219 (97%)   | 0.06   | 3 (1%) 75 77   | 27, 42, 60, 80        | 0     |
| 1   | E     | 215/219 (98%)   | 0.07   | 3 (1%) 75 77   | 30, 45, 64, 84        | 0     |
| 1   | F     | 212/219 (96%)   | 0.12   | 5 (2%) 59 62   | 29, 45, 62, 74        | 0     |
| 1   | G     | 213/219 (97%)   | 0.13   | 4 (1%) 66 69   | 31, 41, 59, 69        | 0     |
| 1   | H     | 216/219 (98%)   | 0.08   | 7 (3%) 47 51   | 19, 37, 52, 72        | 0     |
| 1   | I     | 214/219 (97%)   | 0.19   | 3 (1%) 75 77   | 32, 44, 62, 72        | 0     |
| 1   | J     | 211/219 (96%)   | 0.65   | 27 (12%) 3 3   | 38, 55, 77, 81        | 0     |
| 1   | K     | 212/219 (96%)   | 0.63   | 23 (10%) 5 5   | 43, 59, 76, 88        | 0     |
| 1   | L     | 210/219 (95%)   | 0.74   | 28 (13%) 3 2   | 40, 55, 74, 84        | 0     |
| All | All   | 2558/2628 (97%) | 0.21   | 108 (4%) 36 39 | 19, 44, 69, 88        | 0     |

All (108) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 124 | VAL  | 6.0  |
| 1   | J     | 125 | ALA  | 5.5  |
| 1   | H     | 5   | ILE  | 4.7  |
| 1   | J     | 6   | THR  | 4.5  |
| 1   | L     | 6   | THR  | 4.5  |
| 1   | J     | 46  | LYS  | 4.0  |
| 1   | G     | 15  | GLN  | 3.9  |
| 1   | K     | 158 | LEU  | 3.9  |
| 1   | L     | 15  | GLN  | 3.8  |
| 1   | L     | 115 | GLN  | 3.8  |
| 1   | K     | 215 | TRP  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 122 | GLN  | 3.7  |
| 1   | H     | 218 | GLY  | 3.5  |
| 1   | K     | 114 | ARG  | 3.5  |
| 1   | F     | 173 | MET  | 3.5  |
| 1   | K     | 98  | GLN  | 3.5  |
| 1   | L     | 113 | PHE  | 3.5  |
| 1   | L     | 181 | ASP  | 3.4  |
| 1   | L     | 125 | ALA  | 3.4  |
| 1   | L     | 118 | HIS  | 3.3  |
| 1   | L     | 131 | LEU  | 3.3  |
| 1   | K     | 50  | LYS  | 3.2  |
| 1   | J     | 43  | ALA  | 3.2  |
| 1   | L     | 114 | ARG  | 3.2  |
| 1   | D     | 46  | LYS  | 3.2  |
| 1   | J     | 181 | ASP  | 3.1  |
| 1   | F     | 77  | MET  | 3.1  |
| 1   | L     | 112 | ASP  | 3.0  |
| 1   | I     | 124 | VAL  | 3.0  |
| 1   | H     | 219 | ALA  | 3.0  |
| 1   | L     | 122 | GLN  | 3.0  |
| 1   | G     | 6   | THR  | 2.9  |
| 1   | F     | 211 | TYR  | 2.8  |
| 1   | G     | 98  | GLN  | 2.8  |
| 1   | C     | 118 | HIS  | 2.8  |
| 1   | J     | 50  | LYS  | 2.7  |
| 1   | L     | 23  | GLU  | 2.7  |
| 1   | L     | 71  | PRO  | 2.7  |
| 1   | J     | 14  | SER  | 2.7  |
| 1   | K     | 46  | LYS  | 2.7  |
| 1   | J     | 156 | PHE  | 2.6  |
| 1   | L     | 14  | SER  | 2.6  |
| 1   | K     | 22  | PHE  | 2.6  |
| 1   | J     | 15  | GLN  | 2.6  |
| 1   | L     | 188 | ALA  | 2.6  |
| 1   | L     | 89  | HIS  | 2.5  |
| 1   | H     | 6   | THR  | 2.5  |
| 1   | J     | 97  | GLU  | 2.5  |
| 1   | K     | 173 | MET  | 2.5  |
| 1   | L     | 179 | GLN  | 2.5  |
| 1   | J     | 34  | ASN  | 2.5  |
| 1   | J     | 180 | GLY  | 2.5  |
| 1   | L     | 45  | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 157 | ASP  | 2.4  |
| 1   | L     | 77  | MET  | 2.4  |
| 1   | K     | 15  | GLN  | 2.4  |
| 1   | H     | 154 | THR  | 2.4  |
| 1   | F     | 181 | ASP  | 2.4  |
| 1   | J     | 51  | ASN  | 2.4  |
| 1   | J     | 118 | HIS  | 2.4  |
| 1   | E     | 12  | ASP  | 2.4  |
| 1   | E     | 155 | SER  | 2.4  |
| 1   | A     | 181 | ASP  | 2.4  |
| 1   | L     | 189 | ILE  | 2.3  |
| 1   | J     | 95  | PHE  | 2.3  |
| 1   | J     | 138 | PHE  | 2.3  |
| 1   | J     | 99  | THR  | 2.3  |
| 1   | J     | 98  | GLN  | 2.3  |
| 1   | J     | 188 | ALA  | 2.3  |
| 1   | K     | 42  | THR  | 2.3  |
| 1   | L     | 130 | ASN  | 2.3  |
| 1   | K     | 211 | TYR  | 2.3  |
| 1   | H     | 155 | SER  | 2.3  |
| 1   | L     | 180 | GLY  | 2.3  |
| 1   | K     | 36  | THR  | 2.2  |
| 1   | K     | 17  | HIS  | 2.2  |
| 1   | K     | 180 | GLY  | 2.2  |
| 1   | L     | 50  | LYS  | 2.2  |
| 1   | C     | 115 | GLN  | 2.2  |
| 1   | D     | 217 | GLY  | 2.2  |
| 1   | J     | 121 | SER  | 2.2  |
| 1   | K     | 44  | PHE  | 2.2  |
| 1   | B     | 216 | GLN  | 2.2  |
| 1   | J     | 130 | ASN  | 2.2  |
| 1   | J     | 13  | ILE  | 2.2  |
| 1   | D     | 98  | GLN  | 2.1  |
| 1   | K     | 110 | HIS  | 2.1  |
| 1   | K     | 34  | ASN  | 2.1  |
| 1   | K     | 12  | ASP  | 2.1  |
| 1   | K     | 81  | GLU  | 2.1  |
| 1   | C     | 52  | LYS  | 2.1  |
| 1   | E     | 173 | MET  | 2.1  |
| 1   | H     | 15  | GLN  | 2.1  |
| 1   | K     | 127 | TYR  | 2.1  |
| 1   | L     | 8   | TYR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 201 | VAL  | 2.1  |
| 1   | K     | 48  | VAL  | 2.1  |
| 1   | L     | 172 | THR  | 2.1  |
| 1   | J     | 126 | CYS  | 2.1  |
| 1   | I     | 52  | LYS  | 2.1  |
| 1   | F     | 156 | PHE  | 2.0  |
| 1   | K     | 130 | ASN  | 2.0  |
| 1   | K     | 159 | ASN  | 2.0  |
| 1   | J     | 127 | TYR  | 2.0  |
| 1   | G     | 157 | ASP  | 2.0  |
| 1   | L     | 83  | VAL  | 2.0  |
| 1   | L     | 7   | GLY  | 2.0  |
| 1   | L     | 127 | TYR  | 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.