



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:18 PM UTC

PDB ID : 4Z7F / pdb\_00004z7f  
Title : Crystal structure of FolT bound with folic acid  
Authors : Zhao, Q.; Wang, C.C.; Wang, C.Y.; Zhang, P.  
Deposited on : 2015-04-07  
Resolution : 3.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

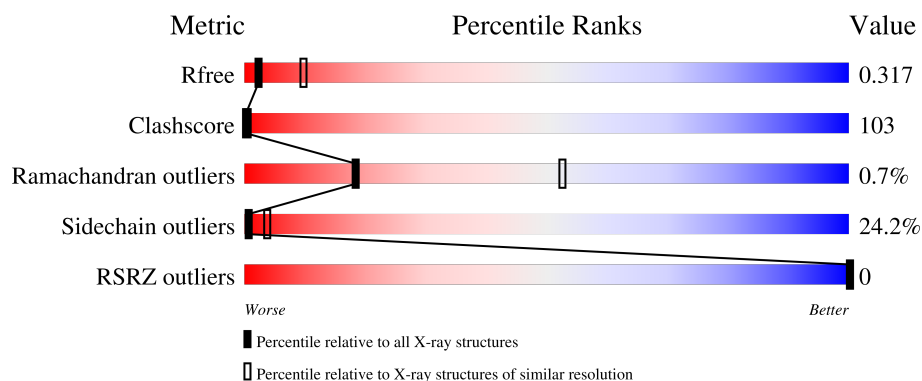
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 199    |                  |
| 1   | B     | 199    |                  |
| 1   | C     | 199    |                  |
| 1   | D     | 199    |                  |
| 1   | E     | 199    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | F     | 199    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | FOL  | A     | 201 | -         | -        | X       | -                |
| 2   | FOL  | B     | 201 | -         | -        | X       | -                |
| 2   | FOL  | D     | 201 | -         | -        | X       | -                |
| 2   | FOL  | E     | 201 | -         | -        | X       | -                |
| 2   | FOL  | F     | 201 | -         | -        | X       | -                |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7862 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 Folate ECF transporter.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1300  | 899 | 192 | 204 | 5 |         |         |       |
| 1   | B     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1341  | 927 | 197 | 212 | 5 |         |         |       |
| 1   | C     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1331  | 920 | 199 | 207 | 5 |         |         |       |
| 1   | D     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 919 | 196 | 210 | 5 |         |         |       |
| 1   | E     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1175  | 817 | 173 | 181 | 4 |         |         |       |
| 1   | F     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1193  | 827 | 175 | 186 | 5 |         |         |       |

There are 120 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -19     | MET      | -      | expression tag | UNP Q837A3 |
| A     | -18     | GLY      | -      | expression tag | UNP Q837A3 |
| A     | -17     | SER      | -      | expression tag | UNP Q837A3 |
| A     | -16     | SER      | -      | expression tag | UNP Q837A3 |
| A     | -15     | HIS      | -      | expression tag | UNP Q837A3 |
| A     | -14     | HIS      | -      | expression tag | UNP Q837A3 |
| A     | -13     | HIS      | -      | expression tag | UNP Q837A3 |
| A     | -12     | HIS      | -      | expression tag | UNP Q837A3 |
| A     | -11     | HIS      | -      | expression tag | UNP Q837A3 |
| A     | -10     | HIS      | -      | expression tag | UNP Q837A3 |
| A     | -9      | SER      | -      | expression tag | UNP Q837A3 |
| A     | -8      | SER      | -      | expression tag | UNP Q837A3 |
| A     | -7      | GLY      | -      | expression tag | UNP Q837A3 |
| A     | -6      | LEU      | -      | expression tag | UNP Q837A3 |
| A     | -5      | VAL      | -      | expression tag | UNP Q837A3 |
| A     | -4      | PRO      | -      | expression tag | UNP Q837A3 |
| A     | -3      | ARG      | -      | expression tag | UNP Q837A3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | GLY      | -      | expression tag | UNP Q837A3 |
| A     | -1      | SER      | -      | expression tag | UNP Q837A3 |
| A     | 0       | HIS      | -      | expression tag | UNP Q837A3 |
| B     | -19     | MET      | -      | expression tag | UNP Q837A3 |
| B     | -18     | GLY      | -      | expression tag | UNP Q837A3 |
| B     | -17     | SER      | -      | expression tag | UNP Q837A3 |
| B     | -16     | SER      | -      | expression tag | UNP Q837A3 |
| B     | -15     | HIS      | -      | expression tag | UNP Q837A3 |
| B     | -14     | HIS      | -      | expression tag | UNP Q837A3 |
| B     | -13     | HIS      | -      | expression tag | UNP Q837A3 |
| B     | -12     | HIS      | -      | expression tag | UNP Q837A3 |
| B     | -11     | HIS      | -      | expression tag | UNP Q837A3 |
| B     | -10     | HIS      | -      | expression tag | UNP Q837A3 |
| B     | -9      | SER      | -      | expression tag | UNP Q837A3 |
| B     | -8      | SER      | -      | expression tag | UNP Q837A3 |
| B     | -7      | GLY      | -      | expression tag | UNP Q837A3 |
| B     | -6      | LEU      | -      | expression tag | UNP Q837A3 |
| B     | -5      | VAL      | -      | expression tag | UNP Q837A3 |
| B     | -4      | PRO      | -      | expression tag | UNP Q837A3 |
| B     | -3      | ARG      | -      | expression tag | UNP Q837A3 |
| B     | -2      | GLY      | -      | expression tag | UNP Q837A3 |
| B     | -1      | SER      | -      | expression tag | UNP Q837A3 |
| B     | 0       | HIS      | -      | expression tag | UNP Q837A3 |
| C     | -19     | MET      | -      | expression tag | UNP Q837A3 |
| C     | -18     | GLY      | -      | expression tag | UNP Q837A3 |
| C     | -17     | SER      | -      | expression tag | UNP Q837A3 |
| C     | -16     | SER      | -      | expression tag | UNP Q837A3 |
| C     | -15     | HIS      | -      | expression tag | UNP Q837A3 |
| C     | -14     | HIS      | -      | expression tag | UNP Q837A3 |
| C     | -13     | HIS      | -      | expression tag | UNP Q837A3 |
| C     | -12     | HIS      | -      | expression tag | UNP Q837A3 |
| C     | -11     | HIS      | -      | expression tag | UNP Q837A3 |
| C     | -10     | HIS      | -      | expression tag | UNP Q837A3 |
| C     | -9      | SER      | -      | expression tag | UNP Q837A3 |
| C     | -8      | SER      | -      | expression tag | UNP Q837A3 |
| C     | -7      | GLY      | -      | expression tag | UNP Q837A3 |
| C     | -6      | LEU      | -      | expression tag | UNP Q837A3 |
| C     | -5      | VAL      | -      | expression tag | UNP Q837A3 |
| C     | -4      | PRO      | -      | expression tag | UNP Q837A3 |
| C     | -3      | ARG      | -      | expression tag | UNP Q837A3 |
| C     | -2      | GLY      | -      | expression tag | UNP Q837A3 |
| C     | -1      | SER      | -      | expression tag | UNP Q837A3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 0       | HIS      | -      | expression tag | UNP Q837A3 |
| D     | -19     | MET      | -      | expression tag | UNP Q837A3 |
| D     | -18     | GLY      | -      | expression tag | UNP Q837A3 |
| D     | -17     | SER      | -      | expression tag | UNP Q837A3 |
| D     | -16     | SER      | -      | expression tag | UNP Q837A3 |
| D     | -15     | HIS      | -      | expression tag | UNP Q837A3 |
| D     | -14     | HIS      | -      | expression tag | UNP Q837A3 |
| D     | -13     | HIS      | -      | expression tag | UNP Q837A3 |
| D     | -12     | HIS      | -      | expression tag | UNP Q837A3 |
| D     | -11     | HIS      | -      | expression tag | UNP Q837A3 |
| D     | -10     | HIS      | -      | expression tag | UNP Q837A3 |
| D     | -9      | SER      | -      | expression tag | UNP Q837A3 |
| D     | -8      | SER      | -      | expression tag | UNP Q837A3 |
| D     | -7      | GLY      | -      | expression tag | UNP Q837A3 |
| D     | -6      | LEU      | -      | expression tag | UNP Q837A3 |
| D     | -5      | VAL      | -      | expression tag | UNP Q837A3 |
| D     | -4      | PRO      | -      | expression tag | UNP Q837A3 |
| D     | -3      | ARG      | -      | expression tag | UNP Q837A3 |
| D     | -2      | GLY      | -      | expression tag | UNP Q837A3 |
| D     | -1      | SER      | -      | expression tag | UNP Q837A3 |
| D     | 0       | HIS      | -      | expression tag | UNP Q837A3 |
| E     | -19     | MET      | -      | expression tag | UNP Q837A3 |
| E     | -18     | GLY      | -      | expression tag | UNP Q837A3 |
| E     | -17     | SER      | -      | expression tag | UNP Q837A3 |
| E     | -16     | SER      | -      | expression tag | UNP Q837A3 |
| E     | -15     | HIS      | -      | expression tag | UNP Q837A3 |
| E     | -14     | HIS      | -      | expression tag | UNP Q837A3 |
| E     | -13     | HIS      | -      | expression tag | UNP Q837A3 |
| E     | -12     | HIS      | -      | expression tag | UNP Q837A3 |
| E     | -11     | HIS      | -      | expression tag | UNP Q837A3 |
| E     | -10     | HIS      | -      | expression tag | UNP Q837A3 |
| E     | -9      | SER      | -      | expression tag | UNP Q837A3 |
| E     | -8      | SER      | -      | expression tag | UNP Q837A3 |
| E     | -7      | GLY      | -      | expression tag | UNP Q837A3 |
| E     | -6      | LEU      | -      | expression tag | UNP Q837A3 |
| E     | -5      | VAL      | -      | expression tag | UNP Q837A3 |
| E     | -4      | PRO      | -      | expression tag | UNP Q837A3 |
| E     | -3      | ARG      | -      | expression tag | UNP Q837A3 |
| E     | -2      | GLY      | -      | expression tag | UNP Q837A3 |
| E     | -1      | SER      | -      | expression tag | UNP Q837A3 |
| E     | 0       | HIS      | -      | expression tag | UNP Q837A3 |
| F     | -19     | MET      | -      | expression tag | UNP Q837A3 |

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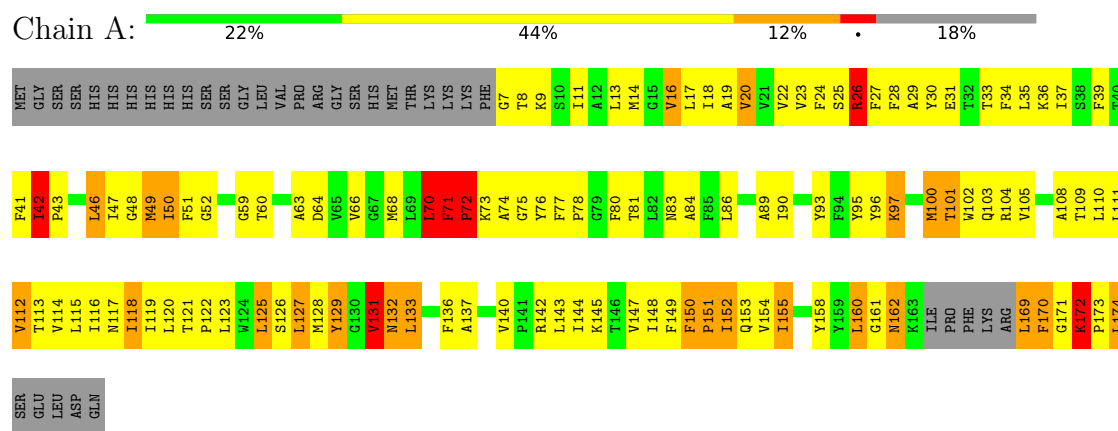
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 32    | 19 | 7 | 6 |         |         |
| 2   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 32    | 19 | 7 | 6 |         |         |
| 2   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 32    | 19 | 7 | 6 |         |         |
| 2   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 32    | 19 | 7 | 6 |         |         |



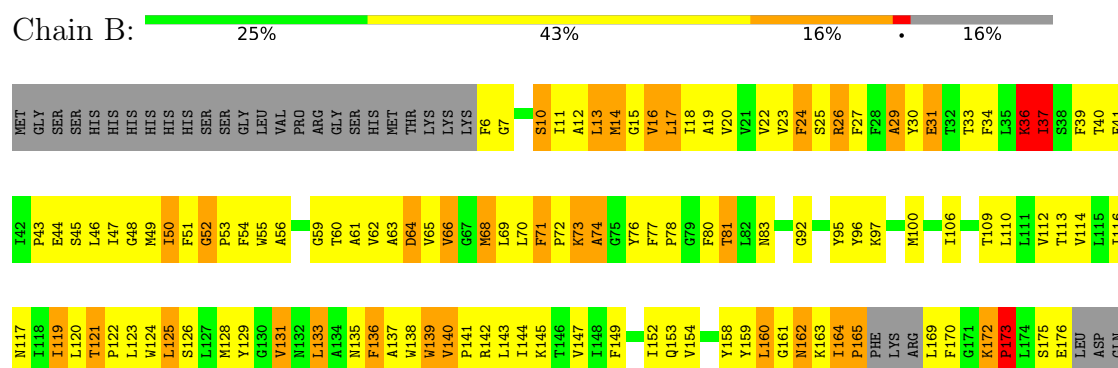
### 3 Residue-property plots

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

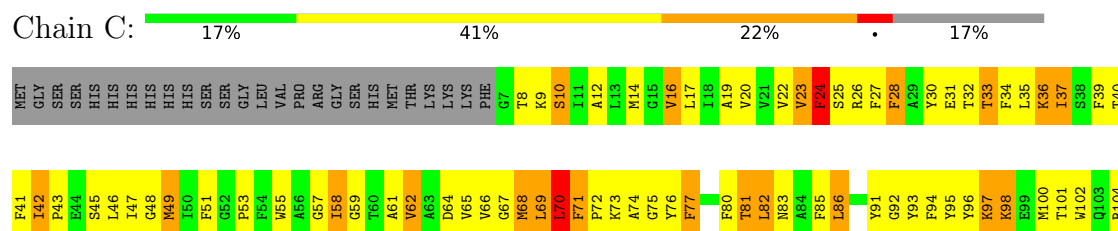
#### • Molecule 1: Folate ECF transporter

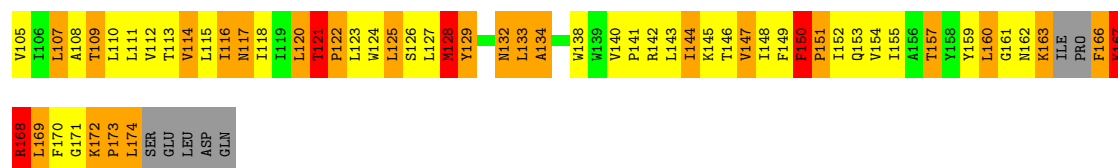


#### • Molecule 1: Folate ECF transporter



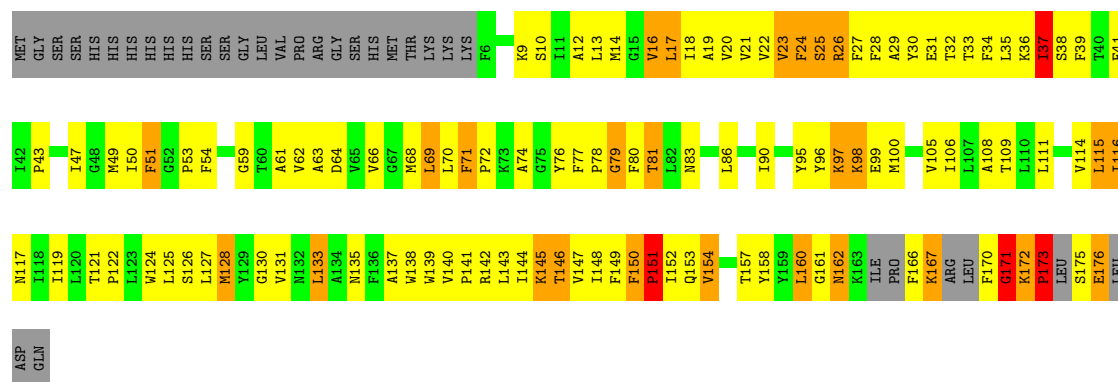
#### • Molecule 1: Folate ECF transporter





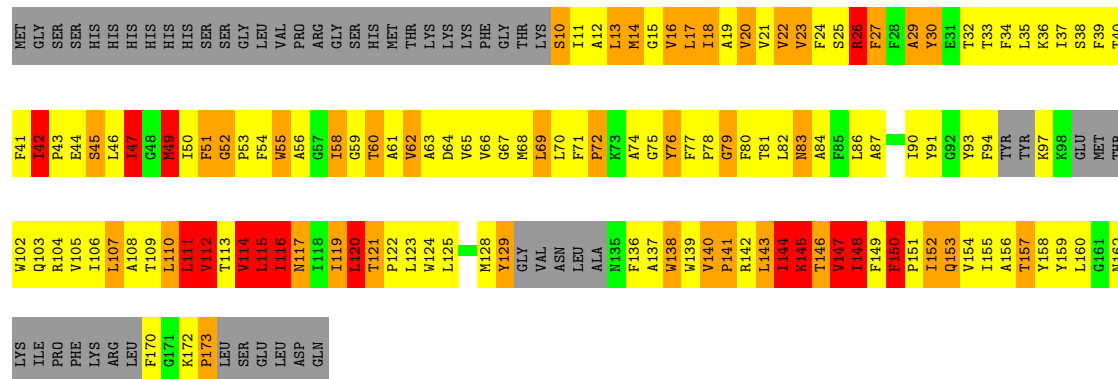
• Molecule 1: Folate ECF transporter

Chain D: 25% 43% 13% 17%



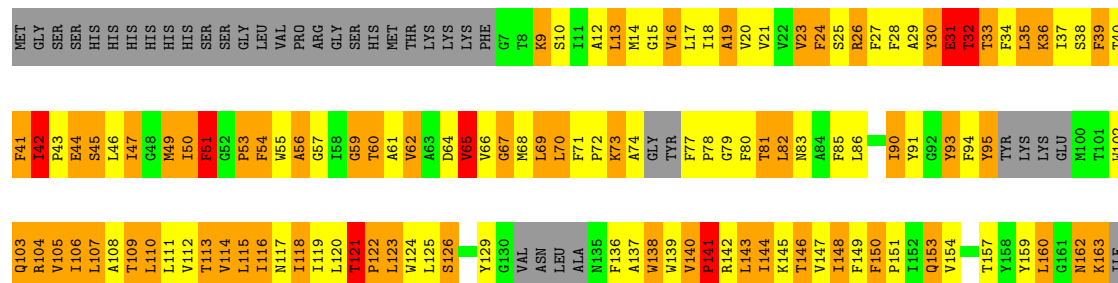
• Molecule 1: Folate ECF transporter

Chain E: 8% 39% 20% 8% 26%



• Molecule 1: Folate ECF transporter

Chain F: 13% 29% 30% 25%



|     |     |     |     |      |      |      |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | PHE | LYS | ARG | L169 | F170 | G171 | LYS | PRO | PRO | LEU | SER | GLU | LEU | ASP | GLN |
|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 31                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 92.75Å 92.75Å 183.44Å<br>90.00° 90.00° 120.00°                 | Depositor        |
| Resolution (Å)                                                          | 33.57 – 3.19<br>33.57 – 3.19                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 76.1 (33.57-3.19)<br>68.3 (33.57-3.19)                         | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                           | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 5.79 (at 3.18Å)                                                | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.9_1692)                               | Depositor        |
| R, $R_{free}$                                                           | 0.293 , 0.356<br>0.287 , 0.317                                 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2011 reflections (8.97%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 68.8                                                           | Xtriage          |
| Anisotropy                                                              | 0.857                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.15 , 42.7                                                    | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$    | Xtriage          |
| Estimated twinning fraction                                             | 0.034 for -h,-k,l<br>0.380 for h,-h-k,-l<br>0.035 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                           | EDS              |
| Total number of atoms                                                   | 7862                                                           | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 108.0                                                          | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FOL

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     | 1.09         | 3/1342 (0.2%)  | 1.56        | 26/1830 (1.4%)   |
| 1   | B     | 0.98         | 2/1385 (0.1%)  | 1.49        | 36/1889 (1.9%)   |
| 1   | C     | 1.22         | 7/1374 (0.5%)  | 1.57        | 25/1871 (1.3%)   |
| 1   | D     | 1.11         | 1/1372 (0.1%)  | 1.43        | 17/1865 (0.9%)   |
| 1   | E     | 1.09         | 9/1212 (0.7%)  | 2.00        | 48/1650 (2.9%)   |
| 1   | F     | 1.15         | 9/1229 (0.7%)  | 1.81        | 46/1673 (2.7%)   |
| All | All   | 1.11         | 31/7914 (0.4%) | 1.64        | 198/10778 (1.8%) |

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   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 6                   |
| 1   | F     | 0                   | 5                   |
| All | All   | 0                   | 15                  |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 71  | PHE  | C-N   | 7.08 | 1.40        | 1.33     |
| 1   | F     | 62  | VAL  | CA-CB | 7.05 | 1.62        | 1.54     |
| 1   | F     | 122 | PRO  | N-CD  | 6.80 | 1.57        | 1.47     |
| 1   | F     | 121 | THR  | C-N   | 6.73 | 1.44        | 1.33     |
| 1   | D     | 150 | PHE  | C-N   | 6.59 | 1.43        | 1.34     |
| 1   | C     | 121 | THR  | C-N   | 6.54 | 1.43        | 1.33     |
| 1   | C     | 122 | PRO  | N-CD  | 6.26 | 1.56        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 115 | LEU  | CA-C  | -6.15 | 1.45        | 1.52     |
| 1   | F     | 62  | VAL  | C-O   | 5.84  | 1.30        | 1.24     |
| 1   | E     | 47  | ILE  | CA-CB | 5.73  | 1.61        | 1.54     |
| 1   | E     | 42  | ILE  | C-N   | 5.72  | 1.41        | 1.34     |
| 1   | E     | 116 | ILE  | CA-CB | 5.49  | 1.60        | 1.54     |
| 1   | F     | 71  | PHE  | C-N   | 5.42  | 1.40        | 1.33     |
| 1   | C     | 173 | PRO  | N-CD  | 5.41  | 1.55        | 1.47     |
| 1   | C     | 172 | LYS  | C-N   | 5.40  | 1.40        | 1.34     |
| 1   | E     | 140 | VAL  | C-N   | 5.40  | 1.41        | 1.34     |
| 1   | B     | 165 | PRO  | N-CD  | 5.31  | 1.55        | 1.47     |
| 1   | A     | 52  | GLY  | C-N   | 5.29  | 1.40        | 1.34     |
| 1   | A     | 72  | PRO  | N-CD  | 5.27  | 1.55        | 1.47     |
| 1   | E     | 72  | PRO  | N-CD  | 5.24  | 1.55        | 1.47     |
| 1   | F     | 42  | ILE  | C-N   | 5.23  | 1.41        | 1.34     |
| 1   | B     | 172 | LYS  | C-N   | 5.22  | 1.39        | 1.33     |
| 1   | F     | 72  | PRO  | N-CD  | 5.21  | 1.55        | 1.47     |
| 1   | E     | 147 | VAL  | CA-C  | 5.20  | 1.59        | 1.52     |
| 1   | E     | 173 | PRO  | N-CD  | 5.19  | 1.55        | 1.47     |
| 1   | E     | 45  | SER  | CA-C  | 5.14  | 1.59        | 1.52     |
| 1   | F     | 56  | ALA  | CA-CB | -5.12 | 1.45        | 1.53     |
| 1   | C     | 120 | LEU  | CA-C  | -5.08 | 1.46        | 1.52     |
| 1   | E     | 141 | PRO  | N-CD  | 5.06  | 1.54        | 1.47     |
| 1   | F     | 149 | PHE  | CA-C  | -5.04 | 1.45        | 1.52     |
| 1   | C     | 151 | PRO  | N-CD  | 5.01  | 1.54        | 1.47     |

All (198) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | E     | 30  | TYR  | N-CA-C  | 27.07  | 142.58      | 110.91   |
| 1   | E     | 115 | LEU  | N-CA-C  | 17.59  | 132.48      | 111.02   |
| 1   | F     | 31  | GLU  | N-CA-C  | 17.38  | 129.91      | 111.14   |
| 1   | C     | 167 | LYS  | N-CA-C  | 14.13  | 126.76      | 111.36   |
| 1   | F     | 50  | ILE  | N-CA-C  | 13.00  | 122.75      | 110.53   |
| 1   | C     | 168 | ARG  | N-CA-C  | 12.04  | 124.14      | 108.24   |
| 1   | C     | 129 | TYR  | N-CA-C  | -11.82 | 91.17       | 109.85   |
| 1   | E     | 143 | LEU  | CB-CA-C | -11.73 | 95.68       | 111.63   |
| 1   | F     | 150 | PHE  | CA-C-N  | -11.28 | 106.88      | 119.28   |
| 1   | F     | 150 | PHE  | C-N-CA  | -11.28 | 106.88      | 119.28   |
| 1   | F     | 32  | THR  | N-CA-C  | 10.89  | 123.25      | 108.23   |
| 1   | E     | 115 | LEU  | CB-CA-C | -9.92  | 95.14       | 110.92   |
| 1   | D     | 79  | GLY  | N-CA-C  | 9.86   | 124.86      | 112.83   |
| 1   | A     | 172 | LYS  | N-CA-C  | 9.81   | 131.49      | 109.81   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 148 | ILE  | CB-CA-C | -9.60 | 99.47       | 112.04   |
| 1   | C     | 128 | MET  | N-CA-C  | 9.49  | 121.22      | 111.07   |
| 1   | B     | 50  | ILE  | N-CA-C  | 9.41  | 119.38      | 110.53   |
| 1   | C     | 70  | LEU  | N-CA-C  | -9.37 | 96.59       | 110.46   |
| 1   | E     | 146 | THR  | N-CA-C  | -9.27 | 100.88      | 113.30   |
| 1   | D     | 71  | PHE  | CA-C-N  | 9.23  | 128.96      | 119.64   |
| 1   | D     | 71  | PHE  | C-N-CA  | 9.23  | 128.96      | 119.64   |
| 1   | A     | 105 | VAL  | N-CA-C  | -9.20 | 101.24      | 110.62   |
| 1   | B     | 36  | LYS  | N-CA-C  | 9.15  | 123.22      | 108.76   |
| 1   | B     | 173 | PRO  | N-CA-CB | -9.04 | 93.14       | 102.72   |
| 1   | C     | 122 | PRO  | CA-N-CD | -9.03 | 99.36       | 112.00   |
| 1   | D     | 150 | PHE  | CA-C-N  | -8.80 | 109.28      | 119.05   |
| 1   | D     | 150 | PHE  | C-N-CA  | -8.80 | 109.28      | 119.05   |
| 1   | A     | 129 | TYR  | N-CA-C  | -8.76 | 95.65       | 109.50   |
| 1   | E     | 30  | TYR  | CB-CA-C | -8.71 | 97.04       | 112.27   |
| 1   | F     | 36  | LYS  | N-CA-C  | 8.68  | 121.71      | 108.52   |
| 1   | F     | 51  | PHE  | N-CA-C  | 8.56  | 123.53      | 112.41   |
| 1   | A     | 121 | THR  | CA-C-N  | -8.32 | 110.37      | 119.19   |
| 1   | A     | 121 | THR  | C-N-CA  | -8.32 | 110.37      | 119.19   |
| 1   | C     | 134 | ALA  | N-CA-C  | 8.18  | 120.20      | 111.28   |
| 1   | F     | 122 | PRO  | CA-N-CD | -7.99 | 100.82      | 112.00   |
| 1   | C     | 75  | GLY  | N-CA-C  | -7.98 | 102.62      | 112.68   |
| 1   | C     | 10  | SER  | N-CA-C  | -7.97 | 102.60      | 111.28   |
| 1   | E     | 29  | ALA  | N-CA-C  | 7.93  | 122.16      | 108.76   |
| 1   | F     | 105 | VAL  | CB-CA-C | -7.89 | 98.35       | 111.29   |
| 1   | E     | 30  | TYR  | CA-C-N  | 7.87  | 132.00      | 120.90   |
| 1   | E     | 30  | TYR  | C-N-CA  | 7.87  | 132.00      | 120.90   |
| 1   | C     | 77  | PHE  | CA-C-N  | 7.76  | 128.47      | 119.47   |
| 1   | C     | 77  | PHE  | C-N-CA  | 7.76  | 128.47      | 119.47   |
| 1   | E     | 144 | ILE  | CA-C-N  | -7.69 | 111.28      | 122.44   |
| 1   | E     | 144 | ILE  | C-N-CA  | -7.69 | 111.28      | 122.44   |
| 1   | C     | 67  | GLY  | N-CA-C  | 7.67  | 121.77      | 112.49   |
| 1   | E     | 144 | ILE  | N-CA-C  | -7.62 | 93.48       | 109.34   |
| 1   | E     | 103 | GLN  | N-CA-C  | 7.40  | 120.22      | 111.71   |
| 1   | E     | 145 | LYS  | N-CA-C  | 7.38  | 120.56      | 107.80   |
| 1   | B     | 10  | SER  | N-CA-C  | -7.38 | 103.24      | 111.28   |
| 1   | E     | 147 | VAL  | N-CA-C  | 7.36  | 124.66      | 109.34   |
| 1   | B     | 31  | GLU  | N-CA-C  | 7.27  | 120.25      | 108.76   |
| 1   | F     | 138 | TRP  | N-CA-C  | 7.24  | 119.25      | 111.36   |
| 1   | D     | 69  | LEU  | N-CA-C  | -7.18 | 103.45      | 111.28   |
| 1   | E     | 117 | ASN  | CA-C-N  | -7.17 | 114.18      | 122.14   |
| 1   | E     | 117 | ASN  | C-N-CA  | -7.17 | 114.18      | 122.14   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 71  | PHE  | CA-C-N    | -7.01 | 112.75      | 119.76   |
| 1   | F     | 71  | PHE  | C-N-CA    | -7.01 | 112.75      | 119.76   |
| 1   | B     | 136 | PHE  | N-CA-C    | -6.97 | 97.86       | 108.67   |
| 1   | E     | 82  | LEU  | N-CA-C    | -6.97 | 103.70      | 111.71   |
| 1   | D     | 151 | PRO  | CA-N-CD   | -6.91 | 102.33      | 112.00   |
| 1   | A     | 26  | ARG  | N-CA-C    | 6.90  | 118.45      | 111.07   |
| 1   | D     | 72  | PRO  | N-CA-C    | 6.88  | 123.74      | 114.18   |
| 1   | B     | 163 | LYS  | N-CA-C    | 6.86  | 120.99      | 110.36   |
| 1   | E     | 114 | VAL  | N-CA-C    | -6.80 | 103.85      | 110.72   |
| 1   | A     | 50  | ILE  | N-CA-C    | 6.80  | 116.92      | 110.53   |
| 1   | A     | 42  | ILE  | CA-C-N    | -6.62 | 111.70      | 119.05   |
| 1   | A     | 42  | ILE  | C-N-CA    | -6.62 | 111.70      | 119.05   |
| 1   | F     | 54  | PHE  | N-CA-C    | 6.60  | 118.26      | 111.14   |
| 1   | F     | 121 | THR  | CA-C-N    | -6.59 | 111.81      | 119.32   |
| 1   | F     | 121 | THR  | C-N-CA    | -6.59 | 111.81      | 119.32   |
| 1   | E     | 116 | ILE  | N-CA-C    | 6.53  | 116.63      | 110.30   |
| 1   | C     | 121 | THR  | CA-C-N    | -6.53 | 111.88      | 119.32   |
| 1   | C     | 121 | THR  | C-N-CA    | -6.53 | 111.88      | 119.32   |
| 1   | F     | 146 | THR  | N-CA-C    | -6.49 | 104.29      | 111.82   |
| 1   | F     | 65  | VAL  | N-CA-C    | 6.47  | 117.26      | 110.72   |
| 1   | B     | 27  | PHE  | N-CA-C    | 6.44  | 120.34      | 112.23   |
| 1   | D     | 171 | GLY  | N-CA-C    | 6.42  | 128.40      | 113.18   |
| 1   | A     | 71  | PHE  | CA-C-N    | -6.40 | 113.14      | 120.89   |
| 1   | A     | 71  | PHE  | C-N-CA    | -6.40 | 113.14      | 120.89   |
| 1   | E     | 119 | ILE  | N-CA-C    | -6.38 | 102.89      | 111.44   |
| 1   | E     | 42  | ILE  | CA-C-N    | -6.34 | 112.38      | 118.97   |
| 1   | E     | 42  | ILE  | C-N-CA    | -6.34 | 112.38      | 118.97   |
| 1   | F     | 150 | PHE  | N-CA-C    | 6.26  | 123.65      | 109.81   |
| 1   | C     | 71  | PHE  | C-N-CD    | -6.25 | 99.39       | 125.00   |
| 1   | B     | 70  | LEU  | N-CA-C    | -6.23 | 102.49      | 110.53   |
| 1   | E     | 15  | GLY  | N-CA-C    | -6.21 | 105.28      | 112.73   |
| 1   | F     | 67  | GLY  | N-CA-C    | -6.21 | 105.28      | 112.73   |
| 1   | B     | 74  | ALA  | N-CA-CB   | -6.19 | 104.12      | 114.27   |
| 1   | E     | 143 | LEU  | N-CA-C    | -6.10 | 103.75      | 111.92   |
| 1   | F     | 105 | VAL  | N-CA-C    | -6.08 | 96.69       | 109.34   |
| 1   | F     | 62  | VAL  | CA-CB-CG2 | 6.04  | 120.67      | 110.40   |
| 1   | A     | 49  | MET  | N-CA-C    | 6.03  | 117.52      | 111.07   |
| 1   | B     | 15  | GLY  | N-CA-C    | -5.97 | 105.56      | 112.73   |
| 1   | F     | 143 | LEU  | N-CA-C    | -5.97 | 105.08      | 112.90   |
| 1   | F     | 126 | SER  | N-CA-C    | -5.96 | 104.78      | 111.28   |
| 1   | B     | 69  | LEU  | N-CA-C    | -5.96 | 104.70      | 111.07   |
| 1   | B     | 68  | MET  | N-CA-C    | 5.94  | 120.59      | 113.23   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 106 | ILE  | N-CA-C   | 5.93  | 121.68      | 109.34   |
| 1   | E     | 62  | VAL  | N-CA-C   | -5.90 | 104.61      | 110.62   |
| 1   | B     | 71  | PHE  | CA-C-N   | 5.89  | 125.28      | 118.85   |
| 1   | B     | 71  | PHE  | C-N-CA   | 5.89  | 125.28      | 118.85   |
| 1   | B     | 25  | SER  | N-CA-C   | 5.89  | 117.50      | 111.14   |
| 1   | D     | 81  | THR  | N-CA-C   | -5.89 | 104.81      | 112.23   |
| 1   | B     | 160 | LEU  | N-CA-C   | -5.87 | 104.95      | 111.71   |
| 1   | B     | 68  | MET  | CA-CB-CG | -5.86 | 102.38      | 114.10   |
| 1   | E     | 111 | LEU  | CA-CB-CG | 5.86  | 136.79      | 116.30   |
| 1   | B     | 81  | THR  | N-CA-C   | -5.82 | 105.68      | 112.89   |
| 1   | F     | 105 | VAL  | CA-C-N   | 5.81  | 132.44      | 121.97   |
| 1   | F     | 105 | VAL  | C-N-CA   | 5.81  | 132.44      | 121.97   |
| 1   | F     | 149 | PHE  | CA-C-N   | -5.81 | 107.63      | 121.80   |
| 1   | F     | 149 | PHE  | C-N-CA   | -5.81 | 107.63      | 121.80   |
| 1   | B     | 7   | GLY  | N-CA-C   | -5.80 | 101.83      | 110.71   |
| 1   | F     | 95  | TYR  | CA-CB-CG | -5.80 | 103.46      | 113.90   |
| 1   | F     | 79  | GLY  | N-CA-C   | -5.78 | 105.80      | 112.50   |
| 1   | E     | 120 | LEU  | CA-CB-CG | 5.77  | 136.50      | 116.30   |
| 1   | A     | 52  | GLY  | CA-C-N   | -5.77 | 112.97      | 118.97   |
| 1   | A     | 52  | GLY  | C-N-CA   | -5.77 | 112.97      | 118.97   |
| 1   | F     | 42  | ILE  | CA-C-N   | -5.76 | 112.66      | 119.05   |
| 1   | F     | 42  | ILE  | C-N-CA   | -5.76 | 112.66      | 119.05   |
| 1   | F     | 77  | PHE  | CA-C-N   | -5.75 | 112.65      | 119.84   |
| 1   | F     | 77  | PHE  | C-N-CA   | -5.75 | 112.65      | 119.84   |
| 1   | C     | 24  | PHE  | N-CA-C   | -5.75 | 105.02      | 111.28   |
| 1   | D     | 37  | ILE  | N-CA-C   | -5.74 | 100.07      | 108.11   |
| 1   | B     | 31  | GLU  | CA-C-N   | 5.70  | 131.45      | 122.21   |
| 1   | B     | 31  | GLU  | C-N-CA   | 5.70  | 131.45      | 122.21   |
| 1   | A     | 108 | ALA  | N-CA-C   | -5.69 | 104.71      | 111.03   |
| 1   | C     | 49  | MET  | N-CA-C   | 5.69  | 117.56      | 111.36   |
| 1   | C     | 144 | ILE  | CB-CA-C  | -5.69 | 104.57      | 112.02   |
| 1   | E     | 152 | ILE  | N-CA-C   | 5.69  | 118.20      | 111.09   |
| 1   | C     | 102 | TRP  | N-CA-C   | -5.66 | 105.11      | 111.28   |
| 1   | A     | 172 | LYS  | CB-CA-C  | -5.64 | 99.07       | 110.17   |
| 1   | A     | 118 | ILE  | N-CA-C   | -5.63 | 108.01      | 113.53   |
| 1   | D     | 31  | GLU  | N-CA-C   | 5.62  | 118.07      | 108.90   |
| 1   | E     | 140 | VAL  | CA-C-N   | -5.62 | 112.81      | 119.05   |
| 1   | E     | 140 | VAL  | C-N-CA   | -5.62 | 112.81      | 119.05   |
| 1   | E     | 51  | PHE  | N-CA-C   | 5.62  | 119.47      | 108.18   |
| 1   | E     | 112 | VAL  | N-CA-C   | 5.61  | 117.82      | 111.88   |
| 1   | E     | 138 | TRP  | N-CA-C   | -5.59 | 103.62      | 110.61   |
| 1   | F     | 39  | PHE  | N-CA-C   | -5.59 | 106.04      | 112.86   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 70  | LEU  | N-CA-C   | 5.58  | 117.44      | 111.36   |
| 1   | A     | 136 | PHE  | N-CA-C   | -5.58 | 106.27      | 112.57   |
| 1   | B     | 52  | GLY  | CA-C-N   | -5.56 | 112.89      | 119.84   |
| 1   | B     | 52  | GLY  | C-N-CA   | -5.56 | 112.89      | 119.84   |
| 1   | B     | 121 | THR  | CA-C-N   | -5.51 | 113.35      | 119.19   |
| 1   | B     | 121 | THR  | C-N-CA   | -5.51 | 113.35      | 119.19   |
| 1   | D     | 173 | PRO  | CA-N-CD  | -5.51 | 104.29      | 112.00   |
| 1   | B     | 125 | LEU  | N-CA-C   | -5.48 | 106.09      | 112.89   |
| 1   | B     | 172 | LYS  | CA-C-N   | -5.47 | 113.62      | 120.51   |
| 1   | B     | 172 | LYS  | C-N-CA   | -5.47 | 113.62      | 120.51   |
| 1   | E     | 52  | GLY  | N-CA-C   | 5.47  | 123.50      | 112.34   |
| 1   | C     | 150 | PHE  | CA-C-N   | -5.46 | 112.99      | 119.05   |
| 1   | C     | 150 | PHE  | C-N-CA   | -5.46 | 112.99      | 119.05   |
| 1   | C     | 98  | LYS  | N-CA-C   | -5.44 | 100.80      | 109.23   |
| 1   | A     | 133 | LEU  | N-CA-C   | -5.42 | 105.37      | 111.28   |
| 1   | C     | 157 | THR  | N-CA-C   | -5.42 | 105.37      | 111.28   |
| 1   | F     | 50  | ILE  | CB-CA-C  | -5.40 | 104.95      | 112.02   |
| 1   | E     | 114 | VAL  | CA-C-O   | -5.38 | 115.15      | 120.85   |
| 1   | B     | 140 | VAL  | CA-C-N   | -5.37 | 113.19      | 119.32   |
| 1   | B     | 140 | VAL  | C-N-CA   | -5.37 | 113.19      | 119.32   |
| 1   | C     | 114 | VAL  | N-CA-C   | -5.37 | 105.27      | 110.42   |
| 1   | A     | 131 | VAL  | N-CA-C   | 5.36  | 116.20      | 108.48   |
| 1   | B     | 29  | ALA  | N-CA-C   | 5.34  | 118.29      | 109.85   |
| 1   | E     | 148 | ILE  | CA-C-N   | 5.32  | 131.13      | 121.92   |
| 1   | E     | 148 | ILE  | C-N-CA   | 5.32  | 131.13      | 121.92   |
| 1   | B     | 173 | PRO  | CA-N-CD  | -5.32 | 104.55      | 112.00   |
| 1   | D     | 150 | PHE  | O-C-N    | 5.31  | 125.21      | 120.48   |
| 1   | E     | 49  | MET  | CB-CA-C  | -5.31 | 102.47      | 110.92   |
| 1   | E     | 144 | ILE  | N-CA-CB  | 5.28  | 119.93      | 111.23   |
| 1   | E     | 49  | MET  | CA-CB-CG | 5.27  | 124.65      | 114.10   |
| 1   | F     | 51  | PHE  | CA-C-N   | 5.26  | 130.13      | 121.87   |
| 1   | F     | 51  | PHE  | C-N-CA   | 5.26  | 130.13      | 121.87   |
| 1   | F     | 141 | PRO  | N-CA-C   | -5.24 | 106.58      | 113.65   |
| 1   | C     | 82  | LEU  | N-CA-C   | -5.23 | 105.69      | 111.71   |
| 1   | F     | 59  | GLY  | CA-C-N   | -5.22 | 112.36      | 122.06   |
| 1   | F     | 59  | GLY  | C-N-CA   | -5.22 | 112.36      | 122.06   |
| 1   | E     | 121 | THR  | CA-C-N   | -5.21 | 113.67      | 119.19   |
| 1   | E     | 121 | THR  | C-N-CA   | -5.21 | 113.67      | 119.19   |
| 1   | B     | 172 | LYS  | CB-CA-C  | -5.21 | 102.88      | 109.65   |
| 1   | F     | 19  | ALA  | N-CA-C   | -5.17 | 105.64      | 111.28   |
| 1   | A     | 25  | SER  | CA-C-N   | 5.17  | 127.15      | 120.44   |
| 1   | A     | 25  | SER  | C-N-CA   | 5.17  | 127.15      | 120.44   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 152 | ILE  | CB-CA-C  | -5.15 | 105.18      | 112.14   |
| 1   | E     | 87  | ALA  | N-CA-C   | -5.15 | 105.56      | 111.07   |
| 1   | F     | 16  | VAL  | N-CA-C   | -5.14 | 105.38      | 110.62   |
| 1   | F     | 49  | MET  | N-CA-C   | -5.12 | 105.69      | 111.28   |
| 1   | F     | 150 | PHE  | CA-CB-CG | 5.12  | 118.92      | 113.80   |
| 1   | D     | 70  | LEU  | N-CA-C   | 5.11  | 117.97      | 111.69   |
| 1   | A     | 150 | PHE  | CA-C-N   | -5.10 | 113.39      | 119.05   |
| 1   | A     | 150 | PHE  | C-N-CA   | -5.10 | 113.39      | 119.05   |
| 1   | E     | 173 | PRO  | CA-N-CD  | -5.09 | 104.88      | 112.00   |
| 1   | E     | 145 | LYS  | CA-CB-CG | -5.08 | 103.93      | 114.10   |
| 1   | E     | 157 | THR  | N-CA-C   | -5.08 | 106.35      | 112.54   |
| 1   | D     | 154 | VAL  | CB-CA-C  | -5.07 | 105.30      | 112.14   |
| 1   | B     | 37  | ILE  | CA-C-N   | -5.06 | 113.42      | 122.07   |
| 1   | B     | 37  | ILE  | C-N-CA   | -5.06 | 113.42      | 122.07   |
| 1   | D     | 53  | PRO  | N-CA-C   | 5.06  | 122.89      | 112.47   |
| 1   | E     | 26  | ARG  | N-CA-C   | 5.05  | 116.79      | 111.28   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 139 | TRP  | Peptide   |
| 1   | C     | 117 | ASN  | Mainchain |
| 1   | D     | 171 | GLY  | Peptide   |
| 1   | D     | 32  | THR  | Peptide   |
| 1   | E     | 112 | VAL  | Peptide   |
| 1   | E     | 144 | ILE  | Peptide   |
| 1   | E     | 145 | LYS  | Peptide   |
| 1   | E     | 150 | PHE  | Peptide   |
| 1   | E     | 49  | MET  | Peptide   |
| 1   | E     | 79  | GLY  | Peptide   |
| 1   | F     | 105 | VAL  | Peptide   |
| 1   | F     | 141 | PRO  | Peptide   |
| 1   | F     | 30  | TYR  | Peptide   |
| 1   | F     | 31  | GLU  | Peptide   |
| 1   | F     | 51  | PHE  | 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     | 1300  | 0        | 1357     | 225     | 4            |
| 1   | B     | 1341  | 0        | 1395     | 203     | 4            |
| 1   | C     | 1331  | 0        | 1392     | 276     | 0            |
| 1   | D     | 1330  | 0        | 1375     | 191     | 0            |
| 1   | E     | 1175  | 0        | 1222     | 403     | 0            |
| 1   | F     | 1193  | 0        | 1239     | 357     | 0            |
| 2   | A     | 32    | 0        | 17       | 13      | 0            |
| 2   | B     | 32    | 0        | 17       | 15      | 0            |
| 2   | C     | 32    | 0        | 17       | 6       | 0            |
| 2   | D     | 32    | 0        | 17       | 10      | 0            |
| 2   | E     | 32    | 0        | 17       | 27      | 0            |
| 2   | F     | 32    | 0        | 17       | 46      | 0            |
| All | All   | 7862  | 0        | 8082     | 1645    | 4            |

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 103.

All (1645) 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:D:14:MET:HE2   | 1:D:51:PHE:CE2  | 1.24                     | 1.69              |
| 1:B:96:TYR:CZ    | 1:B:97:LYS:HE3  | 1.19                     | 1.66              |
| 1:C:49:MET:HE2   | 1:C:100:MET:CE  | 1.19                     | 1.66              |
| 1:D:14:MET:HE1   | 1:D:51:PHE:CD2  | 1.33                     | 1.61              |
| 1:D:14:MET:CE    | 1:D:51:PHE:CE2  | 1.82                     | 1.57              |
| 1:B:96:TYR:CE2   | 1:B:97:LYS:HE3  | 1.38                     | 1.56              |
| 1:D:33:THR:HG22  | 1:D:34:PHE:CE1  | 1.39                     | 1.54              |
| 1:C:10:SER:HB3   | 1:C:170:PHE:CE1 | 1.43                     | 1.53              |
| 1:E:40:THR:HG21  | 1:E:44:GLU:CD   | 1.33                     | 1.51              |
| 1:E:40:THR:CG2   | 1:E:44:GLU:HG2  | 1.38                     | 1.51              |
| 1:E:39:PHE:CD1   | 1:E:41:PHE:CE1  | 2.00                     | 1.50              |
| 1:E:54:PHE:CE2   | 1:E:55:TRP:HZ3  | 1.32                     | 1.48              |
| 1:E:40:THR:HG21  | 1:E:44:GLU:CG   | 1.44                     | 1.46              |
| 1:D:14:MET:CE    | 1:D:51:PHE:CD2  | 1.91                     | 1.43              |
| 1:C:49:MET:CE    | 1:C:100:MET:HE3 | 1.47                     | 1.43              |
| 1:E:115:LEU:HD13 | 1:E:116:ILE:N   | 1.28                     | 1.42              |
| 1:E:69:LEU:HD13  | 1:E:70:LEU:N    | 1.21                     | 1.41              |
| 1:E:68:MET:CE    | 2:E:201:FOL:C2  | 2.01                     | 1.39              |
| 1:A:50:ILE:O     | 1:A:173:PRO:CB  | 1.73                     | 1.37              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:30:TYR:N    | 1:F:36:LYS:HZ1   | 1.23                     | 1.36              |
| 1:D:10:SER:OG   | 1:D:172:LYS:CB   | 1.72                     | 1.36              |
| 1:F:30:TYR:O    | 1:F:36:LYS:HD3   | 1.23                     | 1.35              |
| 1:E:68:MET:CE   | 2:E:201:FOL:N3   | 1.92                     | 1.32              |
| 1:B:96:TYR:CE2  | 1:B:97:LYS:CE    | 2.10                     | 1.32              |
| 1:F:30:TYR:N    | 1:F:36:LYS:NZ    | 1.78                     | 1.31              |
| 1:C:112:VAL:O   | 1:C:116:ILE:HG22 | 1.22                     | 1.31              |
| 1:B:96:TYR:CZ   | 1:B:97:LYS:CE    | 2.13                     | 1.30              |
| 1:E:54:PHE:CE2  | 1:E:55:TRP:CZ3   | 2.20                     | 1.29              |
| 1:A:100:MET:SD  | 1:A:161:GLY:HA3  | 1.70                     | 1.29              |
| 1:E:39:PHE:HD1  | 1:E:41:PHE:CE1   | 1.43                     | 1.28              |
| 1:E:54:PHE:CD2  | 1:E:55:TRP:CZ3   | 2.20                     | 1.28              |
| 1:E:40:THR:HG21 | 1:E:44:GLU:OE2   | 1.27                     | 1.28              |
| 1:F:73:LYS:HD2  | 2:F:201:FOL:C7   | 1.63                     | 1.27              |
| 1:A:50:ILE:O    | 1:A:173:PRO:HB2  | 1.28                     | 1.26              |
| 1:E:115:LEU:O   | 1:E:119:ILE:HG12 | 1.25                     | 1.26              |
| 1:E:139:TRP:CZ3 | 1:E:142:ARG:HD2  | 1.67                     | 1.26              |
| 1:C:49:MET:CE   | 1:C:95:TYR:CD2   | 2.17                     | 1.25              |
| 1:C:49:MET:HE3  | 1:C:95:TYR:CD2   | 1.73                     | 1.24              |
| 1:F:39:PHE:HA   | 1:F:41:PHE:CE2   | 1.72                     | 1.24              |
| 1:C:10:SER:CB   | 1:C:170:PHE:CE1  | 2.18                     | 1.24              |
| 1:E:39:PHE:CD1  | 1:E:41:PHE:HE1   | 1.46                     | 1.23              |
| 1:F:68:MET:SD   | 2:F:201:FOL:N1   | 2.10                     | 1.23              |
| 1:C:49:MET:CE   | 1:C:100:MET:CE   | 2.05                     | 1.22              |
| 1:E:18:ILE:HG23 | 1:E:63:ALA:CB    | 1.67                     | 1.22              |
| 1:D:33:THR:CG2  | 1:D:34:PHE:CE1   | 2.22                     | 1.21              |
| 1:E:68:MET:HE3  | 2:E:201:FOL:C2   | 1.62                     | 1.21              |
| 1:C:70:LEU:C    | 1:C:72:PRO:HD3   | 1.64                     | 1.21              |
| 1:E:40:THR:CG2  | 1:E:44:GLU:OE2   | 1.88                     | 1.21              |
| 1:F:80:PHE:HE1  | 2:F:201:FOL:OE2  | 1.21                     | 1.20              |
| 1:E:18:ILE:CG2  | 1:E:63:ALA:HB2   | 1.72                     | 1.19              |
| 1:D:10:SER:OG   | 1:D:172:LYS:HB2  | 1.03                     | 1.19              |
| 1:A:126:SER:HA  | 1:A:131:VAL:CG2  | 1.72                     | 1.19              |
| 1:F:83:ASN:OD1  | 1:F:116:ILE:HD11 | 1.36                     | 1.18              |
| 1:D:33:THR:HG22 | 1:D:34:PHE:CD1   | 1.79                     | 1.18              |
| 1:B:96:TYR:OH   | 1:B:97:LYS:HE3   | 1.37                     | 1.18              |
| 1:F:80:PHE:CD2  | 2:F:201:FOL:N3   | 2.12                     | 1.17              |
| 1:E:40:THR:CG2  | 1:E:44:GLU:CG    | 2.09                     | 1.17              |
| 1:F:13:LEU:HD21 | 1:F:51:PHE:CE2   | 1.80                     | 1.16              |
| 1:C:71:PHE:N    | 1:C:72:PRO:CD    | 2.10                     | 1.14              |
| 1:F:160:LEU:O   | 1:F:163:LYS:HG3  | 1.46                     | 1.14              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:61:ALA:HB2  | 1:F:85:PHE:CD1   | 1.82                     | 1.13              |
| 1:C:49:MET:HE3  | 1:C:95:TYR:CG    | 1.84                     | 1.13              |
| 1:E:69:LEU:CD1  | 1:E:70:LEU:N     | 2.11                     | 1.13              |
| 1:F:80:PHE:CE2  | 2:F:201:FOL:N3   | 2.16                     | 1.13              |
| 1:B:36:LYS:HE2  | 1:B:37:ILE:H     | 1.02                     | 1.13              |
| 1:E:35:LEU:CD2  | 1:E:142:ARG:HG2  | 1.78                     | 1.12              |
| 1:F:61:ALA:O    | 1:F:65:VAL:HG23  | 1.47                     | 1.12              |
| 1:E:35:LEU:HD21 | 1:E:142:ARG:CG   | 1.79                     | 1.12              |
| 1:F:73:LYS:HD2  | 2:F:201:FOL:C6   | 1.79                     | 1.12              |
| 1:B:30:TYR:N    | 1:B:36:LYS:NZ    | 1.98                     | 1.11              |
| 1:F:95:TYR:OH   | 1:F:108:ALA:HB3  | 1.48                     | 1.11              |
| 1:E:68:MET:HE1  | 2:E:201:FOL:C2   | 1.74                     | 1.11              |
| 1:E:115:LEU:CD1 | 1:E:116:ILE:N    | 2.12                     | 1.11              |
| 1:E:18:ILE:CG2  | 1:E:63:ALA:CB    | 2.28                     | 1.10              |
| 1:B:30:TYR:N    | 1:B:36:LYS:HZ1   | 1.46                     | 1.10              |
| 1:B:30:TYR:HB3  | 1:B:36:LYS:HE3   | 1.24                     | 1.10              |
| 1:E:68:MET:HE1  | 2:E:201:FOL:C4   | 1.82                     | 1.10              |
| 1:C:98:LYS:NZ   | 1:C:104:ARG:NH1  | 1.98                     | 1.10              |
| 1:E:23:VAL:HA   | 1:E:26:ARG:HD2   | 1.16                     | 1.09              |
| 1:A:126:SER:HA  | 1:A:131:VAL:HG21 | 1.25                     | 1.09              |
| 1:B:96:TYR:OH   | 1:B:97:LYS:CE    | 1.96                     | 1.09              |
| 1:D:12:ALA:O    | 1:D:16:VAL:HG22  | 1.53                     | 1.09              |
| 1:F:64:ASP:HB2  | 1:F:80:PHE:CE2   | 1.87                     | 1.08              |
| 1:F:122:PRO:HA  | 1:F:125:LEU:HD12 | 1.15                     | 1.08              |
| 1:F:94:PHE:HD2  | 1:F:108:ALA:HB2  | 1.10                     | 1.08              |
| 1:A:23:VAL:O    | 1:A:26:ARG:NE    | 1.87                     | 1.08              |
| 1:F:39:PHE:HA   | 1:F:41:PHE:HE2   | 0.98                     | 1.08              |
| 1:A:100:MET:SD  | 1:A:161:GLY:CA   | 2.42                     | 1.07              |
| 1:E:54:PHE:HD2  | 1:E:55:TRP:CE3   | 1.70                     | 1.07              |
| 1:F:16:VAL:HG23 | 1:F:17:LEU:HD22  | 1.37                     | 1.07              |
| 1:A:26:ARG:HG2  | 1:A:27:PHE:CD1   | 1.90                     | 1.06              |
| 1:E:77:PHE:CG   | 1:E:78:PRO:HD2   | 1.89                     | 1.06              |
| 1:E:115:LEU:O   | 1:E:115:LEU:HD22 | 1.53                     | 1.06              |
| 1:D:54:PHE:CZ   | 1:D:176:GLU:HB2  | 1.90                     | 1.06              |
| 1:E:112:VAL:HB  | 1:E:115:LEU:HB3  | 1.38                     | 1.06              |
| 1:F:94:PHE:CD2  | 1:F:108:ALA:HB2  | 1.88                     | 1.06              |
| 1:C:25:SER:OG   | 1:C:26:ARG:NH1   | 1.88                     | 1.06              |
| 1:E:141:PRO:O   | 1:E:144:ILE:HG22 | 1.53                     | 1.06              |
| 1:D:10:SER:CB   | 1:D:172:LYS:HG3  | 1.85                     | 1.06              |
| 1:C:105:VAL:O   | 1:C:109:THR:OG1  | 1.74                     | 1.05              |
| 1:E:23:VAL:HA   | 1:E:26:ARG:CD    | 1.87                     | 1.05              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:77:PHE:CD1   | 1:E:78:PRO:HD2   | 1.91                     | 1.05              |
| 1:C:49:MET:HE1   | 1:C:95:TYR:CD2   | 1.86                     | 1.04              |
| 1:F:32:THR:O     | 1:F:35:LEU:CD2   | 2.04                     | 1.04              |
| 1:E:30:TYR:HB2   | 1:E:37:ILE:HG22  | 1.38                     | 1.04              |
| 1:A:68:MET:CE    | 1:A:75:GLY:O     | 2.05                     | 1.04              |
| 1:F:94:PHE:HD2   | 1:F:108:ALA:CB   | 1.69                     | 1.04              |
| 1:F:102:TRP:O    | 1:F:103:GLN:NE2  | 1.91                     | 1.03              |
| 1:B:135:ASN:O    | 1:B:138:TRP:N    | 1.91                     | 1.03              |
| 1:C:148:ILE:O    | 1:C:151:PRO:HD2  | 1.59                     | 1.03              |
| 1:F:30:TYR:C     | 1:F:36:LYS:HZ2   | 1.67                     | 1.03              |
| 1:F:80:PHE:CE1   | 2:F:201:FOL:OE2  | 2.12                     | 1.03              |
| 1:B:30:TYR:CB    | 1:B:36:LYS:HE3   | 1.85                     | 1.02              |
| 1:C:49:MET:HE3   | 1:C:95:TYR:CB    | 1.90                     | 1.02              |
| 1:D:33:THR:C     | 1:D:34:PHE:HD1   | 1.66                     | 1.02              |
| 1:C:34:PHE:CD2   | 1:C:138:TRP:NE1  | 2.25                     | 1.02              |
| 1:F:10:SER:O     | 1:F:14:MET:HG2   | 1.59                     | 1.02              |
| 1:E:14:MET:CE    | 1:E:18:ILE:HD11  | 1.89                     | 1.01              |
| 1:E:23:VAL:O     | 1:E:26:ARG:HB2   | 1.60                     | 1.01              |
| 1:C:30:TYR:HB2   | 1:C:37:ILE:HG13  | 1.38                     | 1.01              |
| 1:C:71:PHE:N     | 1:C:72:PRO:HD2   | 1.71                     | 1.01              |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:H    | 1.19                     | 1.01              |
| 1:F:30:TYR:O     | 1:F:36:LYS:CD    | 2.07                     | 1.01              |
| 1:B:96:TYR:CE2   | 1:B:97:LYS:CD    | 2.44                     | 1.01              |
| 1:F:32:THR:HG22  | 1:F:33:THR:H     | 1.25                     | 1.01              |
| 1:C:122:PRO:HA   | 1:C:125:LEU:HD12 | 1.40                     | 1.00              |
| 1:A:26:ARG:CZ    | 1:A:27:PHE:HB2   | 1.91                     | 1.00              |
| 1:C:27:PHE:HE1   | 1:C:71:PHE:CZ    | 1.78                     | 1.00              |
| 1:D:10:SER:HB3   | 1:D:172:LYS:CG   | 1.90                     | 1.00              |
| 1:E:69:LEU:CD1   | 1:E:70:LEU:H     | 1.69                     | 1.00              |
| 1:E:141:PRO:O    | 1:E:144:ILE:CG2  | 2.10                     | 1.00              |
| 1:F:68:MET:SD    | 2:F:201:FOL:C2   | 2.50                     | 1.00              |
| 1:C:70:LEU:HD23  | 1:C:70:LEU:H     | 1.26                     | 1.00              |
| 1:F:95:TYR:OH    | 1:F:108:ALA:CB   | 2.08                     | 0.99              |
| 1:A:103:GLN:OE1  | 1:A:104:ARG:HD3  | 1.59                     | 0.99              |
| 1:F:122:PRO:CA   | 1:F:125:LEU:HD12 | 1.91                     | 0.99              |
| 1:E:68:MET:HE1   | 2:E:201:FOL:N3   | 1.68                     | 0.99              |
| 1:C:112:VAL:O    | 1:C:116:ILE:CG2  | 2.11                     | 0.99              |
| 1:C:10:SER:HB3   | 1:C:170:PHE:CZ   | 1.98                     | 0.99              |
| 1:E:18:ILE:HG23  | 1:E:63:ALA:HB2   | 1.02                     | 0.99              |
| 1:E:40:THR:CB    | 1:E:44:GLU:OE2   | 2.11                     | 0.99              |
| 1:F:94:PHE:CD2   | 1:F:108:ALA:CB   | 2.44                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:42:ILE:HG23  | 1:F:43:PRO:HD3   | 1.45                     | 0.98              |
| 1:E:115:LEU:O    | 1:E:119:ILE:CG1  | 2.10                     | 0.98              |
| 1:C:168:ARG:HH21 | 1:C:170:PHE:HD2  | 1.10                     | 0.98              |
| 1:A:173:PRO:O    | 1:A:174:LEU:HB2  | 1.60                     | 0.98              |
| 1:F:30:TYR:HB2   | 1:F:36:LYS:HE3   | 1.44                     | 0.98              |
| 1:E:19:ALA:O     | 1:E:23:VAL:HG12  | 1.64                     | 0.98              |
| 1:F:118:ILE:HG22 | 1:F:119:ILE:HD12 | 1.44                     | 0.98              |
| 1:A:97:LYS:CE    | 1:A:170:PHE:HD1  | 1.75                     | 0.98              |
| 1:D:121:THR:O    | 1:D:125:LEU:HD12 | 1.63                     | 0.98              |
| 1:F:116:ILE:HA   | 1:F:120:LEU:HD13 | 1.45                     | 0.98              |
| 1:A:49:MET:HE3   | 1:A:100:MET:HE1  | 1.46                     | 0.97              |
| 1:D:54:PHE:CE2   | 1:D:176:GLU:HB2  | 1.98                     | 0.97              |
| 1:E:128:MET:C    | 1:E:129:TYR:HD2  | 1.72                     | 0.97              |
| 1:E:40:THR:HG22  | 1:E:44:GLU:HG2   | 1.47                     | 0.97              |
| 1:E:115:LEU:HD13 | 1:E:115:LEU:C    | 1.88                     | 0.97              |
| 1:D:35:LEU:HD23  | 1:D:36:LYS:N     | 1.80                     | 0.97              |
| 1:E:13:LEU:H     | 1:E:13:LEU:HD22  | 1.25                     | 0.97              |
| 1:F:32:THR:O     | 1:F:35:LEU:HD23  | 1.65                     | 0.97              |
| 1:B:36:LYS:HE2   | 1:B:37:ILE:N     | 1.79                     | 0.97              |
| 1:C:98:LYS:HZ2   | 1:C:104:ARG:NH1  | 1.61                     | 0.96              |
| 1:E:54:PHE:CD2   | 1:E:55:TRP:CE3   | 2.47                     | 0.96              |
| 1:C:122:PRO:HA   | 1:C:125:LEU:CD1  | 1.94                     | 0.96              |
| 1:E:35:LEU:HD21  | 1:E:142:ARG:HG2  | 0.97                     | 0.96              |
| 1:D:10:SER:CB    | 1:D:172:LYS:CG   | 2.41                     | 0.96              |
| 1:E:112:VAL:HB   | 1:E:115:LEU:CB   | 1.94                     | 0.96              |
| 1:E:145:LYS:HB2  | 1:E:148:ILE:HG22 | 1.46                     | 0.96              |
| 1:D:12:ALA:O     | 1:D:16:VAL:CG2   | 2.14                     | 0.95              |
| 1:C:30:TYR:CB    | 1:C:37:ILE:HG13  | 1.95                     | 0.95              |
| 1:F:14:MET:HE3   | 1:F:14:MET:HA    | 1.46                     | 0.95              |
| 1:E:139:TRP:CZ3  | 1:E:142:ARG:CD   | 2.48                     | 0.95              |
| 1:E:143:LEU:CD2  | 1:E:146:THR:HG22 | 1.95                     | 0.95              |
| 1:C:10:SER:CB    | 1:C:170:PHE:HE1  | 1.69                     | 0.95              |
| 1:F:61:ALA:HB2   | 1:F:85:PHE:HD1   | 1.24                     | 0.95              |
| 1:C:98:LYS:NZ    | 1:C:104:ARG:HH12 | 1.65                     | 0.94              |
| 1:F:162:ASN:O    | 1:F:162:ASN:ND2  | 1.99                     | 0.94              |
| 1:A:49:MET:HE3   | 1:A:100:MET:CE   | 1.97                     | 0.94              |
| 1:A:70:LEU:H     | 1:A:70:LEU:HD12  | 1.31                     | 0.94              |
| 1:D:14:MET:CE    | 1:D:51:PHE:HE2   | 1.42                     | 0.94              |
| 1:E:56:ALA:O     | 1:E:60:THR:OG1   | 1.85                     | 0.94              |
| 1:E:128:MET:C    | 1:E:129:TYR:CD2  | 2.46                     | 0.94              |
| 1:C:32:THR:OG1   | 1:C:35:LEU:O     | 1.85                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:128:MET:O    | 1:E:129:TYR:HD2  | 1.50                     | 0.94              |
| 1:E:145:LYS:HZ2  | 1:E:149:PHE:HD2  | 1.10                     | 0.94              |
| 1:E:17:LEU:O     | 1:E:20:VAL:HG23  | 1.67                     | 0.93              |
| 1:E:90:ILE:HG12  | 1:E:112:VAL:HG11 | 1.51                     | 0.93              |
| 1:A:18:ILE:O     | 1:A:22:VAL:HG23  | 1.68                     | 0.93              |
| 1:E:68:MET:CE    | 2:E:201:FOL:C4   | 2.42                     | 0.93              |
| 1:F:13:LEU:HD21  | 1:F:51:PHE:HE2   | 1.29                     | 0.93              |
| 1:E:68:MET:HE1   | 2:E:201:FOL:C4A  | 1.99                     | 0.92              |
| 1:F:118:ILE:CG2  | 1:F:119:ILE:HD12 | 1.99                     | 0.92              |
| 1:E:14:MET:HA    | 1:E:17:LEU:CD2   | 1.99                     | 0.92              |
| 1:A:70:LEU:HB2   | 1:A:71:PHE:CD1   | 2.05                     | 0.92              |
| 1:C:49:MET:HE2   | 1:C:100:MET:HE1  | 1.52                     | 0.92              |
| 1:F:160:LEU:O    | 1:F:163:LYS:CG   | 2.18                     | 0.92              |
| 1:D:30:TYR:HE2   | 1:D:39:PHE:CE2   | 1.88                     | 0.91              |
| 1:C:77:PHE:H     | 2:C:201:FOL:HN1  | 1.09                     | 0.91              |
| 1:F:120:LEU:HD23 | 1:F:124:TRP:CZ3  | 2.04                     | 0.91              |
| 1:D:30:TYR:HE2   | 1:D:39:PHE:HE2   | 1.18                     | 0.91              |
| 1:E:115:LEU:HD13 | 1:E:116:ILE:CA   | 2.00                     | 0.91              |
| 1:C:162:ASN:O    | 1:C:163:LYS:C    | 2.14                     | 0.91              |
| 1:D:26:ARG:HH11  | 1:D:26:ARG:HG2   | 1.33                     | 0.91              |
| 1:E:36:LYS:HE3   | 1:E:38:SER:OG    | 1.69                     | 0.91              |
| 1:C:168:ARG:NH2  | 1:C:170:PHE:HD2  | 1.68                     | 0.91              |
| 1:D:33:THR:HG22  | 1:D:34:PHE:HE1   | 1.08                     | 0.91              |
| 1:E:23:VAL:CA    | 1:E:26:ARG:HD2   | 2.01                     | 0.91              |
| 1:C:49:MET:CE    | 1:C:95:TYR:HD2   | 1.75                     | 0.91              |
| 1:E:54:PHE:HE2   | 1:E:55:TRP:CZ3   | 1.73                     | 0.91              |
| 1:C:49:MET:HE3   | 1:C:95:TYR:HB3   | 1.52                     | 0.90              |
| 1:C:114:VAL:HG21 | 1:D:144:ILE:HD11 | 1.53                     | 0.90              |
| 1:E:36:LYS:O     | 2:E:201:FOL:HG1  | 1.71                     | 0.90              |
| 1:E:145:LYS:HD3  | 1:E:149:PHE:H    | 1.33                     | 0.90              |
| 1:D:33:THR:C     | 1:D:34:PHE:CD1   | 2.50                     | 0.90              |
| 1:F:116:ILE:HD12 | 1:F:120:LEU:HD13 | 1.54                     | 0.90              |
| 1:B:30:TYR:H     | 1:B:36:LYS:HZ1   | 1.20                     | 0.90              |
| 1:E:16:VAL:O     | 1:E:20:VAL:HG22  | 1.70                     | 0.90              |
| 1:F:23:VAL:HA    | 1:F:27:PHE:CD2   | 2.06                     | 0.90              |
| 1:D:14:MET:O     | 1:D:18:ILE:HG13  | 1.72                     | 0.90              |
| 1:E:172:LYS:HB3  | 1:E:173:PRO:HA   | 1.52                     | 0.90              |
| 1:D:10:SER:HG    | 1:D:172:LYS:HB2  | 1.25                     | 0.90              |
| 1:F:112:VAL:O    | 1:F:116:ILE:HG22 | 1.72                     | 0.90              |
| 1:E:23:VAL:C     | 1:E:26:ARG:HB2   | 1.97                     | 0.89              |
| 1:F:35:LEU:HB2   | 1:F:145:LYS:NZ   | 1.87                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:26:ARG:HD2   | 1:A:27:PHE:CD2   | 2.07                     | 0.89              |
| 1:E:68:MET:HE1   | 2:E:201:FOL:C8A  | 2.02                     | 0.89              |
| 1:E:68:MET:HE2   | 2:E:201:FOL:N3   | 1.86                     | 0.89              |
| 1:A:50:ILE:O     | 1:A:173:PRO:HB3  | 1.70                     | 0.89              |
| 1:F:61:ALA:HB1   | 1:F:85:PHE:HE1   | 1.38                     | 0.89              |
| 1:E:112:VAL:CB   | 1:E:115:LEU:HB3  | 2.02                     | 0.89              |
| 1:D:117:ASN:ND2  | 2:D:201:FOL:O1   | 2.06                     | 0.89              |
| 1:C:96:TYR:OH    | 1:C:169:LEU:HD23 | 1.71                     | 0.89              |
| 1:E:40:THR:HG23  | 1:E:44:GLU:HG2   | 1.51                     | 0.89              |
| 1:E:47:ILE:HA    | 1:E:50:ILE:HG22  | 1.54                     | 0.89              |
| 1:E:69:LEU:HD13  | 1:E:70:LEU:CA    | 2.01                     | 0.89              |
| 1:F:61:ALA:CB    | 1:F:85:PHE:CE1   | 2.56                     | 0.89              |
| 1:B:164:ILE:HG12 | 1:B:165:PRO:HD2  | 1.53                     | 0.89              |
| 1:A:68:MET:HE1   | 1:A:75:GLY:O     | 1.72                     | 0.88              |
| 1:A:158:TYR:O    | 1:A:162:ASN:ND2  | 2.06                     | 0.88              |
| 1:A:171:GLY:C    | 1:A:173:PRO:HD3  | 1.97                     | 0.88              |
| 1:A:96:TYR:OH    | 1:A:174:LEU:HD11 | 1.73                     | 0.88              |
| 1:D:50:ILE:HG22  | 1:D:51:PHE:CD1   | 2.08                     | 0.88              |
| 1:F:19:ALA:O     | 1:F:23:VAL:HG12  | 1.74                     | 0.88              |
| 1:B:74:ALA:HB1   | 2:B:201:FOL:H92  | 1.55                     | 0.88              |
| 1:B:96:TYR:HE2   | 1:B:97:LYS:CE    | 1.85                     | 0.88              |
| 1:E:119:ILE:HG13 | 1:E:120:LEU:HB3  | 1.52                     | 0.88              |
| 1:D:33:THR:O     | 1:D:34:PHE:HD1   | 1.57                     | 0.88              |
| 1:F:14:MET:O     | 1:F:18:ILE:HG23  | 1.74                     | 0.88              |
| 1:A:132:ASN:O    | 1:A:132:ASN:ND2  | 2.07                     | 0.88              |
| 1:F:65:VAL:O     | 1:F:69:LEU:HD12  | 1.74                     | 0.88              |
| 1:E:139:TRP:HZ3  | 1:E:142:ARG:CD   | 1.87                     | 0.88              |
| 1:D:10:SER:HB3   | 1:D:172:LYS:CD   | 2.04                     | 0.87              |
| 1:F:103:GLN:HE21 | 1:F:103:GLN:HA   | 1.36                     | 0.87              |
| 1:C:151:PRO:O    | 1:C:155:ILE:HG12 | 1.74                     | 0.87              |
| 1:B:135:ASN:HB2  | 1:B:138:TRP:HB2  | 1.55                     | 0.87              |
| 1:F:73:LYS:CD    | 2:F:201:FOL:C7   | 2.51                     | 0.87              |
| 1:E:143:LEU:CD2  | 1:E:146:THR:CG2  | 2.53                     | 0.87              |
| 1:A:97:LYS:HE3   | 1:A:170:PHE:CD1  | 2.08                     | 0.87              |
| 1:E:13:LEU:O     | 1:E:16:VAL:HG23  | 1.75                     | 0.87              |
| 1:F:74:ALA:HB2   | 2:F:201:FOL:H7   | 1.57                     | 0.87              |
| 1:E:54:PHE:HD2   | 1:E:55:TRP:CZ3   | 1.72                     | 0.86              |
| 1:F:43:PRO:O     | 1:F:47:ILE:HD13  | 1.75                     | 0.86              |
| 1:F:116:ILE:CD1  | 1:F:120:LEU:HD13 | 2.05                     | 0.86              |
| 1:F:141:PRO:HB2  | 1:F:142:ARG:HG3  | 1.56                     | 0.86              |
| 1:E:68:MET:HE3   | 2:E:201:FOL:NA2  | 1.90                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:139:TRP:HZ3  | 1:E:142:ARG:HD2  | 1.32                     | 0.86              |
| 1:C:70:LEU:C     | 1:C:72:PRO:CD    | 2.42                     | 0.86              |
| 1:E:14:MET:HA    | 1:E:17:LEU:HD23  | 1.54                     | 0.86              |
| 1:F:74:ALA:CB    | 2:F:201:FOL:H7   | 2.05                     | 0.86              |
| 1:E:36:LYS:HB2   | 2:E:201:FOL:C12  | 2.05                     | 0.86              |
| 1:F:16:VAL:HG23  | 1:F:17:LEU:CD2   | 2.05                     | 0.86              |
| 1:F:16:VAL:O     | 1:F:20:VAL:HG23  | 1.76                     | 0.86              |
| 1:F:160:LEU:HA   | 1:F:163:LYS:HG2  | 1.58                     | 0.86              |
| 1:F:116:ILE:CD1  | 1:F:120:LEU:HD22 | 2.04                     | 0.86              |
| 1:D:10:SER:HB3   | 1:D:172:LYS:HD2  | 1.58                     | 0.86              |
| 1:E:26:ARG:N     | 1:E:27:PHE:HA    | 1.89                     | 0.86              |
| 1:E:115:LEU:HD22 | 1:E:115:LEU:C    | 1.99                     | 0.86              |
| 1:D:150:PHE:O    | 1:D:154:VAL:HG23 | 1.75                     | 0.85              |
| 1:E:10:SER:OG    | 1:E:170:PHE:CD2  | 2.28                     | 0.85              |
| 1:D:33:THR:CG2   | 1:D:34:PHE:HE1   | 1.76                     | 0.85              |
| 1:E:17:LEU:O     | 1:E:21:VAL:HG23  | 1.76                     | 0.85              |
| 1:F:80:PHE:CE1   | 2:F:201:FOL:O4   | 2.28                     | 0.85              |
| 1:B:135:ASN:HB2  | 1:B:138:TRP:CB   | 2.07                     | 0.85              |
| 1:B:128:MET:HE2  | 1:B:129:TYR:CE2  | 2.10                     | 0.85              |
| 1:C:109:THR:O    | 1:C:113:THR:HG22 | 1.77                     | 0.85              |
| 1:C:109:THR:HG22 | 1:C:153:GLN:NE2  | 1.92                     | 0.85              |
| 1:F:13:LEU:HD22  | 1:F:14:MET:N     | 1.92                     | 0.85              |
| 1:F:80:PHE:HE1   | 2:F:201:FOL:CD   | 1.89                     | 0.85              |
| 1:B:137:ALA:HB1  | 1:B:140:VAL:CG2  | 2.06                     | 0.85              |
| 1:C:27:PHE:CE1   | 1:C:71:PHE:CZ    | 2.64                     | 0.85              |
| 1:F:30:TYR:CA    | 1:F:36:LYS:HZ2   | 1.89                     | 0.84              |
| 1:E:62:VAL:O     | 1:E:66:VAL:HG23  | 1.75                     | 0.84              |
| 1:E:147:VAL:HB   | 1:F:150:PHE:CZ   | 2.12                     | 0.84              |
| 1:F:46:LEU:O     | 1:F:50:ILE:HG12  | 1.76                     | 0.84              |
| 1:E:145:LYS:HD3  | 1:E:149:PHE:HB3  | 1.59                     | 0.84              |
| 1:F:15:GLY:O     | 1:F:18:ILE:HG13  | 1.76                     | 0.84              |
| 1:F:110:LEU:O    | 1:F:114:VAL:HG12 | 1.75                     | 0.84              |
| 1:A:26:ARG:HG2   | 1:A:27:PHE:CG    | 2.12                     | 0.84              |
| 1:B:121:THR:HG21 | 2:B:201:FOL:HA   | 1.58                     | 0.84              |
| 1:E:40:THR:OG1   | 1:E:44:GLU:OE2   | 1.95                     | 0.84              |
| 1:D:10:SER:CB    | 1:D:172:LYS:CB   | 2.55                     | 0.84              |
| 1:D:140:VAL:HG13 | 1:D:141:PRO:HD3  | 1.56                     | 0.84              |
| 1:E:10:SER:HA    | 1:E:170:PHE:HE2  | 1.43                     | 0.84              |
| 1:E:143:LEU:HD23 | 1:E:146:THR:HG22 | 1.57                     | 0.84              |
| 1:F:13:LEU:HD11  | 1:F:51:PHE:HZ    | 1.42                     | 0.84              |
| 1:F:30:TYR:O     | 1:F:36:LYS:NZ    | 2.10                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:145:LYS:HA   | 1:F:148:ILE:HG13 | 1.59                     | 0.84              |
| 1:A:24:PHE:CD2   | 1:A:39:PHE:O     | 2.31                     | 0.84              |
| 1:B:30:TYR:CB    | 1:B:36:LYS:CE    | 2.55                     | 0.84              |
| 1:D:68:MET:HE1   | 1:D:74:ALA:HB3   | 1.59                     | 0.84              |
| 1:D:19:ALA:O     | 1:D:23:VAL:HG22  | 1.77                     | 0.84              |
| 1:E:40:THR:HG23  | 1:E:43:PRO:HG2   | 1.60                     | 0.84              |
| 1:A:50:ILE:HG22  | 1:A:173:PRO:HB3  | 1.60                     | 0.83              |
| 1:F:30:TYR:N     | 1:F:36:LYS:HZ2   | 1.70                     | 0.83              |
| 1:F:86:LEU:O     | 1:F:90:ILE:HG13  | 1.77                     | 0.83              |
| 1:F:122:PRO:HA   | 1:F:125:LEU:CD1  | 2.05                     | 0.83              |
| 1:F:42:ILE:HG23  | 1:F:43:PRO:CD    | 2.07                     | 0.83              |
| 1:F:61:ALA:HB2   | 1:F:85:PHE:CE1   | 2.13                     | 0.83              |
| 1:A:126:SER:CA   | 1:A:131:VAL:HG21 | 2.08                     | 0.83              |
| 1:E:59:GLY:O     | 1:E:62:VAL:HG22  | 1.78                     | 0.83              |
| 1:F:42:ILE:CG2   | 1:F:43:PRO:HD3   | 2.09                     | 0.83              |
| 1:F:138:TRP:O    | 1:F:139:TRP:CE3  | 2.31                     | 0.83              |
| 1:C:124:TRP:O    | 1:C:128:MET:HG2  | 1.79                     | 0.83              |
| 1:E:68:MET:HE1   | 2:E:201:FOL:N1   | 1.93                     | 0.83              |
| 1:C:71:PHE:N     | 1:C:72:PRO:HD3   | 1.85                     | 0.83              |
| 1:C:114:VAL:HG21 | 1:D:144:ILE:CD1  | 2.08                     | 0.83              |
| 1:C:150:PHE:O    | 1:C:153:GLN:HG2  | 1.78                     | 0.83              |
| 1:C:83:ASN:ND2   | 1:C:124:TRP:HE1  | 1.77                     | 0.82              |
| 1:E:145:LYS:HE3  | 1:E:150:PHE:N    | 1.94                     | 0.82              |
| 1:A:14:MET:CE    | 1:A:51:PHE:CE2   | 2.62                     | 0.82              |
| 1:A:97:LYS:CE    | 1:A:170:PHE:CD1  | 2.63                     | 0.82              |
| 1:F:81:THR:HG23  | 1:F:85:PHE:CZ    | 2.13                     | 0.82              |
| 1:E:69:LEU:HD13  | 1:E:70:LEU:H     | 1.00                     | 0.82              |
| 1:F:30:TYR:CA    | 1:F:36:LYS:NZ    | 2.42                     | 0.82              |
| 1:E:13:LEU:HA    | 1:E:16:VAL:CG2   | 2.10                     | 0.82              |
| 1:E:54:PHE:HE2   | 1:E:55:TRP:HZ3   | 0.86                     | 0.82              |
| 1:B:36:LYS:HG3   | 1:B:37:ILE:N     | 1.92                     | 0.82              |
| 1:F:26:ARG:HG3   | 1:F:26:ARG:HH11  | 1.45                     | 0.82              |
| 1:E:142:ARG:O    | 1:E:143:LEU:HB2  | 1.78                     | 0.81              |
| 1:A:97:LYS:HE2   | 1:A:170:PHE:HD1  | 1.42                     | 0.81              |
| 1:D:97:LYS:O     | 1:D:98:LYS:HD3   | 1.81                     | 0.81              |
| 1:F:108:ALA:O    | 1:F:112:VAL:HG23 | 1.79                     | 0.81              |
| 1:F:119:ILE:HG22 | 1:F:123:LEU:CD1  | 2.10                     | 0.81              |
| 1:F:120:LEU:HD23 | 1:F:124:TRP:HZ3  | 1.42                     | 0.81              |
| 1:F:120:LEU:HB3  | 1:F:124:TRP:HZ3  | 1.45                     | 0.81              |
| 1:A:18:ILE:CD1   | 1:A:59:GLY:O     | 2.28                     | 0.81              |
| 1:C:168:ARG:HD3  | 1:C:168:ARG:C    | 2.06                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:55:TRP:HD1   | 1:C:172:LYS:HB2  | 1.46                     | 0.81              |
| 1:E:39:PHE:CE1   | 1:E:41:PHE:HE1   | 1.98                     | 0.81              |
| 1:F:30:TYR:H     | 1:F:36:LYS:HZ1   | 0.84                     | 0.81              |
| 1:A:123:LEU:O    | 1:A:126:SER:OG   | 1.99                     | 0.80              |
| 1:C:111:LEU:HD23 | 1:C:111:LEU:O    | 1.81                     | 0.80              |
| 1:D:148:ILE:HG13 | 1:D:149:PHE:N    | 1.94                     | 0.80              |
| 1:A:170:PHE:HD2  | 1:A:171:GLY:H    | 1.29                     | 0.80              |
| 1:E:39:PHE:CE1   | 1:E:41:PHE:CE1   | 2.68                     | 0.80              |
| 1:F:120:LEU:HB3  | 1:F:124:TRP:CZ3  | 2.16                     | 0.80              |
| 1:A:171:GLY:O    | 1:A:173:PRO:CD   | 2.29                     | 0.80              |
| 1:A:171:GLY:O    | 1:A:173:PRO:HD2  | 1.82                     | 0.80              |
| 1:F:73:LYS:HD2   | 2:F:201:FOL:H7   | 1.62                     | 0.80              |
| 1:D:13:LEU:HA    | 1:D:16:VAL:HG23  | 1.64                     | 0.80              |
| 1:E:14:MET:SD    | 1:E:18:ILE:HD11  | 2.21                     | 0.80              |
| 1:F:64:ASP:HB2   | 1:F:80:PHE:CZ    | 2.16                     | 0.80              |
| 1:C:48:GLY:O     | 1:C:92:GLY:HA2   | 1.82                     | 0.79              |
| 1:F:68:MET:SD    | 2:F:201:FOL:C8A  | 2.71                     | 0.79              |
| 1:A:97:LYS:HE3   | 1:A:170:PHE:HD1  | 1.44                     | 0.79              |
| 1:B:164:ILE:HD13 | 1:B:165:PRO:N    | 1.96                     | 0.79              |
| 1:B:46:LEU:HD12  | 1:B:49:MET:HE3   | 1.63                     | 0.79              |
| 1:A:103:GLN:OE1  | 1:A:104:ARG:CD   | 2.30                     | 0.79              |
| 1:D:125:LEU:HD12 | 1:D:125:LEU:H    | 1.46                     | 0.79              |
| 1:E:29:ALA:HB2   | 1:E:39:PHE:CE2   | 2.17                     | 0.79              |
| 1:A:125:LEU:O    | 1:A:129:TYR:HB2  | 1.83                     | 0.79              |
| 1:C:98:LYS:HZ1   | 1:C:104:ARG:NH1  | 1.76                     | 0.79              |
| 1:E:112:VAL:CA   | 1:E:115:LEU:HB3  | 2.12                     | 0.79              |
| 1:F:117:ASN:O    | 1:F:121:THR:OG1  | 1.99                     | 0.78              |
| 1:F:160:LEU:C    | 1:F:163:LYS:HG3  | 2.06                     | 0.78              |
| 1:D:10:SER:OG    | 1:D:172:LYS:CG   | 2.30                     | 0.78              |
| 1:E:36:LYS:HB2   | 2:E:201:FOL:H12  | 1.65                     | 0.78              |
| 1:A:126:SER:HA   | 1:A:131:VAL:HG22 | 1.64                     | 0.78              |
| 1:D:50:ILE:HG22  | 1:D:51:PHE:HD1   | 1.46                     | 0.78              |
| 1:C:30:TYR:CG    | 1:C:37:ILE:HG13  | 2.19                     | 0.78              |
| 1:E:13:LEU:C     | 1:E:16:VAL:HG23  | 2.07                     | 0.78              |
| 1:D:14:MET:CE    | 1:D:51:PHE:HD2   | 1.58                     | 0.78              |
| 1:F:30:TYR:H     | 1:F:36:LYS:NZ    | 1.61                     | 0.78              |
| 1:C:68:MET:HE3   | 1:C:74:ALA:HB3   | 1.65                     | 0.78              |
| 1:E:52:GLY:O     | 1:E:56:ALA:HB2   | 1.84                     | 0.78              |
| 1:F:68:MET:HE1   | 2:F:201:FOL:N8   | 1.97                     | 0.78              |
| 1:E:30:TYR:HB2   | 1:E:37:ILE:CG2   | 2.12                     | 0.78              |
| 1:D:121:THR:O    | 1:D:125:LEU:CD1  | 2.32                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:168:ARG:NH2  | 1:C:170:PHE:CD2  | 2.52                     | 0.78              |
| 1:A:173:PRO:O    | 1:A:174:LEU:CB   | 2.32                     | 0.77              |
| 1:B:50:ILE:HG22  | 1:B:51:PHE:CD1   | 2.19                     | 0.77              |
| 1:B:145:LYS:NZ   | 2:B:201:FOL:OE1  | 2.18                     | 0.77              |
| 1:C:34:PHE:HE1   | 1:C:129:TYR:HD2  | 1.31                     | 0.77              |
| 1:C:45:SER:O     | 1:C:49:MET:SD    | 2.43                     | 0.77              |
| 1:D:20:VAL:O     | 1:D:23:VAL:HG23  | 1.84                     | 0.77              |
| 1:E:29:ALA:HB2   | 1:E:39:PHE:CD2   | 2.20                     | 0.77              |
| 1:F:28:PHE:HB2   | 1:F:39:PHE:CE2   | 2.18                     | 0.77              |
| 1:F:61:ALA:CB    | 1:F:85:PHE:CD1   | 2.67                     | 0.77              |
| 1:F:64:ASP:OD1   | 1:F:65:VAL:N     | 2.17                     | 0.77              |
| 1:F:73:LYS:HD2   | 2:F:201:FOL:C9   | 2.13                     | 0.77              |
| 1:F:119:ILE:O    | 1:F:123:LEU:HD12 | 1.85                     | 0.77              |
| 1:E:115:LEU:CD2  | 1:E:119:ILE:HD11 | 2.14                     | 0.77              |
| 1:B:30:TYR:CA    | 1:B:36:LYS:HZ1   | 1.94                     | 0.77              |
| 1:D:142:ARG:O    | 1:D:146:THR:OG1  | 2.03                     | 0.77              |
| 1:E:14:MET:O     | 1:E:17:LEU:HD23  | 1.84                     | 0.77              |
| 1:E:153:GLN:OE1  | 1:E:153:GLN:N    | 2.18                     | 0.77              |
| 1:F:18:ILE:HD12  | 1:F:19:ALA:N     | 1.99                     | 0.77              |
| 1:C:96:TYR:CE1   | 1:C:169:LEU:HD21 | 2.20                     | 0.77              |
| 1:B:36:LYS:CE    | 1:B:37:ILE:H     | 1.90                     | 0.76              |
| 1:C:125:LEU:HA   | 1:C:128:MET:HG3  | 1.65                     | 0.76              |
| 1:E:40:THR:HG22  | 1:E:43:PRO:HD2   | 1.68                     | 0.76              |
| 1:B:37:ILE:H     | 1:B:37:ILE:HD12  | 1.48                     | 0.76              |
| 1:E:14:MET:SD    | 1:E:17:LEU:HD21  | 2.24                     | 0.76              |
| 1:F:109:THR:HG22 | 1:F:153:GLN:HE21 | 1.48                     | 0.76              |
| 1:E:109:THR:O    | 1:E:113:THR:OG1  | 2.01                     | 0.76              |
| 1:F:104:ARG:HG2  | 1:F:104:ARG:HH21 | 1.51                     | 0.76              |
| 1:B:30:TYR:CA    | 1:B:36:LYS:NZ    | 2.36                     | 0.76              |
| 1:C:26:ARG:HG2   | 1:C:26:ARG:HH11  | 1.49                     | 0.76              |
| 1:E:25:SER:C     | 1:E:27:PHE:HA    | 2.11                     | 0.76              |
| 1:B:31:GLU:HB3   | 1:B:36:LYS:HD3   | 1.66                     | 0.76              |
| 1:F:61:ALA:CB    | 1:F:85:PHE:HE1   | 1.97                     | 0.76              |
| 1:A:49:MET:SD    | 1:A:95:TYR:HB3   | 2.26                     | 0.76              |
| 1:E:23:VAL:HA    | 1:E:26:ARG:HB2   | 1.67                     | 0.75              |
| 1:B:30:TYR:N     | 1:B:36:LYS:HZ2   | 1.83                     | 0.75              |
| 1:B:77:PHE:H     | 2:B:201:FOL:HN1  | 1.34                     | 0.75              |
| 1:E:74:ALA:HB1   | 1:E:75:GLY:C     | 2.11                     | 0.75              |
| 1:E:139:TRP:C    | 1:E:141:PRO:HD2  | 2.10                     | 0.75              |
| 1:E:17:LEU:HA    | 1:E:20:VAL:CG2   | 2.17                     | 0.75              |
| 1:E:61:ALA:HA    | 1:E:64:ASP:OD2   | 1.87                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:80:PHE:CZ    | 2:F:201:FOL:O4   | 2.40                     | 0.75              |
| 1:F:94:PHE:CD2   | 1:F:108:ALA:HB1  | 2.22                     | 0.75              |
| 1:F:25:SER:O     | 1:F:29:ALA:CB    | 2.34                     | 0.75              |
| 1:C:55:TRP:CD1   | 1:C:172:LYS:HB2  | 2.21                     | 0.75              |
| 1:D:26:ARG:HG2   | 1:D:26:ARG:NH1   | 1.97                     | 0.75              |
| 1:F:17:LEU:O     | 1:F:21:VAL:HG23  | 1.86                     | 0.75              |
| 1:F:39:PHE:CA    | 1:F:41:PHE:CE2   | 2.63                     | 0.75              |
| 1:B:128:MET:HE2  | 1:B:129:TYR:HE2  | 1.50                     | 0.74              |
| 1:C:163:LYS:HE2  | 1:C:166:PHE:HB3  | 1.68                     | 0.74              |
| 1:E:52:GLY:O     | 1:E:56:ALA:CB    | 2.35                     | 0.74              |
| 1:F:14:MET:HE3   | 1:F:14:MET:CA    | 2.15                     | 0.74              |
| 1:C:112:VAL:C    | 1:C:116:ILE:HG22 | 2.11                     | 0.74              |
| 1:E:115:LEU:HD22 | 1:E:119:ILE:CD1  | 2.17                     | 0.74              |
| 1:E:128:MET:O    | 1:E:129:TYR:CD2  | 2.38                     | 0.74              |
| 1:D:36:LYS:HE2   | 1:D:38:SER:HB3   | 1.68                     | 0.74              |
| 1:E:23:VAL:O     | 1:E:26:ARG:CB    | 2.34                     | 0.74              |
| 1:F:116:ILE:HA   | 1:F:120:LEU:CD1  | 2.17                     | 0.74              |
| 1:C:10:SER:HB3   | 1:C:170:PHE:HE1  | 0.92                     | 0.74              |
| 1:C:148:ILE:O    | 1:C:151:PRO:CD   | 2.34                     | 0.74              |
| 1:A:49:MET:O     | 1:A:96:TYR:HD1   | 1.69                     | 0.74              |
| 1:B:12:ALA:O     | 1:B:16:VAL:HG23  | 1.88                     | 0.74              |
| 1:B:73:LYS:O     | 1:B:74:ALA:HB3   | 1.87                     | 0.74              |
| 1:D:26:ARG:HG3   | 1:D:71:PHE:CD2   | 2.22                     | 0.74              |
| 1:E:14:MET:CA    | 1:E:17:LEU:HD23  | 2.18                     | 0.74              |
| 1:B:13:LEU:C     | 1:B:13:LEU:HD23  | 2.12                     | 0.74              |
| 1:D:10:SER:HB3   | 1:D:172:LYS:HG3  | 1.55                     | 0.74              |
| 1:C:30:TYR:HD2   | 1:C:32:THR:HG23  | 1.53                     | 0.74              |
| 1:D:137:ALA:O    | 1:D:140:VAL:HG12 | 1.88                     | 0.74              |
| 1:D:144:ILE:O    | 1:D:147:VAL:HG22 | 1.88                     | 0.74              |
| 1:E:143:LEU:HD22 | 1:E:146:THR:HG22 | 1.69                     | 0.74              |
| 1:A:30:TYR:HB3   | 1:A:37:ILE:HB    | 1.71                     | 0.73              |
| 1:D:30:TYR:CE2   | 1:D:39:PHE:HE2   | 2.02                     | 0.73              |
| 1:C:30:TYR:HB2   | 1:C:37:ILE:CG1   | 2.18                     | 0.73              |
| 1:E:42:ILE:N     | 1:E:42:ILE:HD13  | 2.02                     | 0.73              |
| 1:E:143:LEU:HD23 | 1:E:146:THR:CG2  | 2.15                     | 0.73              |
| 1:A:148:ILE:O    | 1:A:151:PRO:HD2  | 1.88                     | 0.73              |
| 1:C:80:PHE:O     | 1:C:83:ASN:HB2   | 1.87                     | 0.73              |
| 1:D:147:VAL:O    | 1:D:151:PRO:HD2  | 1.87                     | 0.73              |
| 1:B:96:TYR:CE2   | 1:B:97:LYS:HD2   | 2.24                     | 0.73              |
| 1:F:13:LEU:HD22  | 1:F:13:LEU:C     | 2.13                     | 0.73              |
| 1:F:61:ALA:HB1   | 1:F:85:PHE:CE1   | 2.18                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:49:MET:HE1   | 1:B:160:LEU:HG   | 1.70                     | 0.73              |
| 1:C:98:LYS:NZ    | 1:C:104:ARG:HH11 | 1.85                     | 0.73              |
| 1:C:168:ARG:O    | 1:C:169:LEU:HD12 | 1.88                     | 0.73              |
| 1:E:55:TRP:CE3   | 1:E:55:TRP:HA    | 2.23                     | 0.73              |
| 1:F:80:PHE:CD2   | 2:F:201:FOL:C2   | 2.71                     | 0.73              |
| 1:F:109:THR:CG2  | 1:F:153:GLN:HE21 | 2.00                     | 0.73              |
| 1:A:17:LEU:HB3   | 1:A:47:ILE:HD11  | 1.70                     | 0.73              |
| 1:A:169:LEU:HD12 | 1:A:169:LEU:O    | 1.88                     | 0.73              |
| 1:C:61:ALA:HB2   | 1:C:85:PHE:HB2   | 1.71                     | 0.73              |
| 1:C:116:ILE:HG23 | 1:C:117:ASN:N    | 2.02                     | 0.73              |
| 1:E:110:LEU:HD21 | 1:F:144:ILE:HD12 | 1.71                     | 0.72              |
| 1:A:24:PHE:HD2   | 1:A:39:PHE:O     | 1.71                     | 0.72              |
| 1:A:126:SER:CA   | 1:A:131:VAL:CG2  | 2.62                     | 0.72              |
| 1:C:122:PRO:O    | 1:C:126:SER:OG   | 2.03                     | 0.72              |
| 1:E:22:VAL:CG2   | 1:E:67:GLY:CA    | 2.67                     | 0.72              |
| 1:F:116:ILE:HD13 | 1:F:120:LEU:HD22 | 1.69                     | 0.72              |
| 1:A:42:ILE:HD12  | 1:A:160:LEU:HD13 | 1.71                     | 0.72              |
| 1:D:125:LEU:HD12 | 1:D:125:LEU:N    | 2.03                     | 0.72              |
| 1:E:115:LEU:HD13 | 1:E:116:ILE:H    | 1.50                     | 0.72              |
| 1:B:11:ILE:HG13  | 1:B:12:ALA:N     | 2.04                     | 0.72              |
| 1:C:42:ILE:HG22  | 1:C:160:LEU:HD13 | 1.72                     | 0.72              |
| 1:E:70:LEU:HD23  | 1:E:70:LEU:C     | 2.15                     | 0.72              |
| 1:E:153:GLN:NE2  | 1:E:154:VAL:HG13 | 2.05                     | 0.72              |
| 1:B:30:TYR:HB2   | 1:B:36:LYS:HZ1   | 1.54                     | 0.72              |
| 1:C:66:VAL:O     | 1:C:70:LEU:HD23  | 1.90                     | 0.72              |
| 1:C:96:TYR:CE1   | 1:C:169:LEU:CD2  | 2.72                     | 0.72              |
| 1:C:171:GLY:O    | 1:C:172:LYS:HD3  | 1.90                     | 0.72              |
| 1:F:10:SER:O     | 1:F:13:LEU:CD1   | 2.38                     | 0.72              |
| 1:F:51:PHE:O     | 1:F:55:TRP:HB2   | 1.90                     | 0.72              |
| 1:C:30:TYR:CD2   | 1:C:32:THR:HG23  | 2.25                     | 0.72              |
| 1:F:82:LEU:HA    | 1:F:85:PHE:CD2   | 2.25                     | 0.72              |
| 1:A:70:LEU:HB2   | 1:A:71:PHE:CE1   | 2.25                     | 0.72              |
| 1:B:20:VAL:O     | 1:B:23:VAL:HG22  | 1.90                     | 0.72              |
| 1:D:18:ILE:HG23  | 1:D:63:ALA:HB2   | 1.71                     | 0.72              |
| 1:E:13:LEU:N     | 1:E:13:LEU:HD13  | 2.04                     | 0.72              |
| 1:A:170:PHE:HD2  | 1:A:171:GLY:N    | 1.87                     | 0.71              |
| 1:B:133:LEU:N    | 1:B:133:LEU:HD12 | 2.04                     | 0.71              |
| 1:D:122:PRO:HA   | 1:D:125:LEU:HD13 | 1.70                     | 0.71              |
| 1:E:115:LEU:CD1  | 1:E:115:LEU:C    | 2.52                     | 0.71              |
| 1:B:138:TRP:CE3  | 1:B:139:TRP:HA   | 2.25                     | 0.71              |
| 1:E:39:PHE:HD1   | 1:E:41:PHE:CD1   | 2.06                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:105:VAL:O    | 1:E:109:THR:HG23 | 1.90                     | 0.71              |
| 1:A:160:LEU:C    | 1:A:160:LEU:HD23 | 2.15                     | 0.71              |
| 1:B:37:ILE:N     | 1:B:37:ILE:HD12  | 2.05                     | 0.71              |
| 1:C:33:THR:HG22  | 1:C:129:TYR:HE2  | 1.56                     | 0.71              |
| 1:C:46:LEU:HA    | 1:C:49:MET:SD    | 2.30                     | 0.71              |
| 1:D:14:MET:HE1   | 1:D:51:PHE:HD2   | 0.82                     | 0.71              |
| 1:A:122:PRO:HA   | 1:A:125:LEU:HD13 | 1.72                     | 0.71              |
| 1:B:131:VAL:HG12 | 1:B:133:LEU:CD1  | 2.21                     | 0.71              |
| 1:E:42:ILE:O     | 1:E:46:LEU:N     | 2.22                     | 0.71              |
| 1:D:80:PHE:CE1   | 2:D:201:FOL:NA2  | 2.58                     | 0.71              |
| 1:E:36:LYS:CE    | 1:E:38:SER:OG    | 2.38                     | 0.71              |
| 1:F:110:LEU:C    | 1:F:110:LEU:HD23 | 2.15                     | 0.71              |
| 1:F:119:ILE:HG22 | 1:F:123:LEU:HD11 | 1.72                     | 0.71              |
| 1:B:30:TYR:CB    | 1:B:36:LYS:HZ1   | 2.04                     | 0.71              |
| 1:B:95:TYR:HB3   | 1:B:100:MET:HE2  | 1.73                     | 0.71              |
| 1:C:174:LEU:C    | 1:C:174:LEU:HD22 | 2.15                     | 0.71              |
| 1:D:80:PHE:CE1   | 1:D:81:THR:HG23  | 2.25                     | 0.71              |
| 1:F:18:ILE:HD12  | 1:F:18:ILE:C     | 2.16                     | 0.71              |
| 1:E:64:ASP:OD1   | 1:E:65:VAL:N     | 2.23                     | 0.71              |
| 1:E:115:LEU:CD2  | 1:E:119:ILE:CD1  | 2.68                     | 0.71              |
| 1:E:13:LEU:HA    | 1:E:16:VAL:HG23  | 1.73                     | 0.70              |
| 1:F:111:LEU:C    | 1:F:111:LEU:HD23 | 2.15                     | 0.70              |
| 1:C:27:PHE:C     | 1:C:28:PHE:HD1   | 1.99                     | 0.70              |
| 1:B:13:LEU:HD23  | 1:B:14:MET:N     | 2.05                     | 0.70              |
| 1:F:32:THR:HG22  | 1:F:33:THR:N     | 2.04                     | 0.70              |
| 1:E:159:TYR:HA   | 1:E:162:ASN:OD1  | 1.91                     | 0.70              |
| 1:F:38:SER:HB2   | 1:F:40:THR:HG22  | 1.73                     | 0.70              |
| 1:F:104:ARG:HG2  | 1:F:104:ARG:NH2  | 2.05                     | 0.70              |
| 1:A:160:LEU:HD23 | 1:A:161:GLY:N    | 2.05                     | 0.70              |
| 1:C:49:MET:O     | 1:C:96:TYR:CD1   | 2.44                     | 0.70              |
| 1:F:13:LEU:HD21  | 1:F:14:MET:SD    | 2.31                     | 0.70              |
| 1:A:101:THR:O    | 1:A:102:TRP:C    | 2.33                     | 0.70              |
| 1:E:42:ILE:HD11  | 1:E:156:ALA:HB1  | 1.73                     | 0.70              |
| 1:E:115:LEU:CD1  | 1:E:116:ILE:H    | 2.04                     | 0.70              |
| 1:F:116:ILE:HD12 | 1:F:120:LEU:HB2  | 1.74                     | 0.70              |
| 1:A:70:LEU:HB2   | 1:A:71:PHE:HD1   | 1.51                     | 0.70              |
| 1:A:23:VAL:HA    | 1:A:26:ARG:HD3   | 1.73                     | 0.69              |
| 1:E:79:GLY:C     | 1:E:81:THR:H     | 1.99                     | 0.69              |
| 1:E:10:SER:HA    | 1:E:170:PHE:CE2  | 2.26                     | 0.69              |
| 1:F:35:LEU:HD23  | 1:F:35:LEU:O     | 1.92                     | 0.69              |
| 1:C:65:VAL:O     | 1:C:69:LEU:HB2   | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:18:ILE:HG23  | 1:E:63:ALA:HB1   | 1.72                     | 0.69              |
| 1:E:22:VAL:CG2   | 1:E:67:GLY:HA2   | 2.22                     | 0.69              |
| 1:E:29:ALA:HB1   | 1:E:30:TYR:HD2   | 1.56                     | 0.69              |
| 1:A:125:LEU:H    | 1:A:125:LEU:CD1  | 1.97                     | 0.69              |
| 1:C:70:LEU:H     | 1:C:70:LEU:CD2   | 2.04                     | 0.69              |
| 1:F:120:LEU:CB   | 1:F:124:TRP:HZ3  | 2.06                     | 0.69              |
| 1:B:64:ASP:CG    | 1:B:81:THR:HG22  | 2.18                     | 0.69              |
| 1:B:164:ILE:HD13 | 1:B:165:PRO:C    | 2.18                     | 0.69              |
| 1:F:64:ASP:HB2   | 1:F:80:PHE:HE2   | 1.52                     | 0.69              |
| 1:B:30:TYR:HB3   | 1:B:37:ILE:HD13  | 1.75                     | 0.69              |
| 1:D:117:ASN:O    | 1:D:142:ARG:NH1  | 2.25                     | 0.69              |
| 1:A:68:MET:HE2   | 1:A:75:GLY:O     | 1.90                     | 0.68              |
| 1:B:164:ILE:HD13 | 1:B:164:ILE:C    | 2.17                     | 0.68              |
| 1:D:140:VAL:CG1  | 1:D:141:PRO:HD3  | 2.22                     | 0.68              |
| 1:E:23:VAL:CA    | 1:E:26:ARG:HB2   | 2.23                     | 0.68              |
| 1:C:68:MET:HE2   | 1:C:71:PHE:O     | 1.94                     | 0.68              |
| 1:D:36:LYS:N     | 2:D:201:FOL:O    | 2.26                     | 0.68              |
| 1:D:80:PHE:CZ    | 2:D:201:FOL:NA2  | 2.60                     | 0.68              |
| 1:C:68:MET:HE1   | 1:C:72:PRO:C     | 2.18                     | 0.68              |
| 1:E:112:VAL:CB   | 1:E:115:LEU:CB   | 2.66                     | 0.68              |
| 1:A:96:TYR:OH    | 1:A:174:LEU:CD1  | 2.41                     | 0.68              |
| 1:A:101:THR:O    | 1:A:104:ARG:N    | 2.25                     | 0.68              |
| 1:B:131:VAL:HG12 | 1:B:133:LEU:HD11 | 1.75                     | 0.68              |
| 1:D:147:VAL:HG23 | 1:D:148:ILE:N    | 2.08                     | 0.68              |
| 1:F:13:LEU:HD21  | 1:F:51:PHE:CZ    | 2.29                     | 0.68              |
| 1:A:50:ILE:O     | 1:A:173:PRO:CG   | 2.42                     | 0.68              |
| 1:A:50:ILE:HB    | 1:A:51:PHE:CD1   | 2.28                     | 0.68              |
| 1:B:26:ARG:HG3   | 1:B:71:PHE:CG    | 2.29                     | 0.68              |
| 1:C:10:SER:HB2   | 1:C:170:PHE:CE1  | 2.23                     | 0.68              |
| 1:E:112:VAL:HA   | 1:E:115:LEU:H    | 1.58                     | 0.68              |
| 1:E:145:LYS:CD   | 1:E:149:PHE:H    | 2.07                     | 0.68              |
| 1:B:159:TYR:OH   | 1:B:164:ILE:HB   | 1.93                     | 0.68              |
| 1:E:43:PRO:HG2   | 1:E:44:GLU:H     | 1.59                     | 0.68              |
| 1:F:109:THR:O    | 1:F:113:THR:OG1  | 2.11                     | 0.68              |
| 1:F:120:LEU:CD2  | 1:F:124:TRP:HZ3  | 2.06                     | 0.68              |
| 1:A:117:ASN:O    | 1:A:142:ARG:NH1  | 2.26                     | 0.68              |
| 1:E:115:LEU:HD22 | 1:E:119:ILE:HD11 | 1.75                     | 0.68              |
| 1:F:73:LYS:CD    | 2:F:201:FOL:H92  | 2.24                     | 0.68              |
| 1:F:64:ASP:OD1   | 1:F:65:VAL:HG22  | 1.94                     | 0.68              |
| 1:E:66:VAL:O     | 1:E:69:LEU:HD12  | 1.94                     | 0.67              |
| 1:E:79:GLY:O     | 1:E:81:THR:N     | 2.26                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:172:LYS:CB   | 1:E:173:PRO:HA   | 2.21                     | 0.67              |
| 1:F:73:LYS:HD2   | 2:F:201:FOL:H92  | 1.74                     | 0.67              |
| 1:F:13:LEU:HD13  | 1:F:14:MET:H     | 1.59                     | 0.67              |
| 1:F:160:LEU:HA   | 1:F:163:LYS:CG   | 2.24                     | 0.67              |
| 1:B:109:THR:O    | 1:B:113:THR:OG1  | 2.10                     | 0.67              |
| 1:D:18:ILE:HG23  | 1:D:63:ALA:CB    | 2.24                     | 0.67              |
| 1:A:100:MET:CE   | 1:A:161:GLY:HA2  | 2.24                     | 0.67              |
| 1:C:66:VAL:O     | 1:C:70:LEU:CD2   | 2.42                     | 0.67              |
| 1:B:149:PHE:HD1  | 1:B:152:ILE:HD12 | 1.59                     | 0.67              |
| 1:D:160:LEU:C    | 1:D:160:LEU:HD23 | 2.19                     | 0.67              |
| 1:E:153:GLN:O    | 1:E:157:THR:HG23 | 1.95                     | 0.67              |
| 1:F:35:LEU:HB2   | 1:F:145:LYS:HZ3  | 1.57                     | 0.67              |
| 1:C:34:PHE:CE2   | 1:C:138:TRP:NE1  | 2.62                     | 0.67              |
| 1:C:97:LYS:HG3   | 1:C:169:LEU:CD2  | 2.25                     | 0.67              |
| 1:E:20:VAL:HA    | 1:E:23:VAL:CG1   | 2.25                     | 0.67              |
| 1:E:70:LEU:CD2   | 1:E:71:PHE:CD2   | 2.78                     | 0.67              |
| 1:F:103:GLN:HE21 | 1:F:103:GLN:CA   | 2.00                     | 0.67              |
| 1:B:173:PRO:HD2  | 1:B:173:PRO:O    | 1.94                     | 0.66              |
| 1:C:30:TYR:CD1   | 1:C:37:ILE:HD12  | 2.30                     | 0.66              |
| 1:F:26:ARG:HG3   | 1:F:26:ARG:NH1   | 2.11                     | 0.66              |
| 1:A:151:PRO:O    | 1:A:155:ILE:HD13 | 1.94                     | 0.66              |
| 1:D:21:VAL:HG22  | 1:D:43:PRO:HG2   | 1.78                     | 0.66              |
| 1:E:13:LEU:CA    | 1:E:16:VAL:HG23  | 2.26                     | 0.66              |
| 1:A:14:MET:HE3   | 1:A:51:PHE:CE2   | 2.29                     | 0.66              |
| 1:A:36:LYS:HG2   | 2:A:201:FOL:C11  | 2.26                     | 0.66              |
| 1:F:116:ILE:HG23 | 1:F:117:ASN:N    | 2.11                     | 0.66              |
| 1:D:140:VAL:HG13 | 1:D:141:PRO:CD   | 2.26                     | 0.66              |
| 1:E:145:LYS:HE3  | 1:E:150:PHE:H    | 1.59                     | 0.66              |
| 1:F:28:PHE:HB2   | 1:F:39:PHE:HE2   | 1.61                     | 0.66              |
| 1:E:12:ALA:O     | 1:E:16:VAL:HG22  | 1.96                     | 0.66              |
| 1:E:14:MET:HE3   | 1:E:18:ILE:HD11  | 1.77                     | 0.66              |
| 1:F:39:PHE:CA    | 1:F:41:PHE:HE2   | 1.91                     | 0.66              |
| 1:C:117:ASN:OD1  | 1:C:142:ARG:NH2  | 2.30                     | 0.65              |
| 1:E:14:MET:C     | 1:E:17:LEU:HD23  | 2.22                     | 0.65              |
| 1:E:141:PRO:C    | 1:E:144:ILE:HG22 | 2.20                     | 0.65              |
| 1:E:147:VAL:HB   | 1:F:150:PHE:HZ   | 1.58                     | 0.65              |
| 1:A:41:PHE:CE1   | 1:A:42:ILE:HG12  | 2.32                     | 0.65              |
| 1:D:54:PHE:CZ    | 1:D:176:GLU:CB   | 2.73                     | 0.65              |
| 1:E:32:THR:HB    | 1:E:35:LEU:O     | 1.96                     | 0.65              |
| 1:C:98:LYS:CE    | 1:C:104:ARG:HH11 | 2.10                     | 0.65              |
| 1:F:29:ALA:C     | 1:F:36:LYS:NZ    | 2.54                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:14:MET:SD    | 1:D:51:PHE:HE2   | 2.20                     | 0.65              |
| 1:D:33:THR:CG2   | 1:D:34:PHE:CD1   | 2.68                     | 0.65              |
| 1:E:77:PHE:CG    | 1:E:78:PRO:CD    | 2.77                     | 0.65              |
| 1:A:171:GLY:C    | 1:A:173:PRO:CD   | 2.70                     | 0.65              |
| 1:C:83:ASN:ND2   | 1:C:124:TRP:NE1  | 2.45                     | 0.64              |
| 1:F:36:LYS:HG3   | 1:F:37:ILE:N     | 2.11                     | 0.64              |
| 1:D:10:SER:OG    | 1:D:172:LYS:HB3  | 1.92                     | 0.64              |
| 1:A:114:VAL:O    | 1:A:119:ILE:HG13 | 1.98                     | 0.64              |
| 1:B:164:ILE:HD13 | 1:B:165:PRO:O    | 1.97                     | 0.64              |
| 1:C:170:PHE:O    | 1:C:172:LYS:HD3  | 1.97                     | 0.64              |
| 1:D:14:MET:HE1   | 1:D:51:PHE:CE2   | 1.78                     | 0.64              |
| 1:F:64:ASP:OD1   | 1:F:65:VAL:CG2   | 2.45                     | 0.64              |
| 1:C:64:ASP:OD2   | 1:C:81:THR:HG23  | 1.98                     | 0.64              |
| 1:D:143:LEU:O    | 1:D:147:VAL:HG13 | 1.96                     | 0.64              |
| 1:E:58:ILE:O     | 1:E:62:VAL:HG13  | 1.97                     | 0.64              |
| 1:F:30:TYR:O     | 1:F:36:LYS:CE    | 2.46                     | 0.64              |
| 1:B:30:TYR:CB    | 1:B:36:LYS:NZ    | 2.61                     | 0.64              |
| 1:D:35:LEU:HD23  | 1:D:35:LEU:C     | 2.22                     | 0.64              |
| 1:B:77:PHE:O     | 2:B:201:FOL:NA2  | 2.30                     | 0.64              |
| 1:C:153:GLN:O    | 1:C:157:THR:HG23 | 1.96                     | 0.64              |
| 1:A:49:MET:HE3   | 1:A:100:MET:HE2  | 1.79                     | 0.64              |
| 1:D:14:MET:HE2   | 1:D:51:PHE:HE2   | 0.85                     | 0.64              |
| 1:E:55:TRP:HA    | 1:E:58:ILE:CG1   | 2.27                     | 0.64              |
| 1:F:80:PHE:CG    | 2:F:201:FOL:N3   | 2.66                     | 0.64              |
| 1:A:7:GLY:O      | 1:A:11:ILE:HG13  | 1.97                     | 0.64              |
| 1:A:18:ILE:HD11  | 1:A:59:GLY:O     | 1.96                     | 0.64              |
| 1:A:19:ALA:O     | 1:A:23:VAL:HG23  | 1.98                     | 0.64              |
| 1:E:39:PHE:CD1   | 1:E:41:PHE:CZ    | 2.80                     | 0.64              |
| 1:F:150:PHE:CA   | 1:F:153:GLN:HB3  | 2.28                     | 0.64              |
| 1:F:150:PHE:HA   | 1:F:153:GLN:HB3  | 1.79                     | 0.64              |
| 1:A:64:ASP:OD2   | 1:A:81:THR:HG22  | 1.98                     | 0.64              |
| 1:A:95:TYR:O     | 1:A:97:LYS:HA    | 1.98                     | 0.64              |
| 1:C:34:PHE:CD2   | 1:C:138:TRP:CD1  | 2.85                     | 0.64              |
| 1:C:97:LYS:HG3   | 1:C:169:LEU:HD21 | 1.80                     | 0.64              |
| 1:F:45:SER:HA    | 1:F:91:TYR:CD2   | 2.33                     | 0.64              |
| 1:B:50:ILE:HG22  | 1:B:51:PHE:HD1   | 1.62                     | 0.63              |
| 1:C:71:PHE:H     | 1:C:72:PRO:HD2   | 1.62                     | 0.63              |
| 1:D:171:GLY:O    | 1:D:173:PRO:HD3  | 1.98                     | 0.63              |
| 1:E:149:PHE:CD1  | 1:E:152:ILE:HD11 | 2.32                     | 0.63              |
| 1:B:36:LYS:HE2   | 1:B:37:ILE:CD1   | 2.28                     | 0.63              |
| 1:C:94:PHE:CD1   | 1:C:108:ALA:CB   | 2.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:94:PHE:CE1   | 1:C:108:ALA:HA   | 2.33                     | 0.63              |
| 1:D:133:LEU:HG   | 1:D:138:TRP:HZ3  | 1.62                     | 0.63              |
| 1:D:30:TYR:CE2   | 1:D:39:PHE:CE2   | 2.79                     | 0.63              |
| 1:D:77:PHE:O     | 1:D:80:PHE:CE2   | 2.51                     | 0.63              |
| 1:C:58:ILE:O     | 1:C:62:VAL:HG13  | 1.97                     | 0.63              |
| 1:A:39:PHE:HA    | 1:A:41:PHE:CE2   | 2.34                     | 0.63              |
| 1:F:104:ARG:HH21 | 1:F:104:ARG:CG   | 2.11                     | 0.63              |
| 1:A:14:MET:HE2   | 1:A:14:MET:HA    | 1.80                     | 0.63              |
| 1:F:120:LEU:HD23 | 1:F:124:TRP:CH2  | 2.34                     | 0.63              |
| 1:B:137:ALA:HB1  | 1:B:140:VAL:CB   | 2.28                     | 0.63              |
| 1:A:172:LYS:HA   | 1:A:172:LYS:CE   | 2.29                     | 0.63              |
| 1:D:13:LEU:CA    | 1:D:16:VAL:HG23  | 2.28                     | 0.63              |
| 1:E:42:ILE:HD11  | 1:E:156:ALA:CB   | 2.28                     | 0.63              |
| 1:A:171:GLY:O    | 1:A:173:PRO:HD3  | 1.95                     | 0.63              |
| 1:E:91:TYR:OH    | 1:E:109:THR:HG22 | 1.99                     | 0.63              |
| 1:F:142:ARG:HG2  | 1:F:145:LYS:NZ   | 2.14                     | 0.63              |
| 1:B:30:TYR:CB    | 1:B:37:ILE:HD13  | 2.29                     | 0.62              |
| 1:C:33:THR:CG2   | 1:C:129:TYR:HE2  | 2.12                     | 0.62              |
| 1:E:53:PRO:HG3   | 1:E:93:TYR:CD2   | 2.33                     | 0.62              |
| 1:F:36:LYS:HE2   | 1:F:37:ILE:O     | 1.98                     | 0.62              |
| 1:F:150:PHE:HB2  | 1:F:153:GLN:OE1  | 1.99                     | 0.62              |
| 1:B:26:ARG:HG3   | 1:B:71:PHE:CD2   | 2.34                     | 0.62              |
| 1:B:175:SER:O    | 1:B:176:GLU:HB2  | 1.99                     | 0.62              |
| 1:E:55:TRP:O     | 1:E:58:ILE:HG13  | 1.99                     | 0.62              |
| 1:E:66:VAL:O     | 1:E:69:LEU:HB3   | 1.99                     | 0.62              |
| 1:A:170:PHE:CE2  | 1:A:173:PRO:CG   | 2.82                     | 0.62              |
| 1:E:40:THR:CG2   | 1:E:44:GLU:CD    | 2.28                     | 0.62              |
| 1:A:66:VAL:CG1   | 1:A:70:LEU:HD11  | 2.30                     | 0.62              |
| 1:B:96:TYR:OH    | 1:B:97:LYS:HE2   | 1.95                     | 0.62              |
| 1:C:148:ILE:C    | 1:C:151:PRO:HD2  | 2.24                     | 0.62              |
| 1:E:17:LEU:HD11  | 1:E:47:ILE:CD1   | 2.29                     | 0.62              |
| 1:C:33:THR:CG2   | 1:C:129:TYR:CE2  | 2.83                     | 0.62              |
| 1:C:174:LEU:HD13 | 1:C:174:LEU:O    | 2.00                     | 0.62              |
| 1:D:77:PHE:CG    | 1:D:128:MET:HE2  | 2.35                     | 0.62              |
| 1:E:36:LYS:HB3   | 2:E:201:FOL:C    | 2.30                     | 0.62              |
| 1:A:172:LYS:HA   | 1:A:172:LYS:HE2  | 1.82                     | 0.62              |
| 1:C:174:LEU:HD22 | 1:C:174:LEU:O    | 2.00                     | 0.62              |
| 1:D:50:ILE:HG22  | 1:D:51:PHE:CE1   | 2.35                     | 0.62              |
| 1:F:14:MET:HA    | 1:F:14:MET:CE    | 2.19                     | 0.62              |
| 1:F:142:ARG:HG2  | 1:F:145:LYS:HZ1  | 1.64                     | 0.62              |
| 1:B:135:ASN:HB2  | 1:B:138:TRP:HB3  | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:139:TRP:O    | 1:B:142:ARG:HB3  | 2.00                     | 0.62              |
| 1:D:83:ASN:CG    | 1:D:116:ILE:HG23 | 2.24                     | 0.62              |
| 1:E:14:MET:HE1   | 1:E:18:ILE:HD11  | 1.81                     | 0.62              |
| 1:E:64:ASP:OD1   | 1:E:65:VAL:HG23  | 1.99                     | 0.62              |
| 1:E:32:THR:HG22  | 1:E:33:THR:N     | 2.15                     | 0.62              |
| 1:F:142:ARG:HA   | 1:F:145:LYS:HE2  | 1.82                     | 0.62              |
| 1:B:137:ALA:HB1  | 1:B:140:VAL:HB   | 1.81                     | 0.61              |
| 1:B:140:VAL:O    | 1:B:141:PRO:C    | 2.41                     | 0.61              |
| 1:C:68:MET:O     | 1:C:70:LEU:O     | 2.18                     | 0.61              |
| 1:E:145:LYS:HD3  | 1:E:149:PHE:N    | 2.11                     | 0.61              |
| 1:F:80:PHE:CE1   | 2:F:201:FOL:CD   | 2.74                     | 0.61              |
| 1:A:14:MET:HE2   | 1:A:51:PHE:CZ    | 2.36                     | 0.61              |
| 1:B:36:LYS:HE2   | 1:B:37:ILE:HD12  | 1.81                     | 0.61              |
| 1:D:78:PRO:O     | 1:D:81:THR:OG1   | 2.14                     | 0.61              |
| 1:F:81:THR:HG23  | 1:F:85:PHE:CE2   | 2.34                     | 0.61              |
| 1:A:26:ARG:HG2   | 1:A:27:PHE:CE1   | 2.35                     | 0.61              |
| 1:A:100:MET:SD   | 1:A:161:GLY:HA2  | 2.39                     | 0.61              |
| 1:C:57:GLY:C     | 1:C:85:PHE:HD1   | 2.06                     | 0.61              |
| 1:E:69:LEU:HD13  | 1:E:69:LEU:C     | 2.18                     | 0.61              |
| 1:E:145:LYS:NZ   | 1:E:149:PHE:CD2  | 2.67                     | 0.61              |
| 1:A:26:ARG:NE    | 1:A:27:PHE:HB2   | 2.14                     | 0.61              |
| 1:E:46:LEU:O     | 1:E:49:MET:HB2   | 1.98                     | 0.61              |
| 1:A:112:VAL:HG23 | 1:A:116:ILE:HD11 | 1.83                     | 0.61              |
| 1:C:49:MET:CE    | 1:C:100:MET:HE2  | 2.25                     | 0.61              |
| 1:E:145:LYS:NZ   | 1:E:149:PHE:HD2  | 1.92                     | 0.61              |
| 1:D:109:THR:HG21 | 1:D:154:VAL:HG22 | 1.83                     | 0.61              |
| 1:E:141:PRO:O    | 1:E:144:ILE:HG23 | 1.98                     | 0.61              |
| 1:F:25:SER:O     | 1:F:29:ALA:HB2   | 2.00                     | 0.61              |
| 1:C:132:ASN:N    | 1:C:132:ASN:OD1  | 2.32                     | 0.61              |
| 1:F:68:MET:HE1   | 1:F:73:LYS:HG3   | 1.81                     | 0.61              |
| 1:A:33:THR:HG22  | 1:A:34:PHE:CD1   | 2.35                     | 0.61              |
| 1:D:131:VAL:HG13 | 1:D:133:LEU:CD1  | 2.29                     | 0.61              |
| 1:E:68:MET:CE    | 2:E:201:FOL:N1   | 2.55                     | 0.61              |
| 1:C:27:PHE:CE1   | 1:C:71:PHE:HZ    | 2.17                     | 0.61              |
| 1:C:49:MET:CE    | 1:C:95:TYR:CG    | 2.65                     | 0.61              |
| 1:E:42:ILE:HG23  | 1:E:45:SER:HB2   | 1.83                     | 0.61              |
| 1:A:23:VAL:HG13  | 1:A:26:ARG:HD3   | 1.83                     | 0.60              |
| 1:A:80:PHE:CE1   | 2:A:201:FOL:H16  | 2.36                     | 0.60              |
| 1:E:53:PRO:HG3   | 1:E:93:TYR:HD2   | 1.67                     | 0.60              |
| 1:E:149:PHE:O    | 1:E:152:ILE:HG13 | 2.01                     | 0.60              |
| 1:F:20:VAL:O     | 1:F:23:VAL:HG13  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:144:ILE:O    | 1:A:148:ILE:HG12 | 2.01                     | 0.60              |
| 1:C:116:ILE:HG23 | 1:C:117:ASN:H    | 1.65                     | 0.60              |
| 1:F:45:SER:HA    | 1:F:91:TYR:HD2   | 1.65                     | 0.60              |
| 1:E:10:SER:HA    | 1:E:13:LEU:HD23  | 1.82                     | 0.60              |
| 1:E:18:ILE:CG2   | 1:E:63:ALA:HB1   | 2.25                     | 0.60              |
| 1:F:119:ILE:CG2  | 1:F:123:LEU:HD11 | 2.31                     | 0.60              |
| 1:F:73:LYS:CD    | 2:F:201:FOL:C6   | 2.69                     | 0.60              |
| 1:A:31:GLU:N     | 1:A:31:GLU:OE1   | 2.34                     | 0.60              |
| 1:C:122:PRO:HA   | 1:C:125:LEU:HD11 | 1.83                     | 0.60              |
| 1:F:160:LEU:O    | 1:F:163:LYS:CD   | 2.48                     | 0.60              |
| 1:F:160:LEU:C    | 1:F:163:LYS:CG   | 2.72                     | 0.60              |
| 1:F:10:SER:O     | 1:F:13:LEU:HD11  | 2.01                     | 0.60              |
| 1:F:38:SER:OG    | 2:F:201:FOL:O1   | 2.19                     | 0.60              |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:N    | 2.04                     | 0.60              |
| 1:D:79:GLY:O     | 1:D:124:TRP:CZ3  | 2.55                     | 0.60              |
| 1:F:140:VAL:N    | 1:F:141:PRO:HD3  | 2.17                     | 0.60              |
| 1:A:42:ILE:HD12  | 1:A:160:LEU:CD1  | 2.31                     | 0.60              |
| 1:C:64:ASP:OD2   | 1:C:81:THR:HA    | 2.02                     | 0.60              |
| 1:F:44:GLU:OE2   | 1:F:60:THR:HG21  | 2.00                     | 0.60              |
| 2:F:201:FOL:H15  | 2:F:201:FOL:N5   | 2.16                     | 0.60              |
| 1:C:70:LEU:HD23  | 1:C:70:LEU:N     | 2.08                     | 0.60              |
| 1:C:140:VAL:O    | 1:C:144:ILE:HG13 | 2.02                     | 0.60              |
| 1:E:42:ILE:CG2   | 1:E:45:SER:HB2   | 2.31                     | 0.60              |
| 1:C:42:ILE:HB    | 1:C:43:PRO:HD3   | 1.83                     | 0.59              |
| 1:C:121:THR:O    | 1:C:125:LEU:HG   | 2.02                     | 0.59              |
| 1:D:26:ARG:HH11  | 1:D:26:ARG:CG    | 2.12                     | 0.59              |
| 1:F:141:PRO:O    | 1:F:144:ILE:HG23 | 2.01                     | 0.59              |
| 1:B:61:ALA:O     | 1:B:65:VAL:HG23  | 2.02                     | 0.59              |
| 1:B:73:LYS:O     | 1:B:74:ALA:CB    | 2.49                     | 0.59              |
| 1:C:98:LYS:HZ1   | 1:C:104:ARG:HH12 | 1.38                     | 0.59              |
| 1:D:133:LEU:CD1  | 1:D:138:TRP:CZ3  | 2.85                     | 0.59              |
| 1:F:81:THR:CG2   | 1:F:85:PHE:CZ    | 2.85                     | 0.59              |
| 1:F:83:ASN:OD1   | 1:F:116:ILE:CD1  | 2.30                     | 0.59              |
| 1:A:26:ARG:CD    | 1:A:27:PHE:CD2   | 2.85                     | 0.59              |
| 1:C:150:PHE:HA   | 1:C:153:GLN:HG2  | 1.84                     | 0.59              |
| 1:C:168:ARG:HD3  | 1:C:169:LEU:N    | 2.17                     | 0.59              |
| 1:D:166:PHE:CD1  | 1:D:167:LYS:N    | 2.71                     | 0.59              |
| 1:A:14:MET:CE    | 1:A:51:PHE:CZ    | 2.85                     | 0.59              |
| 1:B:96:TYR:O     | 1:B:97:LYS:HB2   | 2.01                     | 0.59              |
| 1:A:132:ASN:HD22 | 1:A:132:ASN:C    | 2.02                     | 0.59              |
| 1:C:30:TYR:HD2   | 1:C:32:THR:CG2   | 2.16                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:109:THR:HG21 | 1:E:154:VAL:HG12 | 1.84                     | 0.59              |
| 1:F:160:LEU:O    | 1:F:163:LYS:HD2  | 2.02                     | 0.59              |
| 1:A:101:THR:O    | 1:A:103:GLN:N    | 2.36                     | 0.59              |
| 1:A:148:ILE:HD11 | 1:B:110:LEU:HD22 | 1.85                     | 0.59              |
| 1:C:166:PHE:CE2  | 1:C:167:LYS:CE   | 2.85                     | 0.59              |
| 1:D:95:TYR:HB3   | 1:D:100:MET:HE2  | 1.84                     | 0.59              |
| 1:C:30:TYR:CD2   | 1:C:32:THR:CG2   | 2.86                     | 0.59              |
| 1:C:33:THR:O     | 1:C:34:PHE:HB2   | 2.00                     | 0.59              |
| 1:C:59:GLY:O     | 1:C:62:VAL:HG22  | 2.03                     | 0.59              |
| 1:C:166:PHE:CE2  | 1:C:167:LYS:CD   | 2.85                     | 0.59              |
| 1:D:13:LEU:HA    | 1:D:16:VAL:CG2   | 2.31                     | 0.59              |
| 1:E:113:THR:HG21 | 1:E:150:PHE:CD2  | 2.37                     | 0.59              |
| 1:A:27:PHE:O     | 1:A:28:PHE:HD1   | 1.84                     | 0.59              |
| 1:B:77:PHE:N     | 2:B:201:FOL:HN1  | 2.00                     | 0.59              |
| 1:E:39:PHE:CD1   | 1:E:41:PHE:CD1   | 2.83                     | 0.59              |
| 1:F:36:LYS:HG3   | 1:F:37:ILE:C     | 2.27                     | 0.59              |
| 1:F:95:TYR:OH    | 1:F:108:ALA:HB2  | 2.01                     | 0.59              |
| 1:B:24:PHE:CD2   | 1:B:39:PHE:O     | 2.55                     | 0.59              |
| 1:D:133:LEU:HG   | 1:D:138:TRP:CZ3  | 2.38                     | 0.59              |
| 1:B:16:VAL:O     | 1:B:20:VAL:HG23  | 2.03                     | 0.58              |
| 1:B:122:PRO:HA   | 1:B:125:LEU:HD12 | 1.85                     | 0.58              |
| 1:F:29:ALA:C     | 1:F:36:LYS:HZ1   | 2.03                     | 0.58              |
| 1:F:74:ALA:HB3   | 2:F:201:FOL:C7   | 2.33                     | 0.58              |
| 1:C:30:TYR:CD1   | 1:C:37:ILE:CD1   | 2.86                     | 0.58              |
| 1:A:172:LYS:HA   | 1:A:172:LYS:NZ   | 2.18                     | 0.58              |
| 1:E:20:VAL:O     | 1:E:23:VAL:HG13  | 2.03                     | 0.58              |
| 1:E:17:LEU:O     | 1:E:20:VAL:CG2   | 2.46                     | 0.58              |
| 1:E:143:LEU:CD2  | 1:E:146:THR:HG21 | 2.33                     | 0.58              |
| 1:E:145:LYS:HE2  | 1:E:146:THR:C    | 2.28                     | 0.58              |
| 1:F:13:LEU:HD11  | 1:F:51:PHE:CZ    | 2.31                     | 0.58              |
| 1:C:28:PHE:HD1   | 1:C:28:PHE:N     | 2.01                     | 0.58              |
| 1:E:76:TYR:CD1   | 1:E:77:PHE:N     | 2.72                     | 0.58              |
| 1:D:64:ASP:CG    | 1:D:81:THR:HG22  | 2.28                     | 0.58              |
| 1:D:64:ASP:OD2   | 1:D:81:THR:HG22  | 2.03                     | 0.58              |
| 1:E:115:LEU:C    | 1:E:119:ILE:HG12 | 2.20                     | 0.58              |
| 1:A:14:MET:HE2   | 1:A:51:PHE:CE2   | 2.38                     | 0.58              |
| 1:E:66:VAL:HA    | 1:E:69:LEU:HB3   | 1.84                     | 0.58              |
| 1:F:32:THR:CG2   | 1:F:33:THR:H     | 2.06                     | 0.58              |
| 1:D:33:THR:O     | 1:D:34:PHE:CD1   | 2.49                     | 0.58              |
| 1:B:36:LYS:CE    | 1:B:37:ILE:CD1   | 2.82                     | 0.58              |
| 1:E:77:PHE:CD2   | 1:E:78:PRO:HD2   | 2.37                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:74:ALA:CB    | 2:F:201:FOL:C7   | 2.82                     | 0.58              |
| 1:C:109:THR:CG2  | 1:C:153:GLN:NE2  | 2.66                     | 0.57              |
| 1:C:111:LEU:HD23 | 1:C:111:LEU:C    | 2.28                     | 0.57              |
| 1:A:77:PHE:H     | 2:A:201:FOL:HN1  | 1.51                     | 0.57              |
| 1:D:37:ILE:CG1   | 1:D:145:LYS:HG3  | 2.34                     | 0.57              |
| 1:E:94:PHE:HD2   | 1:E:108:ALA:HB2  | 1.69                     | 0.57              |
| 1:E:142:ARG:O    | 1:E:143:LEU:CB   | 2.51                     | 0.57              |
| 1:F:41:PHE:O     | 1:F:45:SER:OG    | 2.21                     | 0.57              |
| 1:F:116:ILE:HD12 | 1:F:120:LEU:CD1  | 2.30                     | 0.57              |
| 1:F:120:LEU:CB   | 1:F:124:TRP:CZ3  | 2.85                     | 0.57              |
| 1:C:28:PHE:N     | 1:C:28:PHE:CD1   | 2.72                     | 0.57              |
| 1:F:13:LEU:HD13  | 1:F:13:LEU:N     | 2.19                     | 0.57              |
| 1:A:36:LYS:O     | 2:A:201:FOL:HG1  | 2.04                     | 0.57              |
| 1:A:70:LEU:CB    | 1:A:71:PHE:CD1   | 2.85                     | 0.57              |
| 1:B:96:TYR:CE2   | 1:B:97:LYS:CG    | 2.88                     | 0.57              |
| 1:C:166:PHE:CE2  | 1:C:167:LYS:NZ   | 2.73                     | 0.57              |
| 1:D:117:ASN:HD21 | 2:D:201:FOL:HG2  | 1.68                     | 0.57              |
| 1:E:40:THR:HG23  | 1:E:43:PRO:CG    | 2.33                     | 0.57              |
| 1:F:24:PHE:O     | 1:F:39:PHE:CD2   | 2.57                     | 0.57              |
| 1:F:142:ARG:O    | 1:F:146:THR:HG23 | 2.04                     | 0.57              |
| 1:B:19:ALA:HA    | 1:B:22:VAL:CG2   | 2.34                     | 0.57              |
| 1:B:124:TRP:O    | 1:B:128:MET:HG2  | 2.03                     | 0.57              |
| 1:C:98:LYS:HZ2   | 1:C:104:ARG:HH12 | 1.32                     | 0.57              |
| 1:A:50:ILE:C     | 1:A:173:PRO:HB3  | 2.30                     | 0.57              |
| 1:B:96:TYR:CE2   | 1:B:97:LYS:HG3   | 2.40                     | 0.57              |
| 1:B:158:TYR:O    | 1:B:162:ASN:ND2  | 2.34                     | 0.57              |
| 1:C:19:ALA:O     | 1:C:22:VAL:HG12  | 2.04                     | 0.57              |
| 1:C:166:PHE:CZ   | 1:C:167:LYS:CD   | 2.88                     | 0.57              |
| 1:E:55:TRP:CE3   | 1:E:55:TRP:CA    | 2.87                     | 0.57              |
| 1:A:90:ILE:HD12  | 1:A:111:LEU:HD22 | 1.87                     | 0.57              |
| 1:B:36:LYS:CG    | 1:B:37:ILE:N     | 2.65                     | 0.57              |
| 1:C:118:ILE:O    | 1:C:122:PRO:HG2  | 2.04                     | 0.57              |
| 1:E:10:SER:CA    | 1:E:13:LEU:HD23  | 2.33                     | 0.57              |
| 1:A:149:PHE:HD1  | 1:A:152:ILE:HD12 | 1.69                     | 0.57              |
| 1:E:125:LEU:O    | 1:E:128:MET:O    | 2.23                     | 0.57              |
| 1:D:160:LEU:HD23 | 1:D:160:LEU:O    | 2.05                     | 0.57              |
| 1:E:43:PRO:HG2   | 1:E:44:GLU:N     | 2.18                     | 0.57              |
| 1:E:129:TYR:CD2  | 1:E:129:TYR:N    | 2.73                     | 0.57              |
| 1:F:150:PHE:O    | 1:F:153:GLN:HB3  | 2.04                     | 0.57              |
| 1:B:34:PHE:O     | 1:B:142:ARG:NH2  | 2.37                     | 0.57              |
| 1:E:119:ILE:O    | 1:E:123:LEU:HD13 | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:10:SER:O     | 1:F:13:LEU:HD13  | 2.05                     | 0.56              |
| 1:C:96:TYR:CZ    | 1:C:169:LEU:HD23 | 2.40                     | 0.56              |
| 1:E:13:LEU:H     | 1:E:13:LEU:CD2   | 2.00                     | 0.56              |
| 1:F:116:ILE:HD13 | 1:F:120:LEU:HD13 | 1.86                     | 0.56              |
| 1:B:23:VAL:HG23  | 1:B:24:PHE:N     | 2.20                     | 0.56              |
| 1:B:143:LEU:O    | 1:B:147:VAL:HG22 | 2.06                     | 0.56              |
| 1:C:49:MET:CE    | 1:C:100:MET:HE1  | 2.18                     | 0.56              |
| 1:C:128:MET:HE2  | 1:C:129:TYR:CE1  | 2.41                     | 0.56              |
| 1:C:150:PHE:HA   | 1:C:153:GLN:OE1  | 2.05                     | 0.56              |
| 1:C:166:PHE:CE2  | 1:C:167:LYS:HD3  | 2.40                     | 0.56              |
| 1:D:14:MET:HE2   | 1:D:51:PHE:CD2   | 1.87                     | 0.56              |
| 1:E:14:MET:SD    | 1:E:18:ILE:CG1   | 2.94                     | 0.56              |
| 1:E:27:PHE:HD2   | 1:E:27:PHE:O     | 1.86                     | 0.56              |
| 1:C:166:PHE:N    | 1:C:166:PHE:CD2  | 2.73                     | 0.56              |
| 1:E:55:TRP:HA    | 1:E:55:TRP:HE3   | 1.68                     | 0.56              |
| 1:A:33:THR:HG22  | 1:A:34:PHE:CE1   | 2.40                     | 0.56              |
| 1:A:149:PHE:CD1  | 1:A:152:ILE:HD12 | 2.41                     | 0.56              |
| 1:B:36:LYS:HE3   | 1:B:37:ILE:HD13  | 1.88                     | 0.56              |
| 1:E:14:MET:SD    | 1:E:17:LEU:CD2   | 2.94                     | 0.56              |
| 1:F:74:ALA:HB3   | 2:F:201:FOL:H7   | 1.82                     | 0.56              |
| 1:F:93:TYR:HD1   | 1:F:93:TYR:O     | 1.89                     | 0.56              |
| 1:D:27:PHE:O     | 1:D:28:PHE:HD2   | 1.89                     | 0.56              |
| 1:F:35:LEU:O     | 1:F:36:LYS:HB2   | 2.05                     | 0.56              |
| 1:F:119:ILE:C    | 1:F:123:LEU:HD12 | 2.30                     | 0.56              |
| 1:B:30:TYR:HB2   | 1:B:36:LYS:NZ    | 2.21                     | 0.56              |
| 2:B:201:FOL:C6   | 2:B:201:FOL:H15  | 2.36                     | 0.56              |
| 1:F:16:VAL:HG23  | 1:F:17:LEU:N     | 2.20                     | 0.56              |
| 1:F:138:TRP:CD1  | 1:F:138:TRP:N    | 2.73                     | 0.56              |
| 1:B:106:ILE:HG13 | 1:B:154:VAL:HG11 | 1.88                     | 0.56              |
| 1:C:57:GLY:C     | 1:C:85:PHE:CD1   | 2.84                     | 0.56              |
| 1:C:114:VAL:CG2  | 1:D:144:ILE:CD1  | 2.83                     | 0.56              |
| 1:A:26:ARG:HE    | 1:A:27:PHE:H     | 1.54                     | 0.56              |
| 1:A:36:LYS:HZ3   | 2:A:201:FOL:HB2  | 1.72                     | 0.56              |
| 1:B:74:ALA:O     | 2:B:201:FOL:H7   | 2.06                     | 0.56              |
| 1:D:80:PHE:O     | 1:D:83:ASN:HB2   | 2.06                     | 0.56              |
| 1:A:26:ARG:CG    | 1:A:27:PHE:CG    | 2.85                     | 0.55              |
| 1:A:36:LYS:HG3   | 2:A:201:FOL:HB2  | 1.87                     | 0.55              |
| 1:B:96:TYR:CD2   | 1:B:97:LYS:HG3   | 2.40                     | 0.55              |
| 1:D:35:LEU:HD21  | 1:D:145:LYS:HD2  | 1.88                     | 0.55              |
| 1:D:131:VAL:HG13 | 1:D:131:VAL:O    | 2.05                     | 0.55              |
| 1:E:68:MET:HE2   | 2:E:201:FOL:C4   | 2.26                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:102:TRP:HB2  | 1:E:158:TYR:OH   | 2.06                     | 0.55              |
| 1:E:110:LEU:O    | 1:E:114:VAL:HG12 | 2.06                     | 0.55              |
| 1:F:13:LEU:CD2   | 1:F:14:MET:SD    | 2.94                     | 0.55              |
| 1:F:160:LEU:CA   | 1:F:163:LYS:HG2  | 2.35                     | 0.55              |
| 1:A:36:LYS:HG2   | 2:A:201:FOL:C12  | 2.36                     | 0.55              |
| 1:A:60:THR:HG22  | 1:A:84:ALA:HB1   | 1.88                     | 0.55              |
| 1:B:131:VAL:CG1  | 1:B:133:LEU:HD11 | 2.36                     | 0.55              |
| 1:C:26:ARG:NH1   | 1:C:26:ARG:HG2   | 2.15                     | 0.55              |
| 1:C:14:MET:HB2   | 1:C:51:PHE:CZ    | 2.41                     | 0.55              |
| 1:C:34:PHE:CE1   | 1:C:129:TYR:HD2  | 2.18                     | 0.55              |
| 1:D:133:LEU:HD11 | 1:D:138:TRP:CZ3  | 2.42                     | 0.55              |
| 1:A:70:LEU:H     | 1:A:70:LEU:CD1   | 2.09                     | 0.55              |
| 1:C:96:TYR:HE1   | 1:C:169:LEU:CD2  | 2.20                     | 0.55              |
| 1:F:31:GLU:HB2   | 1:F:32:THR:OG1   | 2.06                     | 0.55              |
| 1:A:46:LEU:O     | 1:A:50:ILE:HG13  | 2.06                     | 0.55              |
| 1:E:18:ILE:CG2   | 1:E:63:ALA:CA    | 2.85                     | 0.55              |
| 1:E:55:TRP:HA    | 1:E:58:ILE:HD11  | 1.89                     | 0.55              |
| 1:E:83:ASN:OD1   | 1:E:83:ASN:N     | 2.39                     | 0.55              |
| 1:F:94:PHE:HB3   | 1:F:95:TYR:CZ    | 2.41                     | 0.55              |
| 1:B:19:ALA:HA    | 1:B:22:VAL:HG22  | 1.87                     | 0.55              |
| 1:C:49:MET:CE    | 1:C:95:TYR:HB3   | 2.31                     | 0.55              |
| 1:A:70:LEU:HD12  | 1:A:70:LEU:N     | 2.13                     | 0.55              |
| 1:D:143:LEU:HA   | 1:D:146:THR:OG1  | 2.07                     | 0.55              |
| 1:E:14:MET:HE1   | 1:E:59:GLY:HA3   | 1.89                     | 0.55              |
| 1:D:36:LYS:HB3   | 2:D:201:FOL:C    | 2.36                     | 0.55              |
| 1:F:115:LEU:O    | 1:F:119:ILE:HD13 | 2.07                     | 0.55              |
| 1:A:22:VAL:O     | 1:A:26:ARG:HB3   | 2.07                     | 0.55              |
| 1:B:164:ILE:HG12 | 1:B:165:PRO:CD   | 2.30                     | 0.55              |
| 1:C:93:TYR:C     | 1:C:93:TYR:CD2   | 2.85                     | 0.55              |
| 1:D:77:PHE:H     | 1:D:80:PHE:HE2   | 1.55                     | 0.55              |
| 1:B:30:TYR:HB2   | 1:B:36:LYS:CE    | 2.37                     | 0.55              |
| 1:B:71:PHE:N     | 1:B:72:PRO:CD    | 2.69                     | 0.55              |
| 1:E:120:LEU:O    | 1:E:124:TRP:HB2  | 2.07                     | 0.55              |
| 1:F:33:THR:C     | 1:F:34:PHE:CD2   | 2.85                     | 0.55              |
| 1:B:33:THR:HG22  | 1:B:34:PHE:CD2   | 2.42                     | 0.54              |
| 1:D:27:PHE:C     | 1:D:28:PHE:CD2   | 2.85                     | 0.54              |
| 1:D:61:ALA:O     | 1:D:64:ASP:HB3   | 2.06                     | 0.54              |
| 1:E:107:LEU:HD12 | 1:E:107:LEU:O    | 2.07                     | 0.54              |
| 1:F:80:PHE:CZ    | 2:F:201:FOL:N3   | 2.72                     | 0.54              |
| 1:A:30:TYR:CD2   | 1:A:37:ILE:HD12  | 2.43                     | 0.54              |
| 1:A:71:PHE:CD1   | 1:A:71:PHE:N     | 2.75                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:170:PHE:CD2  | 1:A:171:GLY:N    | 2.73                     | 0.54              |
| 1:B:54:PHE:CD1   | 1:B:54:PHE:C     | 2.85                     | 0.54              |
| 1:B:138:TRP:CE3  | 1:B:138:TRP:C    | 2.85                     | 0.54              |
| 1:C:107:LEU:HD13 | 1:C:107:LEU:O    | 2.07                     | 0.54              |
| 1:E:41:PHE:O     | 1:E:42:ILE:HG12  | 2.06                     | 0.54              |
| 1:E:149:PHE:HD1  | 1:E:152:ILE:HD11 | 1.70                     | 0.54              |
| 1:A:140:VAL:O    | 1:A:144:ILE:HG13 | 2.07                     | 0.54              |
| 1:C:143:LEU:O    | 1:C:147:VAL:HG22 | 2.08                     | 0.54              |
| 1:C:30:TYR:HB2   | 1:C:37:ILE:H     | 1.73                     | 0.54              |
| 1:C:94:PHE:CG    | 1:C:108:ALA:HB2  | 2.42                     | 0.54              |
| 1:D:20:VAL:HA    | 1:D:23:VAL:CG2   | 2.37                     | 0.54              |
| 1:D:30:TYR:HD2   | 1:D:37:ILE:HG22  | 1.72                     | 0.54              |
| 1:D:51:PHE:CD1   | 1:D:51:PHE:N     | 2.73                     | 0.54              |
| 1:D:96:TYR:CE2   | 1:D:97:LYS:HG3   | 2.43                     | 0.54              |
| 1:E:69:LEU:HD13  | 1:E:70:LEU:CB    | 2.37                     | 0.54              |
| 1:A:17:LEU:HD13  | 1:A:47:ILE:CG1   | 2.38                     | 0.54              |
| 1:B:24:PHE:CE2   | 1:B:43:PRO:HD3   | 2.42                     | 0.54              |
| 1:E:172:LYS:HB3  | 1:E:173:PRO:CA   | 2.31                     | 0.54              |
| 1:B:31:GLU:CB    | 1:B:36:LYS:HD3   | 2.35                     | 0.54              |
| 1:C:10:SER:CB    | 1:C:170:PHE:CZ   | 2.75                     | 0.54              |
| 1:E:139:TRP:CZ3  | 1:E:142:ARG:NE   | 2.76                     | 0.54              |
| 1:A:97:LYS:HE2   | 1:A:170:PHE:CD1  | 2.33                     | 0.54              |
| 1:A:120:LEU:O    | 1:A:123:LEU:HB3  | 2.07                     | 0.54              |
| 1:D:34:PHE:CD1   | 1:D:34:PHE:N     | 2.72                     | 0.54              |
| 1:E:29:ALA:HB1   | 1:E:30:TYR:CD2   | 2.39                     | 0.54              |
| 1:F:93:TYR:CD1   | 1:F:93:TYR:C     | 2.85                     | 0.54              |
| 1:A:26:ARG:CD    | 1:A:27:PHE:CG    | 2.91                     | 0.54              |
| 1:B:73:LYS:HE2   | 1:B:74:ALA:H     | 1.71                     | 0.54              |
| 1:B:138:TRP:HE3  | 1:B:139:TRP:N    | 2.06                     | 0.54              |
| 1:C:35:LEU:HD11  | 1:C:145:LYS:HD2  | 1.90                     | 0.54              |
| 1:C:150:PHE:C    | 1:C:150:PHE:CD2  | 2.85                     | 0.54              |
| 1:E:137:ALA:C    | 1:E:138:TRP:CD1  | 2.86                     | 0.54              |
| 1:F:33:THR:C     | 1:F:34:PHE:CG    | 2.85                     | 0.54              |
| 1:F:110:LEU:HD23 | 1:F:111:LEU:N    | 2.22                     | 0.54              |
| 1:F:120:LEU:HA   | 1:F:123:LEU:HD13 | 1.88                     | 0.54              |
| 1:A:18:ILE:HD13  | 1:A:63:ALA:HB2   | 1.90                     | 0.54              |
| 1:F:23:VAL:HA    | 1:F:27:PHE:CE2   | 2.43                     | 0.54              |
| 1:A:150:PHE:CD1  | 1:A:150:PHE:C    | 2.86                     | 0.54              |
| 1:B:137:ALA:HB1  | 1:B:140:VAL:HG21 | 1.88                     | 0.54              |
| 1:E:14:MET:SD    | 1:E:18:ILE:CD1   | 2.94                     | 0.54              |
| 1:E:47:ILE:HA    | 1:E:50:ILE:CG2   | 2.32                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:70:LEU:HD23  | 1:E:71:PHE:CG    | 2.43                     | 0.54              |
| 1:E:77:PHE:CD1   | 1:E:78:PRO:CD    | 2.79                     | 0.54              |
| 1:F:94:PHE:CE2   | 1:F:108:ALA:HB2  | 2.40                     | 0.54              |
| 1:E:36:LYS:HE3   | 1:E:38:SER:HG    | 1.70                     | 0.53              |
| 1:E:76:TYR:HE1   | 1:E:78:PRO:HA    | 1.73                     | 0.53              |
| 1:F:129:TYR:CG   | 1:F:129:TYR:O    | 2.60                     | 0.53              |
| 1:A:170:PHE:CD2  | 1:A:173:PRO:HG3  | 2.42                     | 0.53              |
| 1:E:34:PHE:O     | 1:E:35:LEU:HG    | 2.08                     | 0.53              |
| 1:F:13:LEU:HD22  | 1:F:14:MET:CA    | 2.38                     | 0.53              |
| 1:A:70:LEU:CB    | 1:A:71:PHE:CE1   | 2.91                     | 0.53              |
| 1:A:116:ILE:HD12 | 1:A:117:ASN:N    | 2.24                     | 0.53              |
| 1:A:172:LYS:CE   | 1:A:172:LYS:CA   | 2.86                     | 0.53              |
| 1:C:57:GLY:HA3   | 1:C:85:PHE:CE1   | 2.43                     | 0.53              |
| 1:E:112:VAL:HA   | 1:E:115:LEU:CB   | 2.39                     | 0.53              |
| 1:B:49:MET:HG2   | 1:B:95:TYR:HB3   | 1.91                     | 0.53              |
| 1:B:138:TRP:CE3  | 1:B:139:TRP:CA   | 2.91                     | 0.53              |
| 1:C:49:MET:HE2   | 1:C:100:MET:HE3  | 0.55                     | 0.53              |
| 1:E:10:SER:CA    | 1:E:13:LEU:CD2   | 2.86                     | 0.53              |
| 1:A:35:LEU:C     | 2:A:201:FOL:H12  | 2.33                     | 0.53              |
| 1:A:100:MET:CE   | 1:A:161:GLY:CA   | 2.84                     | 0.53              |
| 1:B:37:ILE:H     | 1:B:37:ILE:CD1   | 2.20                     | 0.53              |
| 1:E:139:TRP:HZ3  | 1:E:142:ARG:NE   | 2.07                     | 0.53              |
| 1:A:26:ARG:HE    | 1:A:27:PHE:N     | 2.07                     | 0.53              |
| 1:A:39:PHE:CD2   | 1:A:41:PHE:HZ    | 2.26                     | 0.53              |
| 1:E:116:ILE:HD12 | 1:E:117:ASN:H    | 1.74                     | 0.53              |
| 1:F:140:VAL:O    | 1:F:144:ILE:HG22 | 2.09                     | 0.53              |
| 1:A:150:PHE:O    | 1:A:154:VAL:HG23 | 2.08                     | 0.53              |
| 1:C:55:TRP:CD1   | 1:C:172:LYS:CB   | 2.89                     | 0.53              |
| 1:E:22:VAL:HG22  | 1:E:67:GLY:HA2   | 1.89                     | 0.53              |
| 1:E:150:PHE:CD1  | 1:E:153:GLN:HB3  | 2.44                     | 0.53              |
| 1:F:83:ASN:OD1   | 1:F:120:LEU:HD22 | 2.09                     | 0.53              |
| 1:F:95:TYR:CZ    | 1:F:108:ALA:HB3  | 2.41                     | 0.53              |
| 1:C:100:MET:SD   | 1:C:161:GLY:HA3  | 2.48                     | 0.53              |
| 1:E:86:LEU:HD13  | 1:E:115:LEU:HD21 | 1.91                     | 0.53              |
| 1:F:80:PHE:CD2   | 2:F:201:FOL:NA2  | 2.77                     | 0.53              |
| 1:F:80:PHE:CZ    | 2:F:201:FOL:C4   | 2.92                     | 0.53              |
| 1:B:173:PRO:O    | 1:B:173:PRO:CD   | 2.56                     | 0.53              |
| 1:E:145:LYS:HD2  | 1:E:147:VAL:N    | 2.24                     | 0.53              |
| 1:B:14:MET:O     | 1:B:18:ILE:HG12  | 2.09                     | 0.53              |
| 1:D:37:ILE:HD11  | 1:D:145:LYS:HG3  | 1.90                     | 0.53              |
| 1:E:76:TYR:CD1   | 1:E:76:TYR:C     | 2.86                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:139:TRP:O    | 1:E:141:PRO:HD2  | 2.09                     | 0.53              |
| 1:F:54:PHE:HD2   | 1:F:55:TRP:CD1   | 2.27                     | 0.53              |
| 1:E:77:PHE:CE1   | 1:E:78:PRO:HD2   | 2.41                     | 0.52              |
| 1:E:112:VAL:CA   | 1:E:115:LEU:CB   | 2.84                     | 0.52              |
| 1:F:35:LEU:HD23  | 1:F:35:LEU:H     | 1.72                     | 0.52              |
| 1:F:59:GLY:O     | 1:F:62:VAL:HG22  | 2.09                     | 0.52              |
| 1:F:120:LEU:CG   | 1:F:124:TRP:HZ3  | 2.22                     | 0.52              |
| 1:B:145:LYS:O    | 1:B:149:PHE:HD2  | 1.92                     | 0.52              |
| 1:C:43:PRO:O     | 1:C:46:LEU:N     | 2.43                     | 0.52              |
| 1:F:122:PRO:N    | 1:F:125:LEU:HD12 | 2.24                     | 0.52              |
| 1:B:138:TRP:HE3  | 1:B:139:TRP:CA   | 2.22                     | 0.52              |
| 1:E:17:LEU:HG    | 1:E:18:ILE:N     | 2.24                     | 0.52              |
| 1:E:112:VAL:HB   | 1:E:115:LEU:CG   | 2.39                     | 0.52              |
| 1:E:112:VAL:HA   | 1:E:115:LEU:HB3  | 1.91                     | 0.52              |
| 1:F:30:TYR:CB    | 1:F:36:LYS:HE3   | 2.28                     | 0.52              |
| 1:F:35:LEU:CD2   | 1:F:35:LEU:N     | 2.73                     | 0.52              |
| 1:B:137:ALA:CB   | 1:B:140:VAL:CG2  | 2.85                     | 0.52              |
| 1:D:147:VAL:CG2  | 1:D:148:ILE:N    | 2.73                     | 0.52              |
| 1:E:18:ILE:HG21  | 1:E:63:ALA:HB2   | 1.82                     | 0.52              |
| 1:B:19:ALA:O     | 1:B:22:VAL:HG23  | 2.10                     | 0.52              |
| 1:C:116:ILE:O    | 1:C:120:LEU:HB2  | 2.10                     | 0.52              |
| 1:F:116:ILE:HD11 | 1:F:120:LEU:HD22 | 1.89                     | 0.52              |
| 1:C:8:THR:C      | 1:C:9:LYS:HD3    | 2.35                     | 0.52              |
| 1:C:49:MET:HE1   | 1:C:100:MET:CE   | 2.25                     | 0.52              |
| 1:E:42:ILE:N     | 1:E:43:PRO:CD    | 2.73                     | 0.52              |
| 1:E:110:LEU:HD11 | 1:F:144:ILE:CD1  | 2.39                     | 0.52              |
| 1:E:140:VAL:HG12 | 1:E:140:VAL:O    | 2.10                     | 0.52              |
| 1:C:65:VAL:O     | 1:C:69:LEU:HD12  | 2.10                     | 0.52              |
| 1:C:148:ILE:O    | 1:C:151:PRO:CG   | 2.57                     | 0.52              |
| 1:D:59:GLY:O     | 1:D:62:VAL:HG22  | 2.10                     | 0.52              |
| 1:D:49:MET:SD    | 1:D:100:MET:HE1  | 2.50                     | 0.52              |
| 1:E:40:THR:CG2   | 1:E:43:PRO:HG2   | 2.35                     | 0.52              |
| 1:C:150:PHE:HE2  | 1:D:151:PRO:HG2  | 1.75                     | 0.52              |
| 1:D:12:ALA:O     | 1:D:16:VAL:HG23  | 2.03                     | 0.52              |
| 1:E:145:LYS:CD   | 1:E:149:PHE:HB3  | 2.36                     | 0.52              |
| 1:E:150:PHE:HA   | 1:E:153:GLN:OE1  | 2.10                     | 0.52              |
| 1:A:17:LEU:HD13  | 1:A:47:ILE:HG13  | 1.92                     | 0.51              |
| 1:B:74:ALA:CB    | 2:B:201:FOL:H92  | 2.35                     | 0.51              |
| 1:D:111:LEU:HD11 | 1:D:115:LEU:HD22 | 1.92                     | 0.51              |
| 1:B:55:TRP:O     | 1:B:59:GLY:N     | 2.40                     | 0.51              |
| 1:C:24:PHE:CD2   | 1:C:39:PHE:O     | 2.62                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:22:VAL:HG21  | 1:E:67:GLY:CA    | 2.40                     | 0.51              |
| 1:F:160:LEU:CA   | 1:F:163:LYS:CG   | 2.88                     | 0.51              |
| 1:F:170:PHE:HD2  | 1:F:170:PHE:O    | 1.93                     | 0.51              |
| 1:D:138:TRP:O    | 1:D:141:PRO:HD2  | 2.10                     | 0.51              |
| 1:F:73:LYS:CD    | 2:F:201:FOL:C9   | 2.84                     | 0.51              |
| 1:B:50:ILE:HG22  | 1:B:51:PHE:CE1   | 2.45                     | 0.51              |
| 1:E:70:LEU:HD23  | 1:E:70:LEU:O     | 2.10                     | 0.51              |
| 1:F:32:THR:O     | 1:F:35:LEU:HD22  | 2.03                     | 0.51              |
| 1:D:150:PHE:C    | 1:D:150:PHE:CD2  | 2.88                     | 0.51              |
| 1:F:116:ILE:CA   | 1:F:120:LEU:HD13 | 2.28                     | 0.51              |
| 1:C:36:LYS:HB2   | 2:C:201:FOL:HN   | 1.76                     | 0.51              |
| 1:C:123:LEU:O    | 1:C:127:LEU:HG   | 2.10                     | 0.51              |
| 1:F:13:LEU:CD1   | 1:F:13:LEU:H     | 2.22                     | 0.51              |
| 1:A:109:THR:HA   | 1:A:112:VAL:CG1  | 2.40                     | 0.51              |
| 1:D:66:VAL:HA    | 1:D:69:LEU:HD12  | 1.92                     | 0.51              |
| 1:D:114:VAL:O    | 1:D:119:ILE:HG12 | 2.11                     | 0.51              |
| 1:E:36:LYS:CB    | 2:E:201:FOL:H12  | 2.38                     | 0.51              |
| 1:E:137:ALA:C    | 1:E:138:TRP:HD1  | 2.17                     | 0.51              |
| 1:E:151:PRO:O    | 1:E:154:VAL:HG22 | 2.11                     | 0.51              |
| 1:F:118:ILE:O    | 1:F:122:PRO:HG2  | 2.10                     | 0.51              |
| 1:A:17:LEU:HA    | 1:A:20:VAL:CG2   | 2.41                     | 0.51              |
| 1:A:76:TYR:C     | 1:A:76:TYR:CD2   | 2.89                     | 0.51              |
| 1:B:41:PHE:CD2   | 1:B:153:GLN:HG3  | 2.46                     | 0.51              |
| 1:E:36:LYS:HB3   | 2:E:201:FOL:N    | 2.26                     | 0.51              |
| 1:F:68:MET:CE    | 2:F:201:FOL:N1   | 2.74                     | 0.51              |
| 1:C:33:THR:HG22  | 1:C:129:TYR:CE2  | 2.38                     | 0.51              |
| 1:C:138:TRP:O    | 1:C:141:PRO:HD2  | 2.10                     | 0.51              |
| 1:F:121:THR:O    | 1:F:125:LEU:HG   | 2.10                     | 0.51              |
| 1:B:53:PRO:HG2   | 1:B:54:PHE:N     | 2.26                     | 0.51              |
| 1:B:113:THR:HA   | 1:B:117:ASN:OD1  | 2.11                     | 0.51              |
| 1:F:68:MET:SD    | 2:F:201:FOL:NA2  | 2.83                     | 0.51              |
| 1:A:35:LEU:HD11  | 1:A:145:LYS:HD3  | 1.92                     | 0.50              |
| 1:A:114:VAL:HG21 | 1:B:144:ILE:HG12 | 1.93                     | 0.50              |
| 1:B:164:ILE:CD1  | 1:B:165:PRO:N    | 2.73                     | 0.50              |
| 1:C:34:PHE:CE2   | 1:C:138:TRP:CD1  | 2.99                     | 0.50              |
| 1:C:150:PHE:C    | 1:C:153:GLN:HG2  | 2.35                     | 0.50              |
| 1:E:40:THR:CG2   | 1:E:43:PRO:HD2   | 2.39                     | 0.50              |
| 1:E:115:LEU:C    | 1:E:115:LEU:CD2  | 2.60                     | 0.50              |
| 1:F:13:LEU:CD1   | 1:F:13:LEU:N     | 2.73                     | 0.50              |
| 1:F:32:THR:C     | 1:F:33:THR:OG1   | 2.53                     | 0.50              |
| 1:F:106:ILE:HD13 | 1:F:154:VAL:HG11 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:66:VAL:HG13  | 1:A:70:LEU:HD11  | 1.92                     | 0.50              |
| 1:A:112:VAL:CG2  | 1:A:116:ILE:HD11 | 2.40                     | 0.50              |
| 1:A:118:ILE:HD12 | 1:B:143:LEU:HD13 | 1.93                     | 0.50              |
| 1:B:123:LEU:O    | 1:B:126:SER:OG   | 2.29                     | 0.50              |
| 1:C:49:MET:O     | 1:C:96:TYR:HD1   | 1.91                     | 0.50              |
| 1:A:160:LEU:HD23 | 1:A:161:GLY:CA   | 2.42                     | 0.50              |
| 1:B:36:LYS:HE2   | 1:B:37:ILE:CA    | 2.42                     | 0.50              |
| 1:C:166:PHE:CZ   | 1:C:167:LYS:HD3  | 2.47                     | 0.50              |
| 1:D:80:PHE:CD1   | 1:D:80:PHE:C     | 2.89                     | 0.50              |
| 1:D:97:LYS:HE2   | 1:D:170:PHE:CZ   | 2.46                     | 0.50              |
| 1:D:148:ILE:HG13 | 1:D:149:PHE:H    | 1.73                     | 0.50              |
| 1:E:148:ILE:C    | 1:E:151:PRO:HD2  | 2.36                     | 0.50              |
| 1:F:13:LEU:HD13  | 1:F:14:MET:N     | 2.26                     | 0.50              |
| 1:E:145:LYS:HD2  | 1:E:148:ILE:N    | 2.27                     | 0.50              |
| 1:D:106:ILE:O    | 1:D:109:THR:HG22 | 2.12                     | 0.50              |
| 1:A:26:ARG:NE    | 1:A:27:PHE:N     | 2.60                     | 0.50              |
| 1:C:116:ILE:CG2  | 1:C:117:ASN:N    | 2.73                     | 0.50              |
| 1:C:125:LEU:HA   | 1:C:128:MET:CG   | 2.38                     | 0.50              |
| 1:D:50:ILE:CG2   | 1:D:51:PHE:CE1   | 2.94                     | 0.50              |
| 1:D:126:SER:O    | 1:D:130:GLY:HA2  | 2.11                     | 0.50              |
| 1:E:66:VAL:C     | 1:E:69:LEU:HB3   | 2.36                     | 0.50              |
| 1:E:90:ILE:HG21  | 1:E:112:VAL:HG21 | 1.93                     | 0.50              |
| 1:B:29:ALA:C     | 1:B:36:LYS:HZ2   | 2.19                     | 0.50              |
| 1:C:14:MET:HE2   | 1:C:51:PHE:CD1   | 2.47                     | 0.50              |
| 1:F:103:GLN:NE2  | 1:F:103:GLN:CA   | 2.73                     | 0.50              |
| 1:E:23:VAL:HA    | 1:E:26:ARG:CB    | 2.39                     | 0.50              |
| 1:E:41:PHE:C     | 1:E:43:PRO:CD    | 2.85                     | 0.50              |
| 1:E:45:SER:HB2   | 1:E:160:LEU:CD1  | 2.42                     | 0.50              |
| 1:F:16:VAL:CG2   | 1:F:17:LEU:CD2   | 2.85                     | 0.50              |
| 1:F:61:ALA:O     | 1:F:65:VAL:CG2   | 2.40                     | 0.50              |
| 1:A:26:ARG:O     | 1:A:27:PHE:HD1   | 1.94                     | 0.50              |
| 1:B:64:ASP:OD2   | 1:B:81:THR:HG22  | 2.12                     | 0.50              |
| 1:B:76:TYR:C     | 1:B:76:TYR:CD2   | 2.90                     | 0.50              |
| 1:C:83:ASN:OD1   | 1:C:116:ILE:HG13 | 2.12                     | 0.50              |
| 1:F:67:GLY:HA2   | 1:F:70:LEU:HB2   | 1.93                     | 0.50              |
| 1:F:103:GLN:O    | 1:F:104:ARG:HG2  | 2.12                     | 0.50              |
| 1:E:55:TRP:C     | 1:E:58:ILE:HG13  | 2.36                     | 0.49              |
| 1:F:54:PHE:CD2   | 1:F:55:TRP:HD1   | 2.29                     | 0.49              |
| 1:B:36:LYS:CE    | 1:B:37:ILE:HD12  | 2.41                     | 0.49              |
| 1:C:96:TYR:CZ    | 1:C:169:LEU:CD2  | 2.95                     | 0.49              |
| 1:E:112:VAL:O    | 1:E:115:LEU:HB3  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:116:ILE:HG23 | 1:F:117:ASN:H    | 1.75                     | 0.49              |
| 1:C:70:LEU:CD2   | 1:C:70:LEU:N     | 2.73                     | 0.49              |
| 1:C:96:TYR:O     | 1:C:98:LYS:HG3   | 2.11                     | 0.49              |
| 1:E:22:VAL:HG21  | 1:E:67:GLY:HA2   | 1.91                     | 0.49              |
| 1:E:76:TYR:HD1   | 1:E:77:PHE:N     | 2.10                     | 0.49              |
| 1:F:29:ALA:HB1   | 1:F:36:LYS:HZ3   | 1.77                     | 0.49              |
| 1:A:24:PHE:CE2   | 1:A:43:PRO:HD3   | 2.47                     | 0.49              |
| 1:B:133:LEU:HD12 | 1:B:133:LEU:H    | 1.74                     | 0.49              |
| 1:E:18:ILE:HG21  | 1:E:63:ALA:CB    | 2.37                     | 0.49              |
| 1:E:46:LEU:HD12  | 1:E:49:MET:SD    | 2.52                     | 0.49              |
| 1:F:118:ILE:HG23 | 1:F:119:ILE:HD12 | 1.87                     | 0.49              |
| 1:A:23:VAL:HG13  | 1:A:26:ARG:CD    | 2.42                     | 0.49              |
| 1:B:45:SER:O     | 1:B:49:MET:HG3   | 2.12                     | 0.49              |
| 1:D:79:GLY:O     | 1:D:124:TRP:CH2  | 2.66                     | 0.49              |
| 1:E:32:THR:CG2   | 1:E:33:THR:N     | 2.75                     | 0.49              |
| 1:D:35:LEU:C     | 1:D:35:LEU:CD2   | 2.86                     | 0.49              |
| 1:A:126:SER:HG   | 1:A:127:LEU:N    | 2.11                     | 0.49              |
| 1:B:138:TRP:CE3  | 1:B:139:TRP:N    | 2.81                     | 0.49              |
| 1:A:101:THR:C    | 1:A:103:GLN:N    | 2.66                     | 0.49              |
| 1:A:162:ASN:ND2  | 1:A:162:ASN:N    | 2.60                     | 0.49              |
| 1:A:172:LYS:N    | 1:A:173:PRO:HD3  | 2.25                     | 0.49              |
| 1:B:162:ASN:ND2  | 1:B:162:ASN:N    | 2.60                     | 0.49              |
| 1:E:13:LEU:CA    | 1:E:16:VAL:CG2   | 2.86                     | 0.49              |
| 1:E:115:LEU:HD13 | 1:E:116:ILE:HA   | 1.93                     | 0.49              |
| 1:B:135:ASN:CB   | 1:B:138:TRP:HB2  | 2.35                     | 0.49              |
| 1:C:68:MET:C     | 1:C:70:LEU:O     | 2.56                     | 0.49              |
| 1:C:97:LYS:HG3   | 1:C:169:LEU:HD22 | 1.95                     | 0.49              |
| 1:C:107:LEU:CD1  | 1:C:107:LEU:C    | 2.85                     | 0.49              |
| 1:C:133:LEU:HG   | 1:C:134:ALA:N    | 2.27                     | 0.49              |
| 1:C:125:LEU:CD2  | 2:C:201:FOL:H16  | 2.43                     | 0.49              |
| 1:D:36:LYS:HB2   | 2:D:201:FOL:H12  | 1.94                     | 0.49              |
| 1:E:37:ILE:HG23  | 1:E:37:ILE:O     | 2.13                     | 0.49              |
| 1:E:76:TYR:CE1   | 1:E:78:PRO:HA    | 2.48                     | 0.49              |
| 1:E:76:TYR:HA    | 2:E:201:FOL:N8   | 2.28                     | 0.49              |
| 1:F:36:LYS:CG    | 1:F:37:ILE:N     | 2.76                     | 0.49              |
| 1:A:36:LYS:HG2   | 2:A:201:FOL:C    | 2.43                     | 0.48              |
| 1:A:126:SER:HG   | 1:A:127:LEU:H    | 1.61                     | 0.48              |
| 1:A:137:ALA:HA   | 1:A:140:VAL:HG23 | 1.94                     | 0.48              |
| 1:D:26:ARG:C     | 1:D:27:PHE:HD1   | 2.21                     | 0.48              |
| 1:E:13:LEU:N     | 1:E:13:LEU:CD1   | 2.73                     | 0.48              |
| 1:F:78:PRO:O     | 1:F:81:THR:HG22  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:116:ILE:O    | 1:F:120:LEU:HB2  | 2.13                     | 0.48              |
| 1:C:64:ASP:OD2   | 1:C:81:THR:CA    | 2.61                     | 0.48              |
| 1:F:121:THR:C    | 1:F:125:LEU:HD12 | 2.38                     | 0.48              |
| 2:F:201:FOL:H16  | 2:F:201:FOL:HG1  | 1.94                     | 0.48              |
| 1:C:173:PRO:HG2  | 1:C:174:LEU:N    | 2.28                     | 0.48              |
| 1:F:117:ASN:C    | 1:F:121:THR:HG1  | 2.09                     | 0.48              |
| 1:F:150:PHE:HB2  | 1:F:153:GLN:CD   | 2.38                     | 0.48              |
| 1:C:30:TYR:CB    | 1:C:37:ILE:H     | 2.25                     | 0.48              |
| 1:C:166:PHE:N    | 1:C:166:PHE:HD2  | 2.11                     | 0.48              |
| 1:E:90:ILE:HG21  | 1:E:112:VAL:CG2  | 2.44                     | 0.48              |
| 1:F:150:PHE:CD1  | 1:F:153:GLN:OE1  | 2.67                     | 0.48              |
| 1:C:125:LEU:HD13 | 1:C:138:TRP:CZ2  | 2.49                     | 0.48              |
| 1:E:119:ILE:HG13 | 1:E:120:LEU:CB   | 2.36                     | 0.48              |
| 1:F:138:TRP:CD1  | 1:F:138:TRP:H    | 2.31                     | 0.48              |
| 1:A:170:PHE:CE2  | 1:A:173:PRO:HG2  | 2.48                     | 0.48              |
| 1:C:30:TYR:HB2   | 1:C:37:ILE:N     | 2.28                     | 0.48              |
| 1:D:117:ASN:ND2  | 2:D:201:FOL:OE1  | 2.46                     | 0.48              |
| 1:B:36:LYS:CE    | 1:B:37:ILE:HD13  | 2.44                     | 0.48              |
| 1:B:53:PRO:HG2   | 1:B:54:PHE:H     | 1.78                     | 0.48              |
| 1:C:10:SER:CA    | 1:C:170:PHE:CZ   | 2.96                     | 0.48              |
| 1:E:40:THR:HG22  | 1:E:43:PRO:CD    | 2.42                     | 0.48              |
| 1:B:48:GLY:O     | 1:B:96:TYR:HB2   | 2.14                     | 0.48              |
| 1:B:149:PHE:CD1  | 1:B:152:ILE:HD12 | 2.44                     | 0.48              |
| 1:D:26:ARG:HA    | 1:D:26:ARG:HD3   | 1.53                     | 0.48              |
| 1:E:11:ILE:HG13  | 1:E:12:ALA:N     | 2.29                     | 0.48              |
| 1:E:107:LEU:O    | 1:E:111:LEU:HB2  | 2.13                     | 0.48              |
| 1:C:41:PHE:CZ    | 1:C:42:ILE:HG12  | 2.48                     | 0.48              |
| 1:D:105:VAL:HG21 | 1:D:158:TYR:HB2  | 1.95                     | 0.48              |
| 1:C:51:PHE:HB3   | 1:C:55:TRP:HB2   | 1.96                     | 0.47              |
| 1:E:34:PHE:O     | 1:E:35:LEU:HD23  | 2.13                     | 0.47              |
| 1:F:150:PHE:O    | 1:F:153:GLN:OE1  | 2.32                     | 0.47              |
| 1:A:8:THR:O      | 1:A:9:LYS:C      | 2.58                     | 0.47              |
| 1:A:155:ILE:N    | 1:A:155:ILE:CD1  | 2.77                     | 0.47              |
| 1:D:148:ILE:O    | 1:D:152:ILE:HG13 | 2.14                     | 0.47              |
| 1:E:140:VAL:N    | 1:E:141:PRO:HD2  | 2.28                     | 0.47              |
| 1:F:16:VAL:CG2   | 1:F:17:LEU:N     | 2.77                     | 0.47              |
| 1:F:107:LEU:HD13 | 1:F:107:LEU:HA   | 1.76                     | 0.47              |
| 1:A:14:MET:HE3   | 1:A:51:PHE:CD2   | 2.49                     | 0.47              |
| 1:A:14:MET:HE2   | 1:A:14:MET:CA    | 2.41                     | 0.47              |
| 1:B:135:ASN:C    | 1:B:138:TRP:H    | 2.10                     | 0.47              |
| 1:C:166:PHE:HE2  | 1:C:167:LYS:HZ3  | 1.61                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:41:PHE:C     | 1:E:42:ILE:CG1   | 2.86                     | 0.47              |
| 1:E:51:PHE:CD1   | 1:E:170:PHE:HB3  | 2.49                     | 0.47              |
| 1:F:18:ILE:CD1   | 1:F:19:ALA:N     | 2.73                     | 0.47              |
| 1:F:83:ASN:CG    | 1:F:116:ILE:HD11 | 2.29                     | 0.47              |
| 1:A:8:THR:O      | 1:A:11:ILE:N     | 2.47                     | 0.47              |
| 1:D:41:PHE:CD1   | 1:D:157:THR:OG1  | 2.67                     | 0.47              |
| 1:F:35:LEU:HD23  | 1:F:35:LEU:N     | 2.28                     | 0.47              |
| 1:F:138:TRP:C    | 1:F:139:TRP:CE3  | 2.92                     | 0.47              |
| 1:A:39:PHE:CD2   | 1:A:41:PHE:CZ    | 3.01                     | 0.47              |
| 1:A:51:PHE:CD1   | 1:A:51:PHE:N     | 2.82                     | 0.47              |
| 1:B:62:VAL:O     | 1:B:66:VAL:HG13  | 2.15                     | 0.47              |
| 1:C:118:ILE:O    | 1:C:122:PRO:HD2  | 2.15                     | 0.47              |
| 1:D:95:TYR:CG    | 1:D:100:MET:HE2  | 2.49                     | 0.47              |
| 1:E:145:LYS:HD3  | 1:E:149:PHE:CB   | 2.39                     | 0.47              |
| 1:B:145:LYS:HG2  | 1:B:149:PHE:CD2  | 2.50                     | 0.47              |
| 1:C:112:VAL:CG1  | 1:C:116:ILE:HG21 | 2.44                     | 0.47              |
| 1:D:124:TRP:HD1  | 1:D:127:LEU:HD12 | 1.79                     | 0.47              |
| 1:F:54:PHE:CD2   | 1:F:55:TRP:CD1   | 3.02                     | 0.47              |
| 1:F:114:VAL:HG13 | 1:F:115:LEU:N    | 2.30                     | 0.47              |
| 1:A:17:LEU:O     | 1:A:20:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:172:LYS:NZ   | 1:A:172:LYS:CA   | 2.78                     | 0.47              |
| 1:C:17:LEU:HB3   | 1:C:47:ILE:HD11  | 1.97                     | 0.47              |
| 1:C:70:LEU:O     | 1:C:71:PHE:HB2   | 2.15                     | 0.47              |
| 1:D:24:PHE:CE2   | 1:D:43:PRO:HD3   | 2.50                     | 0.47              |
| 1:D:33:THR:HG21  | 1:D:34:PHE:CE1   | 2.35                     | 0.47              |
| 1:E:86:LEU:O     | 1:E:90:ILE:HD13  | 2.14                     | 0.47              |
| 1:A:36:LYS:HZ2   | 2:A:201:FOL:HN   | 1.63                     | 0.47              |
| 1:B:161:GLY:C    | 1:B:162:ASN:ND2  | 2.73                     | 0.47              |
| 1:E:17:LEU:CA    | 1:E:20:VAL:CG2   | 2.92                     | 0.47              |
| 1:E:145:LYS:NZ   | 1:E:150:PHE:CD2  | 2.82                     | 0.47              |
| 1:F:119:ILE:HD12 | 1:F:119:ILE:N    | 2.30                     | 0.47              |
| 1:A:114:VAL:O    | 1:A:118:ILE:HG12 | 2.15                     | 0.47              |
| 1:B:142:ARG:HH12 | 2:B:201:FOL:HG2  | 1.80                     | 0.47              |
| 1:F:119:ILE:CG2  | 1:F:123:LEU:CD1  | 2.86                     | 0.47              |
| 1:A:16:VAL:O     | 1:A:20:VAL:HG22  | 2.14                     | 0.47              |
| 1:C:86:LEU:HD23  | 1:C:86:LEU:HA    | 1.75                     | 0.47              |
| 1:C:157:THR:O    | 1:C:160:LEU:HB3  | 2.16                     | 0.47              |
| 1:C:174:LEU:C    | 1:C:174:LEU:CD2  | 2.85                     | 0.47              |
| 1:E:23:VAL:CA    | 1:E:26:ARG:CD    | 2.74                     | 0.47              |
| 1:E:52:GLY:O     | 1:E:56:ALA:HB3   | 2.13                     | 0.47              |
| 1:F:80:PHE:HD2   | 2:F:201:FOL:HN22 | 1.63                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:116:ILE:CD1  | 1:F:120:LEU:CD1  | 2.86                     | 0.47              |
| 1:F:170:PHE:N    | 1:F:170:PHE:CD2  | 2.82                     | 0.47              |
| 1:A:77:PHE:CD1   | 1:A:78:PRO:HD2   | 2.50                     | 0.46              |
| 1:B:80:PHE:HD2   | 2:B:201:FOL:C8A  | 2.27                     | 0.46              |
| 1:B:114:VAL:O    | 1:B:119:ILE:HD13 | 2.15                     | 0.46              |
| 1:C:149:PHE:O    | 1:C:152:ILE:N    | 2.48                     | 0.46              |
| 1:D:105:VAL:HG21 | 1:D:158:TYR:HD1  | 1.81                     | 0.46              |
| 1:D:135:ASN:ND2  | 1:D:137:ALA:HB3  | 2.30                     | 0.46              |
| 1:E:27:PHE:CD2   | 1:E:27:PHE:N     | 2.73                     | 0.46              |
| 1:F:17:LEU:HD13  | 1:F:17:LEU:HA    | 1.69                     | 0.46              |
| 1:B:128:MET:CE   | 1:B:129:TYR:CE2  | 2.91                     | 0.46              |
| 1:D:9:LYS:HG3    | 1:D:10:SER:N     | 2.30                     | 0.46              |
| 1:E:117:ASN:HA   | 1:E:121:THR:OG1  | 2.15                     | 0.46              |
| 1:E:128:MET:HB3  | 1:E:129:TYR:CE2  | 2.49                     | 0.46              |
| 1:F:117:ASN:HA   | 1:F:121:THR:OG1  | 2.15                     | 0.46              |
| 1:C:27:PHE:N     | 1:C:27:PHE:HD1   | 2.14                     | 0.46              |
| 1:C:110:LEU:HA   | 1:C:113:THR:CG2  | 2.45                     | 0.46              |
| 1:D:10:SER:HB2   | 1:D:172:LYS:HG3  | 1.90                     | 0.46              |
| 1:E:83:ASN:CG    | 1:E:120:LEU:HD21 | 2.40                     | 0.46              |
| 1:E:153:GLN:CD   | 1:E:154:VAL:N    | 2.73                     | 0.46              |
| 1:B:164:ILE:CG1  | 1:B:165:PRO:HD2  | 2.37                     | 0.46              |
| 1:E:55:TRP:HA    | 1:E:58:ILE:CD1   | 2.45                     | 0.46              |
| 1:F:170:PHE:CD2  | 1:F:170:PHE:C    | 2.92                     | 0.46              |
| 1:B:46:LEU:CD1   | 1:B:49:MET:HE3   | 2.41                     | 0.46              |
| 1:C:112:VAL:HG13 | 1:C:116:ILE:HG21 | 1.97                     | 0.46              |
| 1:F:30:TYR:HB2   | 1:F:36:LYS:CE    | 2.32                     | 0.46              |
| 1:A:23:VAL:CA    | 1:A:26:ARG:HD3   | 2.44                     | 0.46              |
| 1:C:19:ALA:O     | 1:C:23:VAL:HG12  | 2.15                     | 0.46              |
| 1:C:45:SER:HB3   | 1:C:95:TYR:HE2   | 1.80                     | 0.46              |
| 1:B:18:ILE:HG23  | 1:B:63:ALA:HA    | 1.97                     | 0.46              |
| 1:E:18:ILE:HG21  | 1:E:63:ALA:HA    | 1.96                     | 0.46              |
| 1:F:17:LEU:O     | 1:F:20:VAL:HB    | 2.15                     | 0.46              |
| 1:F:111:LEU:O    | 1:F:114:VAL:HG13 | 2.16                     | 0.46              |
| 1:A:80:PHE:O     | 1:A:83:ASN:HB2   | 2.16                     | 0.46              |
| 1:B:18:ILE:O     | 1:B:22:VAL:HG22  | 2.15                     | 0.46              |
| 1:B:48:GLY:HA2   | 1:B:92:GLY:HA2   | 1.98                     | 0.46              |
| 1:B:164:ILE:C    | 1:B:164:ILE:CD1  | 2.86                     | 0.46              |
| 1:F:73:LYS:CG    | 2:F:201:FOL:C7   | 2.94                     | 0.46              |
| 1:B:14:MET:HG2   | 1:B:51:PHE:HZ    | 1.15                     | 0.46              |
| 1:B:49:MET:CE    | 1:B:160:LEU:HG   | 2.42                     | 0.46              |
| 1:C:40:THR:O     | 1:C:43:PRO:HD2   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:17:LEU:N     | 1:D:17:LEU:HD23  | 2.31                     | 0.46              |
| 1:D:108:ALA:O    | 1:D:111:LEU:N    | 2.49                     | 0.46              |
| 1:F:24:PHE:O     | 1:F:39:PHE:HD2   | 1.98                     | 0.46              |
| 1:A:23:VAL:O     | 1:A:26:ARG:HB3   | 2.16                     | 0.46              |
| 1:A:26:ARG:NH1   | 1:A:28:PHE:HB2   | 2.31                     | 0.46              |
| 1:A:29:ALA:C     | 1:A:31:GLU:OE1   | 2.59                     | 0.46              |
| 1:C:150:PHE:N    | 1:C:151:PRO:HD2  | 2.31                     | 0.46              |
| 1:D:18:ILE:O     | 1:D:22:VAL:HG23  | 2.16                     | 0.46              |
| 1:E:40:THR:CG2   | 1:E:43:PRO:CG    | 2.93                     | 0.46              |
| 1:E:152:ILE:HA   | 1:E:155:ILE:HD13 | 1.98                     | 0.46              |
| 1:A:26:ARG:NH2   | 1:A:27:PHE:HB2   | 2.29                     | 0.45              |
| 1:C:94:PHE:CD1   | 1:C:108:ALA:HA   | 2.51                     | 0.45              |
| 1:D:64:ASP:OD1   | 1:D:80:PHE:HE1   | 1.99                     | 0.45              |
| 1:F:116:ILE:CD1  | 1:F:120:LEU:CD2  | 2.85                     | 0.45              |
| 1:F:122:PRO:HD3  | 1:F:142:ARG:HH12 | 1.80                     | 0.45              |
| 1:B:74:ALA:O     | 2:B:201:FOL:C7   | 2.65                     | 0.45              |
| 1:C:70:LEU:CA    | 1:C:72:PRO:HD3   | 2.41                     | 0.45              |
| 1:F:116:ILE:HD13 | 1:F:120:LEU:CD2  | 2.44                     | 0.45              |
| 1:C:48:GLY:O     | 1:C:92:GLY:CA    | 2.57                     | 0.45              |
| 1:C:149:PHE:O    | 1:C:152:ILE:HB   | 2.17                     | 0.45              |
| 1:E:29:ALA:CB    | 1:E:39:PHE:CD2   | 2.94                     | 0.45              |
| 1:E:69:LEU:CD1   | 1:E:70:LEU:HB2   | 2.47                     | 0.45              |
| 1:E:80:PHE:HD2   | 2:E:201:FOL:N1   | 2.15                     | 0.45              |
| 2:F:201:FOL:C6   | 2:F:201:FOL:H15  | 2.46                     | 0.45              |
| 1:C:170:PHE:HD1  | 1:C:172:LYS:CE   | 2.29                     | 0.45              |
| 1:E:18:ILE:CG2   | 1:E:63:ALA:HA    | 2.46                     | 0.45              |
| 1:F:111:LEU:HA   | 1:F:114:VAL:CG1  | 2.46                     | 0.45              |
| 1:F:150:PHE:HA   | 1:F:153:GLN:H    | 1.81                     | 0.45              |
| 1:A:50:ILE:HB    | 1:A:51:PHE:HD1   | 1.77                     | 0.45              |
| 1:A:111:LEU:O    | 1:A:115:LEU:HB3  | 2.17                     | 0.45              |
| 1:A:172:LYS:HA   | 1:A:172:LYS:HZ1  | 1.82                     | 0.45              |
| 1:B:29:ALA:C     | 1:B:36:LYS:NZ    | 2.70                     | 0.45              |
| 1:D:139:TRP:O    | 1:D:142:ARG:HB3  | 2.17                     | 0.45              |
| 1:E:18:ILE:HG21  | 1:E:63:ALA:CA    | 2.46                     | 0.45              |
| 1:E:113:THR:HA   | 1:E:116:ILE:HD11 | 1.98                     | 0.45              |
| 1:F:30:TYR:C     | 1:F:36:LYS:NZ    | 2.52                     | 0.45              |
| 1:B:26:ARG:CD    | 1:B:71:PHE:CD1   | 3.00                     | 0.45              |
| 1:B:81:THR:HG23  | 2:B:201:FOL:HN22 | 1.82                     | 0.45              |
| 1:B:120:LEU:HD22 | 1:B:124:TRP:CZ2  | 2.51                     | 0.45              |
| 1:B:138:TRP:C    | 1:B:138:TRP:CD2  | 2.95                     | 0.45              |
| 1:C:22:VAL:O     | 1:C:26:ARG:HB2   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:76:TYR:CE1   | 1:E:77:PHE:C     | 2.95                     | 0.45              |
| 1:F:25:SER:O     | 1:F:29:ALA:HB3   | 2.14                     | 0.45              |
| 1:F:116:ILE:HD12 | 1:F:120:LEU:CB   | 2.43                     | 0.45              |
| 1:F:120:LEU:HB3  | 1:F:124:TRP:CE3  | 2.51                     | 0.45              |
| 1:C:27:PHE:N     | 1:C:27:PHE:CD1   | 2.84                     | 0.45              |
| 1:C:98:LYS:HE3   | 1:C:104:ARG:HH11 | 1.79                     | 0.45              |
| 1:F:53:PRO:O     | 1:F:56:ALA:HB3   | 2.17                     | 0.45              |
| 1:A:30:TYR:O     | 1:A:36:LYS:HA    | 2.16                     | 0.45              |
| 1:A:49:MET:O     | 1:A:96:TYR:CD1   | 2.60                     | 0.45              |
| 1:C:114:VAL:CG2  | 1:D:144:ILE:HD13 | 2.47                     | 0.45              |
| 1:E:54:PHE:O     | 1:E:58:ILE:HG13  | 2.17                     | 0.45              |
| 1:C:122:PRO:CA   | 1:C:125:LEU:HD12 | 2.28                     | 0.45              |
| 1:C:124:TRP:HE3  | 1:C:124:TRP:HA   | 1.81                     | 0.45              |
| 1:E:80:PHE:HA    | 1:E:124:TRP:CE3  | 2.51                     | 0.45              |
| 1:F:68:MET:HE1   | 2:F:201:FOL:C8A  | 2.47                     | 0.45              |
| 1:A:143:LEU:O    | 1:A:147:VAL:HG12 | 2.17                     | 0.45              |
| 1:C:110:LEU:O    | 1:C:113:THR:HG23 | 2.17                     | 0.45              |
| 1:D:86:LEU:O     | 1:D:90:ILE:HG13  | 2.17                     | 0.45              |
| 1:E:10:SER:OG    | 1:E:170:PHE:HD2  | 1.92                     | 0.45              |
| 1:E:10:SER:C     | 1:E:13:LEU:CD2   | 2.90                     | 0.45              |
| 1:F:81:THR:O     | 1:F:85:PHE:CD1   | 2.70                     | 0.45              |
| 1:F:150:PHE:HB2  | 1:F:153:GLN:HB3  | 1.99                     | 0.45              |
| 1:A:89:ALA:O     | 1:A:93:TYR:N     | 2.44                     | 0.44              |
| 1:D:126:SER:O    | 1:D:130:GLY:N    | 2.50                     | 0.44              |
| 1:E:43:PRO:CG    | 1:E:44:GLU:N     | 2.80                     | 0.44              |
| 1:E:58:ILE:HD12  | 1:E:59:GLY:N     | 2.31                     | 0.44              |
| 1:E:137:ALA:O    | 1:E:138:TRP:CD1  | 2.70                     | 0.44              |
| 1:F:150:PHE:O    | 1:F:151:PRO:C    | 2.57                     | 0.44              |
| 1:B:46:LEU:HD12  | 1:B:46:LEU:HA    | 1.73                     | 0.44              |
| 1:E:76:TYR:CD1   | 1:E:77:PHE:O     | 2.70                     | 0.44              |
| 1:E:151:PRO:O    | 1:E:155:ILE:HD12 | 2.17                     | 0.44              |
| 1:F:120:LEU:O    | 1:F:124:TRP:CE3  | 2.70                     | 0.44              |
| 1:F:153:GLN:OE1  | 1:F:154:VAL:HG23 | 2.17                     | 0.44              |
| 1:B:47:ILE:O     | 1:B:47:ILE:HG22  | 2.16                     | 0.44              |
| 1:C:12:ALA:O     | 1:C:16:VAL:HG13  | 2.17                     | 0.44              |
| 1:D:83:ASN:CG    | 1:D:124:TRP:HZ3  | 2.25                     | 0.44              |
| 1:E:66:VAL:CA    | 1:E:69:LEU:HB3   | 2.48                     | 0.44              |
| 1:F:40:THR:O     | 1:F:43:PRO:HD2   | 2.17                     | 0.44              |
| 1:B:23:VAL:CG2   | 1:B:24:PHE:N     | 2.80                     | 0.44              |
| 1:B:137:ALA:CB   | 1:B:140:VAL:HG21 | 2.48                     | 0.44              |
| 1:D:157:THR:HG22 | 1:D:157:THR:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:114:VAL:HG13 | 1:F:115:LEU:H    | 1.82                     | 0.44              |
| 1:F:116:ILE:HD12 | 1:F:116:ILE:O    | 2.17                     | 0.44              |
| 1:F:118:ILE:CG2  | 1:F:119:ILE:N    | 2.80                     | 0.44              |
| 1:C:91:TYR:HE1   | 1:C:112:VAL:HG21 | 1.81                     | 0.44              |
| 1:E:111:LEU:O    | 1:E:114:VAL:HG13 | 2.18                     | 0.44              |
| 1:F:170:PHE:O    | 1:F:170:PHE:CD2  | 2.70                     | 0.44              |
| 1:B:10:SER:O     | 1:B:14:MET:HB2   | 2.17                     | 0.44              |
| 1:E:153:GLN:CD   | 1:E:154:VAL:H    | 2.25                     | 0.44              |
| 1:B:36:LYS:HE2   | 1:B:37:ILE:CB    | 2.47                     | 0.44              |
| 1:B:40:THR:C     | 1:B:43:PRO:HD2   | 2.42                     | 0.44              |
| 1:C:65:VAL:HG12  | 1:C:69:LEU:HD12  | 1.99                     | 0.44              |
| 1:E:34:PHE:O     | 1:E:35:LEU:CG    | 2.66                     | 0.44              |
| 1:E:76:TYR:CE1   | 1:E:77:PHE:O     | 2.70                     | 0.44              |
| 1:E:115:LEU:HD22 | 1:E:119:ILE:HG12 | 2.00                     | 0.44              |
| 1:B:112:VAL:O    | 1:B:116:ILE:HB   | 2.18                     | 0.44              |
| 1:C:26:ARG:HA    | 1:C:26:ARG:HD3   | 1.72                     | 0.44              |
| 1:C:110:LEU:O    | 1:C:113:THR:CG2  | 2.66                     | 0.44              |
| 1:D:27:PHE:N     | 1:D:27:PHE:CD1   | 2.85                     | 0.44              |
| 1:E:10:SER:OG    | 1:E:170:PHE:CE2  | 2.51                     | 0.44              |
| 1:B:24:PHE:HB3   | 1:B:40:THR:HG22  | 1.98                     | 0.43              |
| 1:B:137:ALA:HB1  | 1:B:140:VAL:HG23 | 1.93                     | 0.43              |
| 1:D:30:TYR:HE2   | 1:D:39:PHE:CD2   | 2.34                     | 0.43              |
| 1:E:55:TRP:HA    | 1:E:58:ILE:HG12  | 2.00                     | 0.43              |
| 1:F:68:MET:CE    | 2:F:201:FOL:C8A  | 2.96                     | 0.43              |
| 1:B:173:PRO:C    | 1:B:175:SER:H    | 2.25                     | 0.43              |
| 1:E:35:LEU:C     | 2:E:201:FOL:H12  | 2.43                     | 0.43              |
| 1:F:18:ILE:C     | 1:F:18:ILE:CD1   | 2.86                     | 0.43              |
| 1:F:33:THR:O     | 1:F:34:PHE:CG    | 2.70                     | 0.43              |
| 1:F:94:PHE:CE2   | 1:F:108:ALA:CB   | 2.99                     | 0.43              |
| 1:B:109:THR:HG23 | 1:B:153:GLN:CD   | 2.43                     | 0.43              |
| 1:B:164:ILE:HD13 | 1:B:165:PRO:CA   | 2.49                     | 0.43              |
| 1:C:76:TYR:CE2   | 2:C:201:FOL:NA2  | 2.87                     | 0.43              |
| 1:C:144:ILE:O    | 1:C:147:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:37:ILE:CD1   | 1:D:145:LYS:HG3  | 2.49                     | 0.43              |
| 1:D:161:GLY:C    | 1:D:162:ASN:CG   | 2.85                     | 0.43              |
| 1:E:14:MET:SD    | 1:E:14:MET:C     | 3.02                     | 0.43              |
| 1:F:66:VAL:O     | 1:F:70:LEU:N     | 2.43                     | 0.43              |
| 1:F:159:TYR:O    | 1:F:163:LYS:HG2  | 2.17                     | 0.43              |
| 1:A:160:LEU:HD23 | 1:A:161:GLY:HA2  | 2.00                     | 0.43              |
| 1:B:96:TYR:HE2   | 1:B:97:LYS:NZ    | 2.16                     | 0.43              |
| 1:D:117:ASN:ND2  | 2:D:201:FOL:HG2  | 2.31                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:13:LEU:HA    | 1:E:16:VAL:HG21  | 1.97                     | 0.43              |
| 1:E:70:LEU:C     | 1:E:70:LEU:CD2   | 2.85                     | 0.43              |
| 1:E:150:PHE:HD1  | 1:E:153:GLN:HB3  | 1.82                     | 0.43              |
| 1:A:26:ARG:NE    | 1:A:27:PHE:CB    | 2.81                     | 0.43              |
| 1:A:41:PHE:HE1   | 1:A:42:ILE:HG12  | 1.82                     | 0.43              |
| 1:B:68:MET:HE1   | 2:B:201:FOL:C4A  | 2.48                     | 0.43              |
| 1:C:27:PHE:C     | 1:C:28:PHE:CD1   | 2.89                     | 0.43              |
| 1:C:118:ILE:O    | 1:C:122:PRO:CD   | 2.67                     | 0.43              |
| 1:C:166:PHE:CZ   | 1:C:167:LYS:HD2  | 2.53                     | 0.43              |
| 1:E:36:LYS:CB    | 2:E:201:FOL:C12  | 2.89                     | 0.43              |
| 1:E:74:ALA:HB1   | 2:E:201:FOL:H7   | 2.00                     | 0.43              |
| 1:B:14:MET:HE2   | 1:B:14:MET:HB3   | 1.94                     | 0.43              |
| 1:D:35:LEU:HD22  | 1:D:37:ILE:HD12  | 1.99                     | 0.43              |
| 1:E:41:PHE:C     | 1:E:42:ILE:HG12  | 2.44                     | 0.43              |
| 1:A:18:ILE:HD12  | 1:A:59:GLY:O     | 2.17                     | 0.43              |
| 1:A:26:ARG:O     | 1:A:27:PHE:CD1   | 2.70                     | 0.43              |
| 1:A:86:LEU:HA    | 1:A:86:LEU:HD23  | 1.73                     | 0.43              |
| 1:C:94:PHE:CD1   | 1:C:108:ALA:HB1  | 2.51                     | 0.43              |
| 1:D:36:LYS:HB2   | 2:D:201:FOL:C12  | 2.49                     | 0.43              |
| 1:E:112:VAL:C    | 1:E:115:LEU:HB3  | 2.42                     | 0.43              |
| 1:E:115:LEU:HD22 | 1:E:119:ILE:CG1  | 2.49                     | 0.43              |
| 1:A:49:MET:CE    | 1:A:100:MET:HE1  | 2.33                     | 0.43              |
| 1:A:122:PRO:HA   | 1:A:125:LEU:CD1  | 2.47                     | 0.43              |
| 1:C:39:PHE:HB3   | 1:C:42:ILE:HD11  | 2.01                     | 0.43              |
| 1:E:42:ILE:N     | 1:E:42:ILE:CD1   | 2.73                     | 0.43              |
| 1:E:104:ARG:NH1  | 1:E:107:LEU:HD23 | 2.34                     | 0.43              |
| 1:E:115:LEU:CD1  | 1:E:116:ILE:HG23 | 2.49                     | 0.43              |
| 1:D:27:PHE:O     | 1:D:28:PHE:CD2   | 2.70                     | 0.43              |
| 1:E:17:LEU:HD11  | 1:E:47:ILE:HD13  | 1.97                     | 0.43              |
| 1:F:26:ARG:HD2   | 1:F:26:ARG:HA    | 1.76                     | 0.43              |
| 1:B:37:ILE:N     | 1:B:37:ILE:CD1   | 2.73                     | 0.43              |
| 1:E:104:ARG:HH11 | 1:E:107:LEU:HD23 | 1.84                     | 0.43              |
| 1:F:74:ALA:HB3   | 2:F:201:FOL:N8   | 2.34                     | 0.43              |
| 1:B:44:GLU:HG2   | 1:B:60:THR:HG21  | 2.01                     | 0.42              |
| 1:E:115:LEU:CD2  | 1:E:119:ILE:HD13 | 2.49                     | 0.42              |
| 1:F:73:LYS:HG3   | 2:F:201:FOL:C7   | 2.49                     | 0.42              |
| 1:A:18:ILE:CD1   | 1:A:63:ALA:HB2   | 2.49                     | 0.42              |
| 1:A:48:GLY:O     | 1:A:96:TYR:HB2   | 2.18                     | 0.42              |
| 1:A:149:PHE:O    | 1:A:153:GLN:N    | 2.40                     | 0.42              |
| 1:C:97:LYS:O     | 1:C:97:LYS:HE3   | 2.19                     | 0.42              |
| 1:D:17:LEU:HB3   | 1:D:47:ILE:HD11  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:81:THR:O     | 1:E:84:ALA:N     | 2.51                     | 0.42              |
| 1:F:13:LEU:C     | 1:F:13:LEU:CD2   | 2.86                     | 0.42              |
| 1:F:44:GLU:O     | 1:F:45:SER:C     | 2.61                     | 0.42              |
| 1:F:80:PHE:CE1   | 2:F:201:FOL:C4   | 3.01                     | 0.42              |
| 1:F:138:TRP:H    | 1:F:138:TRP:HD1  | 1.67                     | 0.42              |
| 1:F:150:PHE:HD1  | 1:F:153:GLN:OE1  | 2.02                     | 0.42              |
| 1:B:64:ASP:OD1   | 1:B:64:ASP:C     | 2.61                     | 0.42              |
| 1:C:68:MET:CE    | 1:C:71:PHE:O     | 2.65                     | 0.42              |
| 1:C:159:TYR:CD1  | 1:C:159:TYR:C    | 2.95                     | 0.42              |
| 1:C:163:LYS:CB   | 1:C:163:LYS:NZ   | 2.83                     | 0.42              |
| 1:E:83:ASN:HB3   | 1:E:116:ILE:HG22 | 2.01                     | 0.42              |
| 1:F:20:VAL:HA    | 1:F:23:VAL:CG1   | 2.50                     | 0.42              |
| 1:A:26:ARG:C     | 1:A:27:PHE:CD1   | 2.97                     | 0.42              |
| 1:A:36:LYS:NZ    | 2:A:201:FOL:HB2  | 2.33                     | 0.42              |
| 1:B:47:ILE:HG22  | 1:B:56:ALA:CB    | 2.48                     | 0.42              |
| 1:B:59:GLY:O     | 1:B:62:VAL:HG22  | 2.20                     | 0.42              |
| 1:C:125:LEU:HD21 | 2:C:201:FOL:H16  | 2.02                     | 0.42              |
| 1:C:150:PHE:O    | 1:C:154:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:51:PHE:HD1   | 1:D:51:PHE:N     | 2.16                     | 0.42              |
| 1:D:76:TYR:CD1   | 1:D:76:TYR:C     | 2.97                     | 0.42              |
| 1:E:43:PRO:CG    | 1:E:44:GLU:H     | 2.29                     | 0.42              |
| 1:F:68:MET:CE    | 2:F:201:FOL:HN1  | 2.33                     | 0.42              |
| 1:A:110:LEU:HD21 | 1:B:144:ILE:HG23 | 2.02                     | 0.42              |
| 1:E:113:THR:HG21 | 1:E:150:PHE:HD2  | 1.82                     | 0.42              |
| 1:F:116:ILE:CG2  | 1:F:117:ASN:N    | 2.81                     | 0.42              |
| 1:F:118:ILE:O    | 1:F:122:PRO:CD   | 2.67                     | 0.42              |
| 1:F:140:VAL:N    | 1:F:141:PRO:CD   | 2.82                     | 0.42              |
| 1:B:77:PHE:HA    | 1:B:78:PRO:HD3   | 1.87                     | 0.42              |
| 1:C:68:MET:HE1   | 1:C:72:PRO:HA    | 2.00                     | 0.42              |
| 1:C:145:LYS:O    | 1:C:145:LYS:HG2  | 2.18                     | 0.42              |
| 1:E:70:LEU:HD23  | 1:E:71:PHE:CD2   | 2.54                     | 0.42              |
| 1:F:35:LEU:O     | 1:F:36:LYS:CB    | 2.68                     | 0.42              |
| 1:F:102:TRP:C    | 1:F:103:GLN:NE2  | 2.73                     | 0.42              |
| 1:F:120:LEU:O    | 1:F:124:TRP:HE3  | 2.02                     | 0.42              |
| 1:A:49:MET:CE    | 1:A:100:MET:CE   | 2.84                     | 0.42              |
| 1:B:52:GLY:HA2   | 1:B:96:TYR:CG    | 2.54                     | 0.42              |
| 1:C:20:VAL:O     | 1:C:23:VAL:HG13  | 2.19                     | 0.42              |
| 1:C:107:LEU:HD13 | 1:C:107:LEU:C    | 2.45                     | 0.42              |
| 1:C:111:LEU:C    | 1:C:111:LEU:CD2  | 2.92                     | 0.42              |
| 1:D:35:LEU:HD23  | 1:D:36:LYS:C     | 2.45                     | 0.42              |
| 1:D:131:VAL:HG13 | 1:D:133:LEU:HD13 | 1.99                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:173:PRO:O   | 1:D:173:PRO:HG2  | 2.19                     | 0.42              |
| 1:F:17:LEU:HD22 | 1:F:17:LEU:N     | 2.34                     | 0.42              |
| 1:F:136:PHE:HA  | 1:F:137:ALA:HA   | 1.65                     | 0.42              |
| 1:A:109:THR:O   | 1:A:112:VAL:HG13 | 2.19                     | 0.42              |
| 1:B:138:TRP:CZ3 | 1:B:139:TRP:HA   | 2.55                     | 0.42              |
| 1:C:30:TYR:HB2  | 1:C:37:ILE:CB    | 2.49                     | 0.42              |
| 1:C:124:TRP:HA  | 1:C:124:TRP:CE3  | 2.54                     | 0.42              |
| 1:D:10:SER:OG   | 1:D:172:LYS:HG3  | 2.04                     | 0.42              |
| 1:E:55:TRP:CA   | 1:E:55:TRP:HE3   | 2.30                     | 0.42              |
| 1:E:58:ILE:HG13 | 1:E:58:ILE:H     | 1.61                     | 0.42              |
| 1:C:35:LEU:HD12 | 1:C:35:LEU:HA    | 1.81                     | 0.42              |
| 1:C:83:ASN:OD1  | 1:C:116:ILE:CG1  | 2.67                     | 0.42              |
| 1:D:150:PHE:CE2 | 1:D:154:VAL:HG21 | 2.55                     | 0.42              |
| 1:F:18:ILE:HD12 | 1:F:19:ALA:CA    | 2.49                     | 0.42              |
| 1:F:81:THR:CG2  | 1:F:85:PHE:HZ    | 2.32                     | 0.42              |
| 1:A:23:VAL:HA   | 1:A:26:ARG:HB3   | 2.02                     | 0.42              |
| 1:C:94:PHE:CD1  | 1:C:108:ALA:HB2  | 2.53                     | 0.42              |
| 1:E:20:VAL:HA   | 1:E:23:VAL:HG12  | 2.00                     | 0.42              |
| 1:E:27:PHE:O    | 1:E:27:PHE:CD2   | 2.70                     | 0.42              |
| 1:F:32:THR:O    | 1:F:33:THR:C     | 2.61                     | 0.42              |
| 1:C:150:PHE:CA  | 1:C:153:GLN:HG2  | 2.48                     | 0.41              |
| 1:E:42:ILE:N    | 1:E:43:PRO:HD2   | 2.34                     | 0.41              |
| 1:F:118:ILE:CG2 | 1:F:119:ILE:CD1  | 2.85                     | 0.41              |
| 1:A:16:VAL:O    | 1:A:19:ALA:HB3   | 2.19                     | 0.41              |
| 1:A:27:PHE:C    | 1:A:28:PHE:HD1   | 2.27                     | 0.41              |
| 1:A:66:VAL:HG12 | 1:A:70:LEU:HD11  | 2.01                     | 0.41              |
| 1:A:170:PHE:CD2 | 1:A:173:PRO:CG   | 3.02                     | 0.41              |
| 1:B:36:LYS:H    | 2:B:201:FOL:HB2  | 1.84                     | 0.41              |
| 1:C:91:TYR:CE1  | 1:C:112:VAL:HG21 | 2.56                     | 0.41              |
| 1:F:35:LEU:N    | 2:F:201:FOL:H12  | 2.34                     | 0.41              |
| 1:D:95:TYR:CB   | 1:D:100:MET:HE2  | 2.48                     | 0.41              |
| 1:D:133:LEU:CG  | 1:D:138:TRP:CZ3  | 3.03                     | 0.41              |
| 1:E:13:LEU:HD22 | 1:E:13:LEU:N     | 2.09                     | 0.41              |
| 1:E:66:VAL:O    | 1:E:66:VAL:HG12  | 2.19                     | 0.41              |
| 1:E:94:PHE:CD2  | 1:E:108:ALA:HB2  | 2.51                     | 0.41              |
| 1:F:64:ASP:OD1  | 1:F:64:ASP:C     | 2.64                     | 0.41              |
| 1:C:80:PHE:O    | 1:C:83:ASN:CB    | 2.63                     | 0.41              |
| 1:E:74:ALA:HB1  | 1:E:75:GLY:CA    | 2.51                     | 0.41              |
| 1:E:75:GLY:O    | 2:E:201:FOL:H7   | 2.20                     | 0.41              |
| 1:F:145:LYS:HA  | 1:F:148:ILE:CG1  | 2.41                     | 0.41              |
| 1:C:25:SER:CB   | 1:C:26:ARG:NH1   | 2.82                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:13:LEU:C     | 1:D:16:VAL:HG23  | 2.45                     | 0.41              |
| 1:E:145:LYS:HD2  | 1:E:148:ILE:H    | 1.83                     | 0.41              |
| 1:F:116:ILE:HD12 | 1:F:116:ILE:C    | 2.44                     | 0.41              |
| 1:A:23:VAL:C     | 1:A:26:ARG:HB3   | 2.45                     | 0.41              |
| 1:B:13:LEU:C     | 1:B:13:LEU:CD2   | 2.85                     | 0.41              |
| 1:F:42:ILE:HG23  | 1:F:43:PRO:N     | 2.36                     | 0.41              |
| 1:F:121:THR:O    | 1:F:125:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:144:ILE:O    | 1:A:147:VAL:HG12 | 2.20                     | 0.41              |
| 1:B:17:LEU:HD13  | 1:B:20:VAL:HG21  | 2.02                     | 0.41              |
| 1:B:26:ARG:HD3   | 1:B:71:PHE:CD1   | 2.56                     | 0.41              |
| 1:C:124:TRP:CE3  | 1:C:124:TRP:CA   | 3.03                     | 0.41              |
| 1:D:24:PHE:CD2   | 1:D:39:PHE:O     | 2.73                     | 0.41              |
| 1:E:39:PHE:CE1   | 1:E:41:PHE:CZ    | 3.07                     | 0.41              |
| 1:F:118:ILE:HG22 | 1:F:119:ILE:CD1  | 2.33                     | 0.41              |
| 1:F:138:TRP:N    | 1:F:138:TRP:HD1  | 2.17                     | 0.41              |
| 1:A:17:LEU:HD13  | 1:A:47:ILE:HG12  | 2.02                     | 0.41              |
| 1:A:74:ALA:HB1   | 2:A:201:FOL:H92  | 2.03                     | 0.41              |
| 1:A:113:THR:HA   | 1:A:117:ASN:ND2  | 2.36                     | 0.41              |
| 1:C:117:ASN:O    | 1:C:121:THR:OG1  | 2.16                     | 0.41              |
| 1:E:47:ILE:HD11  | 1:E:60:THR:HG23  | 2.03                     | 0.41              |
| 1:E:117:ASN:HA   | 1:E:121:THR:HG1  | 1.86                     | 0.41              |
| 1:F:12:ALA:O     | 1:F:13:LEU:C     | 2.61                     | 0.41              |
| 1:A:23:VAL:HA    | 1:A:26:ARG:CD    | 2.47                     | 0.41              |
| 1:C:10:SER:HA    | 1:C:170:PHE:CZ   | 2.56                     | 0.41              |
| 1:C:76:TYR:CD2   | 2:C:201:FOL:NA2  | 2.89                     | 0.41              |
| 1:C:123:LEU:HD12 | 1:C:123:LEU:HA   | 1.80                     | 0.41              |
| 1:E:113:THR:CG2  | 1:E:150:PHE:CD2  | 3.03                     | 0.41              |
| 1:F:143:LEU:O    | 1:F:147:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:14:MET:CE    | 1:A:14:MET:HA    | 2.44                     | 0.41              |
| 1:C:166:PHE:CD2  | 1:C:167:LYS:HD3  | 2.55                     | 0.41              |
| 1:E:81:THR:C     | 1:E:84:ALA:H     | 2.29                     | 0.41              |
| 1:E:140:VAL:C    | 1:E:142:ARG:O    | 2.64                     | 0.41              |
| 1:F:13:LEU:HD22  | 1:F:14:MET:HA    | 2.02                     | 0.41              |
| 1:F:81:THR:OG1   | 1:F:85:PHE:CZ    | 2.70                     | 0.41              |
| 1:B:36:LYS:HA    | 1:B:37:ILE:HD12  | 2.02                     | 0.40              |
| 1:C:45:SER:HB3   | 1:C:95:TYR:CE2   | 2.56                     | 0.40              |
| 1:C:109:THR:HG22 | 1:C:153:GLN:HE21 | 1.82                     | 0.40              |
| 1:D:121:THR:HG22 | 1:D:125:LEU:HD11 | 2.03                     | 0.40              |
| 1:E:14:MET:SD    | 1:E:14:MET:O     | 2.78                     | 0.40              |
| 1:E:23:VAL:HG23  | 1:E:26:ARG:HD3   | 2.03                     | 0.40              |
| 1:E:34:PHE:O     | 1:E:35:LEU:CD2   | 2.68                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:76:TYR:CD1   | 1:E:77:PHE:C     | 2.99                     | 0.40              |
| 1:F:23:VAL:HG23  | 1:F:27:PHE:CG    | 2.56                     | 0.40              |
| 1:F:81:THR:O     | 1:F:85:PHE:CE1   | 2.74                     | 0.40              |
| 1:A:122:PRO:CA   | 1:A:125:LEU:HD13 | 2.49                     | 0.40              |
| 1:B:145:LYS:HG2  | 1:B:149:PHE:HD2  | 1.85                     | 0.40              |
| 1:C:98:LYS:CE    | 1:C:104:ARG:NH1  | 2.71                     | 0.40              |
| 1:D:124:TRP:HD1  | 1:D:127:LEU:CD1  | 2.35                     | 0.40              |
| 1:A:14:MET:CE    | 1:A:51:PHE:CD2   | 3.03                     | 0.40              |
| 1:A:50:ILE:HB    | 1:A:51:PHE:CE1   | 2.55                     | 0.40              |
| 1:C:150:PHE:CE2  | 1:D:151:PRO:HG2  | 2.54                     | 0.40              |
| 1:D:172:LYS:CG   | 1:D:172:LYS:O    | 2.69                     | 0.40              |
| 1:E:42:ILE:O     | 1:E:42:ILE:HG22  | 2.22                     | 0.40              |
| 1:E:115:LEU:HD23 | 1:E:119:ILE:HD13 | 2.03                     | 0.40              |
| 1:F:9:LYS:O      | 1:F:13:LEU:HD12  | 2.21                     | 0.40              |
| 1:A:36:LYS:N     | 2:A:201:FOL:H12  | 2.36                     | 0.40              |
| 1:B:80:PHE:O     | 1:B:83:ASN:HB2   | 2.20                     | 0.40              |
| 1:B:96:TYR:CG    | 1:B:97:LYS:HG3   | 2.57                     | 0.40              |
| 1:D:25:SER:O     | 1:D:29:ALA:CB    | 2.70                     | 0.40              |
| 1:E:34:PHE:C     | 1:E:35:LEU:HG    | 2.47                     | 0.40              |
| 1:E:35:LEU:O     | 2:E:201:FOL:H12  | 2.21                     | 0.40              |
| 1:E:41:PHE:O     | 1:E:42:ILE:CB    | 2.70                     | 0.40              |
| 1:F:57:GLY:O     | 1:F:85:PHE:HA    | 2.22                     | 0.40              |
| 1:B:36:LYS:NZ    | 1:B:37:ILE:O     | 2.40                     | 0.40              |
| 1:B:136:PHE:HA   | 1:B:137:ALA:HA   | 1.81                     | 0.40              |
| 1:E:117:ASN:O    | 1:E:122:PRO:HD3  | 2.22                     | 0.40              |
| 1:F:34:PHE:HB2   | 1:F:125:LEU:CD2  | 2.51                     | 0.40              |
| 1:F:118:ILE:O    | 1:F:122:PRO:HD2  | 2.20                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:A:72:PRO:CB  | 1:B:11:ILE:CD1[2_555] | 1.00                     | 1.20              |
| 1:A:128:MET:CE | 1:B:6:PHE:CZ[2_555]   | 1.92                     | 0.28              |
| 1:A:128:MET:CE | 1:B:6:PHE:CG[2_555]   | 1.98                     | 0.22              |
| 1:A:72:PRO:CG  | 1:B:11:ILE:CD1[2_555] | 2.19                     | 0.01              |

## 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     | 159/199 (80%)  | 151 (95%) | 7 (4%)   | 1 (1%)   | 21          | 56  |
| 1   | B     | 164/199 (82%)  | 157 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 1   | C     | 162/199 (81%)  | 152 (94%) | 9 (6%)   | 1 (1%)   | 21          | 56  |
| 1   | D     | 158/199 (79%)  | 151 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 1   | E     | 137/199 (69%)  | 121 (88%) | 13 (10%) | 3 (2%)   | 5           | 29  |
| 1   | F     | 140/199 (70%)  | 131 (94%) | 8 (6%)   | 1 (1%)   | 18          | 52  |
| All | All   | 920/1194 (77%) | 863 (94%) | 51 (6%)  | 6 (1%)   | 18          | 52  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 172 | LYS  |
| 1   | E     | 42  | ILE  |
| 1   | F     | 53  | PRO  |
| 1   | C     | 53  | PRO  |
| 1   | E     | 72  | PRO  |
| 1   | E     | 150 | PHE  |

### 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     | 135/168 (80%) | 108 (80%) | 27 (20%) | 1           | 7  |
| 1   | B     | 140/168 (83%) | 120 (86%) | 20 (14%) | 3           | 16 |

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| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | C     | 138/168 (82%)  | 100 (72%) | 38 (28%)  | 0           | 2 |
| 1   | D     | 138/168 (82%)  | 112 (81%) | 26 (19%)  | 1           | 9 |
| 1   | E     | 122/168 (73%)  | 86 (70%)  | 36 (30%)  | 0           | 1 |
| 1   | F     | 124/168 (74%)  | 78 (63%)  | 46 (37%)  | 0           | 0 |
| All | All   | 797/1008 (79%) | 604 (76%) | 193 (24%) | 1           | 4 |

All (193) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | LEU  |
| 1   | A     | 16  | VAL  |
| 1   | A     | 20  | VAL  |
| 1   | A     | 26  | ARG  |
| 1   | A     | 42  | ILE  |
| 1   | A     | 46  | LEU  |
| 1   | A     | 70  | LEU  |
| 1   | A     | 71  | PHE  |
| 1   | A     | 72  | PRO  |
| 1   | A     | 73  | LYS  |
| 1   | A     | 97  | LYS  |
| 1   | A     | 100 | MET  |
| 1   | A     | 101 | THR  |
| 1   | A     | 112 | VAL  |
| 1   | A     | 125 | LEU  |
| 1   | A     | 127 | LEU  |
| 1   | A     | 131 | VAL  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 133 | LEU  |
| 1   | A     | 151 | PRO  |
| 1   | A     | 155 | ILE  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 162 | ASN  |
| 1   | A     | 169 | LEU  |
| 1   | A     | 170 | PHE  |
| 1   | A     | 172 | LYS  |
| 1   | A     | 174 | LEU  |
| 1   | B     | 13  | LEU  |
| 1   | B     | 14  | MET  |
| 1   | B     | 16  | VAL  |
| 1   | B     | 17  | LEU  |
| 1   | B     | 24  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 26  | ARG  |
| 1   | B     | 36  | LYS  |
| 1   | B     | 37  | ILE  |
| 1   | B     | 64  | ASP  |
| 1   | B     | 66  | VAL  |
| 1   | B     | 73  | LYS  |
| 1   | B     | 119 | ILE  |
| 1   | B     | 131 | VAL  |
| 1   | B     | 133 | LEU  |
| 1   | B     | 162 | ASN  |
| 1   | B     | 164 | ILE  |
| 1   | B     | 169 | LEU  |
| 1   | B     | 170 | PHE  |
| 1   | B     | 172 | LYS  |
| 1   | B     | 173 | PRO  |
| 1   | C     | 16  | VAL  |
| 1   | C     | 23  | VAL  |
| 1   | C     | 24  | PHE  |
| 1   | C     | 28  | PHE  |
| 1   | C     | 31  | GLU  |
| 1   | C     | 33  | THR  |
| 1   | C     | 36  | LYS  |
| 1   | C     | 37  | ILE  |
| 1   | C     | 42  | ILE  |
| 1   | C     | 58  | ILE  |
| 1   | C     | 62  | VAL  |
| 1   | C     | 68  | MET  |
| 1   | C     | 69  | LEU  |
| 1   | C     | 70  | LEU  |
| 1   | C     | 73  | LYS  |
| 1   | C     | 81  | THR  |
| 1   | C     | 82  | LEU  |
| 1   | C     | 86  | LEU  |
| 1   | C     | 97  | LYS  |
| 1   | C     | 101 | THR  |
| 1   | C     | 107 | LEU  |
| 1   | C     | 109 | THR  |
| 1   | C     | 116 | ILE  |
| 1   | C     | 121 | THR  |
| 1   | C     | 125 | LEU  |
| 1   | C     | 128 | MET  |
| 1   | C     | 132 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 133 | LEU  |
| 1   | C     | 146 | THR  |
| 1   | C     | 147 | VAL  |
| 1   | C     | 150 | PHE  |
| 1   | C     | 160 | LEU  |
| 1   | C     | 163 | LYS  |
| 1   | C     | 166 | PHE  |
| 1   | C     | 167 | LYS  |
| 1   | C     | 168 | ARG  |
| 1   | C     | 169 | LEU  |
| 1   | C     | 174 | LEU  |
| 1   | D     | 16  | VAL  |
| 1   | D     | 17  | LEU  |
| 1   | D     | 23  | VAL  |
| 1   | D     | 24  | PHE  |
| 1   | D     | 25  | SER  |
| 1   | D     | 26  | ARG  |
| 1   | D     | 37  | ILE  |
| 1   | D     | 51  | PHE  |
| 1   | D     | 97  | LYS  |
| 1   | D     | 98  | LYS  |
| 1   | D     | 99  | GLU  |
| 1   | D     | 115 | LEU  |
| 1   | D     | 116 | ILE  |
| 1   | D     | 128 | MET  |
| 1   | D     | 133 | LEU  |
| 1   | D     | 145 | LYS  |
| 1   | D     | 146 | THR  |
| 1   | D     | 151 | PRO  |
| 1   | D     | 153 | GLN  |
| 1   | D     | 160 | LEU  |
| 1   | D     | 162 | ASN  |
| 1   | D     | 167 | LYS  |
| 1   | D     | 172 | LYS  |
| 1   | D     | 173 | PRO  |
| 1   | D     | 175 | SER  |
| 1   | D     | 176 | GLU  |
| 1   | E     | 10  | SER  |
| 1   | E     | 13  | LEU  |
| 1   | E     | 14  | MET  |
| 1   | E     | 16  | VAL  |
| 1   | E     | 17  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 18  | ILE  |
| 1   | E     | 20  | VAL  |
| 1   | E     | 22  | VAL  |
| 1   | E     | 23  | VAL  |
| 1   | E     | 24  | PHE  |
| 1   | E     | 26  | ARG  |
| 1   | E     | 27  | PHE  |
| 1   | E     | 42  | ILE  |
| 1   | E     | 47  | ILE  |
| 1   | E     | 55  | TRP  |
| 1   | E     | 58  | ILE  |
| 1   | E     | 60  | THR  |
| 1   | E     | 69  | LEU  |
| 1   | E     | 76  | TYR  |
| 1   | E     | 83  | ASN  |
| 1   | E     | 97  | LYS  |
| 1   | E     | 106 | ILE  |
| 1   | E     | 107 | LEU  |
| 1   | E     | 110 | LEU  |
| 1   | E     | 111 | LEU  |
| 1   | E     | 114 | VAL  |
| 1   | E     | 115 | LEU  |
| 1   | E     | 116 | ILE  |
| 1   | E     | 120 | LEU  |
| 1   | E     | 129 | TYR  |
| 1   | E     | 136 | PHE  |
| 1   | E     | 144 | ILE  |
| 1   | E     | 145 | LYS  |
| 1   | E     | 147 | VAL  |
| 1   | E     | 148 | ILE  |
| 1   | E     | 153 | GLN  |
| 1   | F     | 9   | LYS  |
| 1   | F     | 13  | LEU  |
| 1   | F     | 23  | VAL  |
| 1   | F     | 24  | PHE  |
| 1   | F     | 26  | ARG  |
| 1   | F     | 31  | GLU  |
| 1   | F     | 32  | THR  |
| 1   | F     | 33  | THR  |
| 1   | F     | 35  | LEU  |
| 1   | F     | 41  | PHE  |
| 1   | F     | 42  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 44  | GLU  |
| 1   | F     | 45  | SER  |
| 1   | F     | 47  | ILE  |
| 1   | F     | 49  | MET  |
| 1   | F     | 60  | THR  |
| 1   | F     | 65  | VAL  |
| 1   | F     | 69  | LEU  |
| 1   | F     | 70  | LEU  |
| 1   | F     | 73  | LYS  |
| 1   | F     | 81  | THR  |
| 1   | F     | 82  | LEU  |
| 1   | F     | 90  | ILE  |
| 1   | F     | 93  | TYR  |
| 1   | F     | 103 | GLN  |
| 1   | F     | 104 | ARG  |
| 1   | F     | 107 | LEU  |
| 1   | F     | 109 | THR  |
| 1   | F     | 110 | LEU  |
| 1   | F     | 113 | THR  |
| 1   | F     | 114 | VAL  |
| 1   | F     | 115 | LEU  |
| 1   | F     | 116 | ILE  |
| 1   | F     | 118 | ILE  |
| 1   | F     | 121 | THR  |
| 1   | F     | 123 | LEU  |
| 1   | F     | 126 | SER  |
| 1   | F     | 140 | VAL  |
| 1   | F     | 144 | ILE  |
| 1   | F     | 153 | GLN  |
| 1   | F     | 157 | THR  |
| 1   | F     | 160 | LEU  |
| 1   | F     | 162 | ASN  |
| 1   | F     | 163 | LYS  |
| 1   | F     | 169 | LEU  |
| 1   | F     | 170 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 83  | ASN  |
| 1   | F     | 103 | GLN  |
| 1   | F     | 153 | 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | FOL  | A     | 201 | -    | 34,34,34     | 1.02 | 2 (5%)      | 43,47,47    | 1.65 | 10 (23%)    |
| 2   | FOL  | F     | 201 | -    | 34,34,34     | 1.14 | 2 (5%)      | 43,47,47    | 1.31 | 4 (9%)      |
| 2   | FOL  | D     | 201 | -    | 34,34,34     | 0.97 | 2 (5%)      | 43,47,47    | 1.28 | 3 (6%)      |
| 2   | FOL  | C     | 201 | -    | 34,34,34     | 1.15 | 2 (5%)      | 43,47,47    | 1.87 | 8 (18%)     |
| 2   | FOL  | B     | 201 | -    | 34,34,34     | 0.99 | 2 (5%)      | 43,47,47    | 1.46 | 5 (11%)     |
| 2   | FOL  | E     | 201 | -    | 34,34,34     | 1.08 | 2 (5%)      | 43,47,47    | 1.58 | 7 (16%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | FOL  | A     | 201 | -    | -       | 9/22/22/22  | 0/3/3/3 |
| 2   | FOL  | F     | 201 | -    | -       | 12/22/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | FOL  | D     | 201 | -    | -       | 11/22/22/22 | 0/3/3/3 |
| 2   | FOL  | C     | 201 | -    | -       | 8/22/22/22  | 0/3/3/3 |
| 2   | FOL  | B     | 201 | -    | -       | 12/22/22/22 | 0/3/3/3 |
| 2   | FOL  | E     | 201 | -    | -       | 12/22/22/22 | 0/3/3/3 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 201 | FOL  | C8A-N1  | -4.02 | 1.33        | 1.38     |
| 2   | F     | 201 | FOL  | C8A-N1  | -3.76 | 1.33        | 1.38     |
| 2   | D     | 201 | FOL  | C8A-N1  | -3.05 | 1.34        | 1.38     |
| 2   | E     | 201 | FOL  | C8A-N1  | -2.90 | 1.34        | 1.38     |
| 2   | B     | 201 | FOL  | C8A-N1  | -2.56 | 1.34        | 1.38     |
| 2   | E     | 201 | FOL  | C4A-C8A | 2.29  | 1.48        | 1.42     |
| 2   | A     | 201 | FOL  | C8A-N1  | -2.28 | 1.35        | 1.38     |
| 2   | F     | 201 | FOL  | C2-N1   | -2.10 | 1.32        | 1.37     |
| 2   | A     | 201 | FOL  | C4A-C8A | 2.10  | 1.48        | 1.42     |
| 2   | C     | 201 | FOL  | C4-N3   | -2.04 | 1.34        | 1.38     |
| 2   | D     | 201 | FOL  | C4A-C8A | 2.04  | 1.48        | 1.42     |
| 2   | B     | 201 | FOL  | C4A-C8A | 2.03  | 1.48        | 1.42     |

All (37) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | C     | 201 | FOL  | C6-C9-N10  | -6.98 | 97.79       | 113.13   |
| 2   | A     | 201 | FOL  | N1-C8A-N8  | 5.27  | 124.25      | 116.38   |
| 2   | E     | 201 | FOL  | C8A-C4A-C4 | -4.82 | 116.44      | 119.56   |
| 2   | C     | 201 | FOL  | C8A-C4A-C4 | -4.64 | 116.55      | 119.56   |
| 2   | B     | 201 | FOL  | N1-C8A-N8  | 4.12  | 122.53      | 116.38   |
| 2   | D     | 201 | FOL  | C8A-C4A-C4 | -3.93 | 117.01      | 119.56   |
| 2   | F     | 201 | FOL  | N1-C8A-N8  | 3.89  | 122.19      | 116.38   |
| 2   | D     | 201 | FOL  | N1-C8A-N8  | 3.87  | 122.15      | 116.38   |
| 2   | B     | 201 | FOL  | C8A-C4A-C4 | -3.79 | 117.10      | 119.56   |
| 2   | E     | 201 | FOL  | N1-C8A-N8  | 3.71  | 121.92      | 116.38   |
| 2   | B     | 201 | FOL  | C4-C4A-N5  | 3.68  | 124.35      | 118.55   |
| 2   | F     | 201 | FOL  | C8A-C4A-C4 | -3.48 | 117.30      | 119.56   |
| 2   | F     | 201 | FOL  | C4-C4A-N5  | 3.44  | 123.97      | 118.55   |
| 2   | C     | 201 | FOL  | C4-C4A-N5  | 3.18  | 123.57      | 118.55   |
| 2   | E     | 201 | FOL  | C4-C4A-N5  | 3.02  | 123.30      | 118.55   |
| 2   | C     | 201 | FOL  | C9-C6-C7   | -2.98 | 116.01      | 121.38   |
| 2   | A     | 201 | FOL  | CT-CA-N    | -2.96 | 103.70      | 110.57   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D     | 201 | FOL  | C4-C4A-N5  | 2.93  | 123.17      | 118.55   |
| 2   | A     | 201 | FOL  | C8A-C4A-C4 | -2.91 | 117.67      | 119.56   |
| 2   | C     | 201 | FOL  | C7-C6-N5   | 2.84  | 122.71      | 120.87   |
| 2   | E     | 201 | FOL  | C9-C6-N5   | 2.47  | 121.23      | 116.56   |
| 2   | A     | 201 | FOL  | CB-CA-CT   | -2.46 | 104.51      | 110.35   |
| 2   | C     | 201 | FOL  | N1-C8A-N8  | 2.45  | 120.03      | 116.38   |
| 2   | C     | 201 | FOL  | C9-C6-N5   | 2.43  | 121.16      | 116.56   |
| 2   | E     | 201 | FOL  | C7-C6-N5   | -2.32 | 119.36      | 120.87   |
| 2   | A     | 201 | FOL  | C7-N8-C8A  | 2.26  | 120.62      | 116.19   |
| 2   | A     | 201 | FOL  | CA-N-C     | 2.24  | 126.93      | 121.56   |
| 2   | B     | 201 | FOL  | C6-C7-N8   | -2.23 | 121.00      | 123.14   |
| 2   | A     | 201 | FOL  | C11-C-N    | 2.20  | 121.12      | 117.04   |
| 2   | C     | 201 | FOL  | CB-CA-N    | -2.19 | 106.58      | 110.91   |
| 2   | A     | 201 | FOL  | C9-N10-C14 | 2.17  | 128.82      | 121.87   |
| 2   | E     | 201 | FOL  | CG-CB-CA   | -2.14 | 109.21      | 113.16   |
| 2   | A     | 201 | FOL  | C4-C4A-N5  | 2.09  | 121.84      | 118.55   |
| 2   | B     | 201 | FOL  | C7-N8-C8A  | 2.06  | 120.23      | 116.19   |
| 2   | A     | 201 | FOL  | NA2-C2-N3  | -2.05 | 115.67      | 119.67   |
| 2   | F     | 201 | FOL  | C6-C7-N8   | -2.03 | 121.19      | 123.14   |
| 2   | E     | 201 | FOL  | CT-CA-N    | 2.02  | 115.25      | 110.57   |

There are no chirality outliers.

All (64) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | B     | 201 | FOL  | N-CA-CB-CG     |
| 2   | E     | 201 | FOL  | N-CA-CB-CG     |
| 2   | F     | 201 | FOL  | C11-C-N-CA     |
| 2   | F     | 201 | FOL  | O-C-N-CA       |
| 2   | A     | 201 | FOL  | C13-C14-N10-C9 |
| 2   | A     | 201 | FOL  | N-CA-CB-CG     |
| 2   | D     | 201 | FOL  | N-CA-CB-CG     |
| 2   | D     | 201 | FOL  | C15-C14-N10-C9 |
| 2   | E     | 201 | FOL  | C13-C14-N10-C9 |
| 2   | E     | 201 | FOL  | N-C-C11-C12    |
| 2   | A     | 201 | FOL  | C15-C14-N10-C9 |
| 2   | B     | 201 | FOL  | C13-C14-N10-C9 |
| 2   | D     | 201 | FOL  | C13-C14-N10-C9 |
| 2   | E     | 201 | FOL  | C15-C14-N10-C9 |
| 2   | C     | 201 | FOL  | O-C-N-CA       |
| 2   | E     | 201 | FOL  | O-C-C11-C12    |
| 2   | A     | 201 | FOL  | CT-CA-CB-CG    |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | B     | 201 | FOL  | CT-CA-CB-CG    |
| 2   | D     | 201 | FOL  | CT-CA-CB-CG    |
| 2   | E     | 201 | FOL  | N-C-C11-C16    |
| 2   | B     | 201 | FOL  | C15-C14-N10-C9 |
| 2   | E     | 201 | FOL  | O-C-C11-C16    |
| 2   | B     | 201 | FOL  | CT-CA-N-C      |
| 2   | C     | 201 | FOL  | C11-C-N-CA     |
| 2   | E     | 201 | FOL  | CT-CA-CB-CG    |
| 2   | F     | 201 | FOL  | C13-C14-N10-C9 |
| 2   | F     | 201 | FOL  | C15-C14-N10-C9 |
| 2   | E     | 201 | FOL  | N-CA-CT-O1     |
| 2   | E     | 201 | FOL  | N-CA-CT-O2     |
| 2   | D     | 201 | FOL  | CA-CB-CG-CD    |
| 2   | A     | 201 | FOL  | N-C-C11-C12    |
| 2   | B     | 201 | FOL  | CB-CA-CT-O2    |
| 2   | B     | 201 | FOL  | CB-CA-N-C      |
| 2   | B     | 201 | FOL  | CB-CA-CT-O1    |
| 2   | D     | 201 | FOL  | C11-C-N-CA     |
| 2   | A     | 201 | FOL  | O-C-C11-C12    |
| 2   | D     | 201 | FOL  | O-C-N-CA       |
| 2   | B     | 201 | FOL  | OE1-CD-CG-CB   |
| 2   | C     | 201 | FOL  | OE1-CD-CG-CB   |
| 2   | C     | 201 | FOL  | C7-C6-C9-N10   |
| 2   | C     | 201 | FOL  | N-CA-CT-O2     |
| 2   | B     | 201 | FOL  | OE2-CD-CG-CB   |
| 2   | F     | 201 | FOL  | OE2-CD-CG-CB   |
| 2   | F     | 201 | FOL  | OE1-CD-CG-CB   |
| 2   | B     | 201 | FOL  | C7-C6-C9-N10   |
| 2   | C     | 201 | FOL  | OE2-CD-CG-CB   |
| 2   | C     | 201 | FOL  | N5-C6-C9-N10   |
| 2   | F     | 201 | FOL  | N-CA-CT-O1     |
| 2   | F     | 201 | FOL  | N-CA-CT-O2     |
| 2   | B     | 201 | FOL  | N5-C6-C9-N10   |
| 2   | A     | 201 | FOL  | N-C-C11-C16    |
| 2   | D     | 201 | FOL  | OE2-CD-CG-CB   |
| 2   | D     | 201 | FOL  | OE1-CD-CG-CB   |
| 2   | F     | 201 | FOL  | CB-CA-CT-O1    |
| 2   | A     | 201 | FOL  | N5-C6-C9-N10   |
| 2   | E     | 201 | FOL  | N5-C6-C9-N10   |
| 2   | F     | 201 | FOL  | N5-C6-C9-N10   |
| 2   | F     | 201 | FOL  | CB-CA-CT-O2    |
| 2   | A     | 201 | FOL  | C7-C6-C9-N10   |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | E     | 201 | FOL  | C7-C6-C9-N10 |
| 2   | D     | 201 | FOL  | N5-C6-C9-N10 |
| 2   | D     | 201 | FOL  | C7-C6-C9-N10 |
| 2   | F     | 201 | FOL  | C7-C6-C9-N10 |
| 2   | C     | 201 | FOL  | N-CA-CT-O1   |

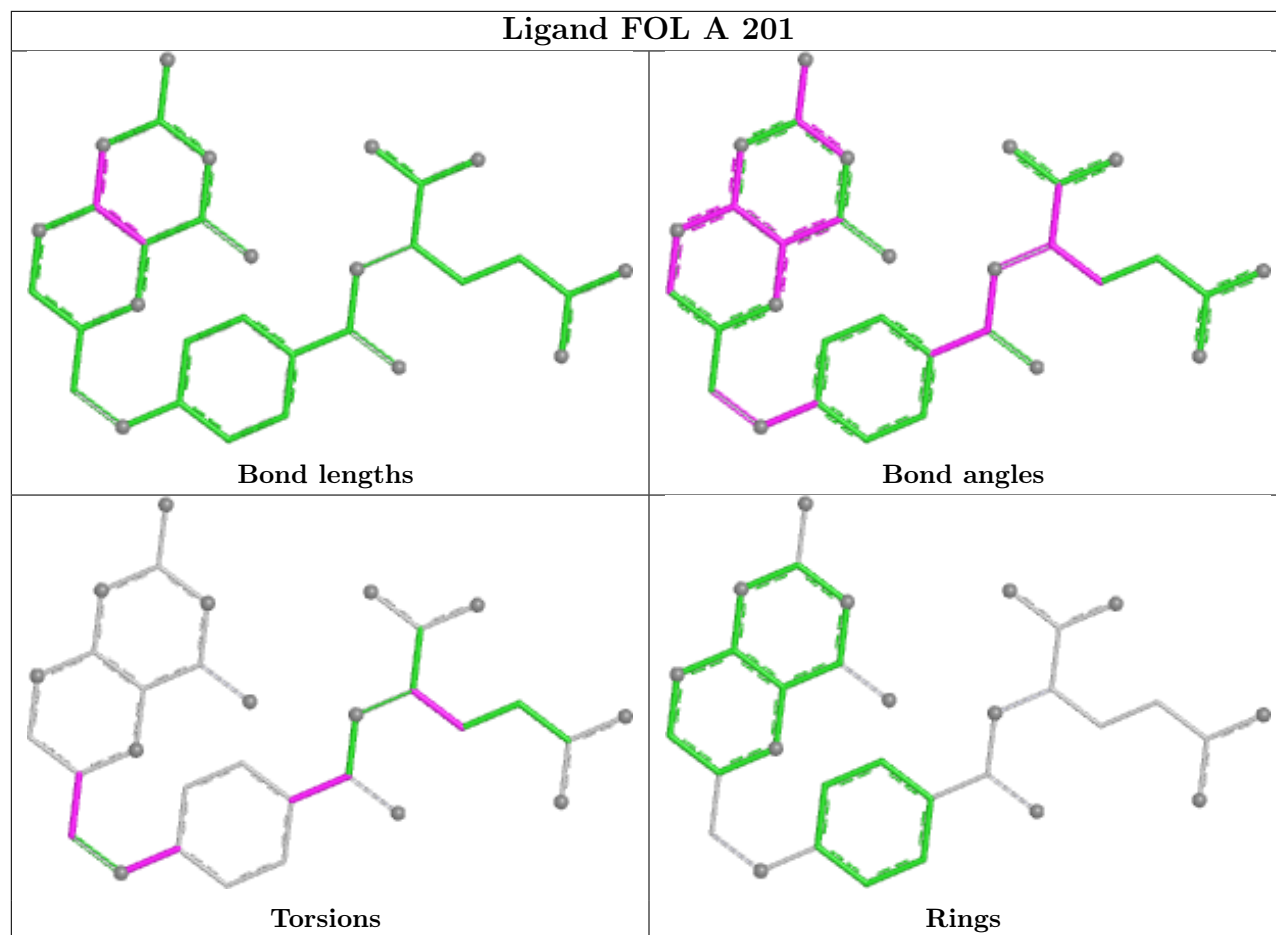
There are no ring outliers.

6 monomers are involved in 117 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 201 | FOL  | 13      | 0            |
| 2   | F     | 201 | FOL  | 46      | 0            |
| 2   | D     | 201 | FOL  | 10      | 0            |
| 2   | C     | 201 | FOL  | 6       | 0            |
| 2   | B     | 201 | FOL  | 15      | 0            |
| 2   | E     | 201 | FOL  | 27      | 0            |

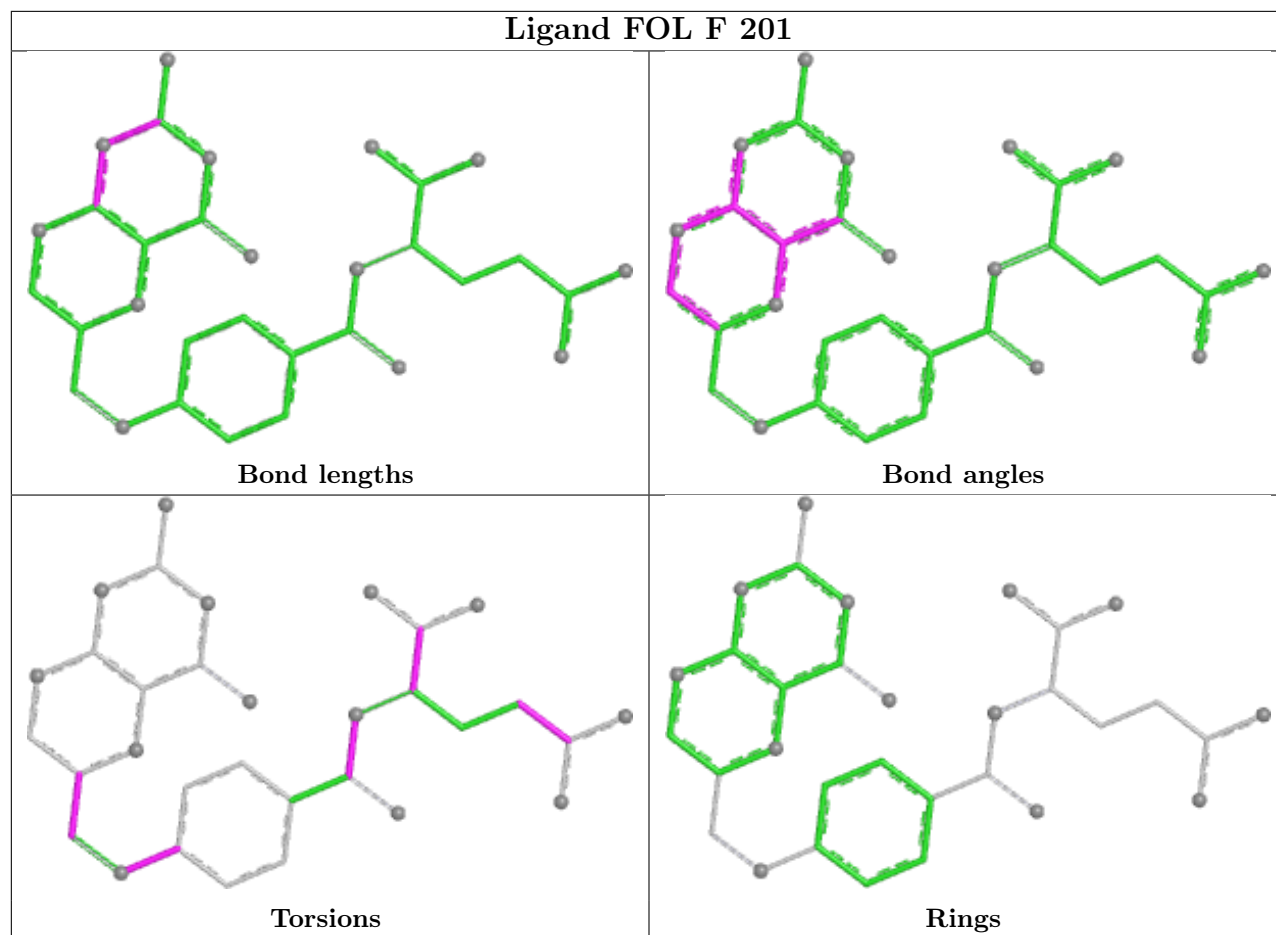
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand FOL A 201

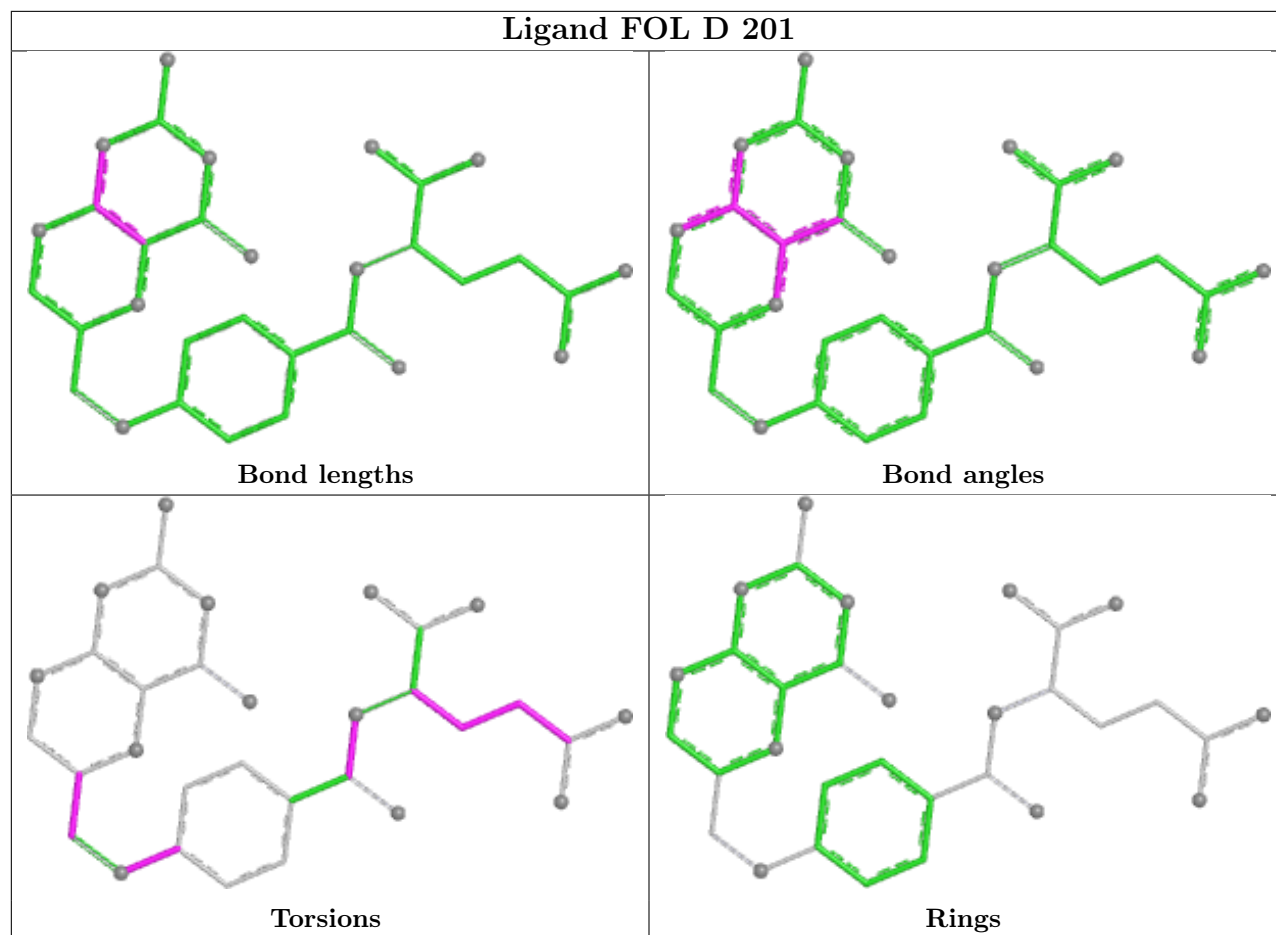




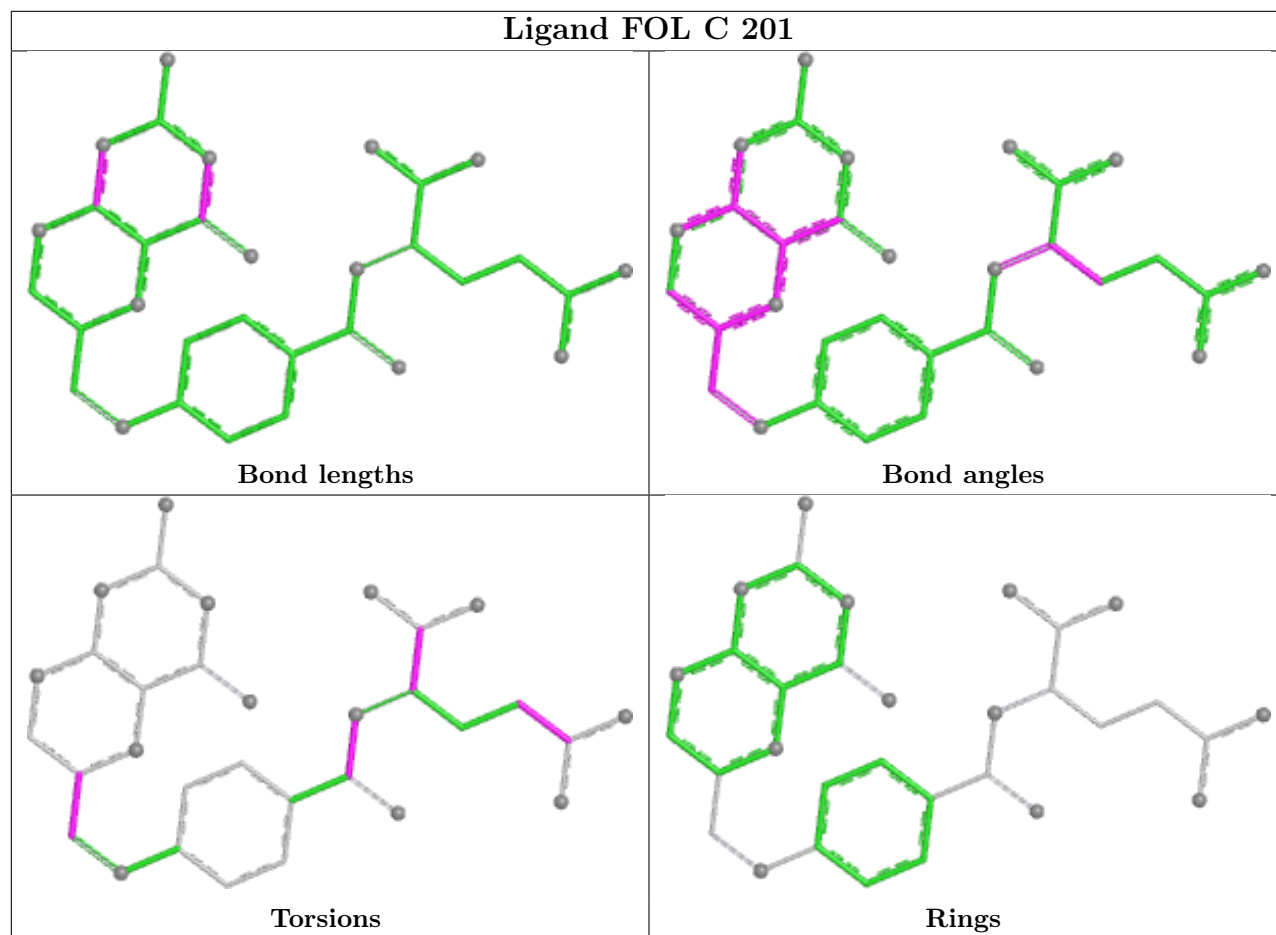
## Ligand FOL F 201



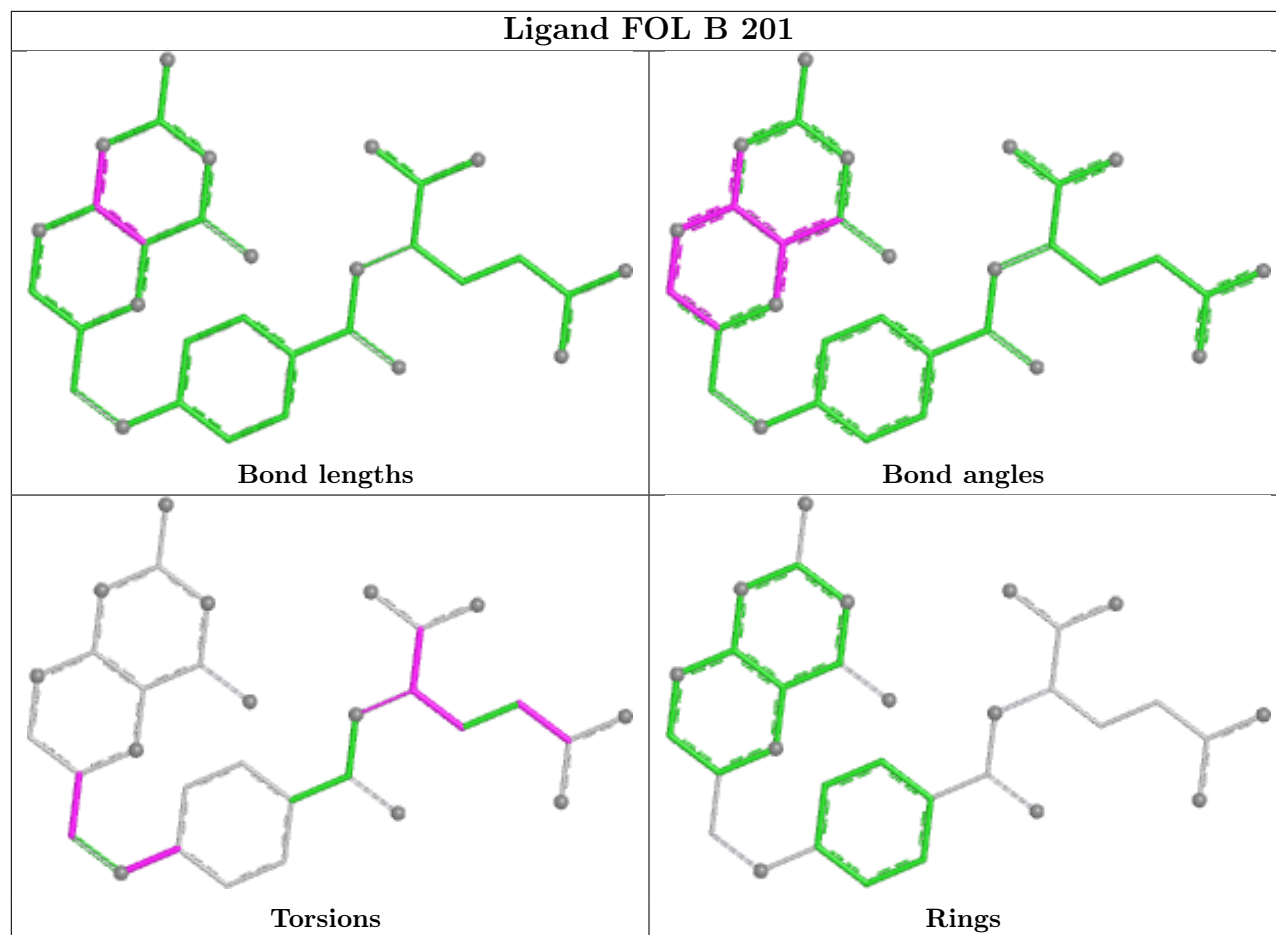
## Ligand FOL D 201

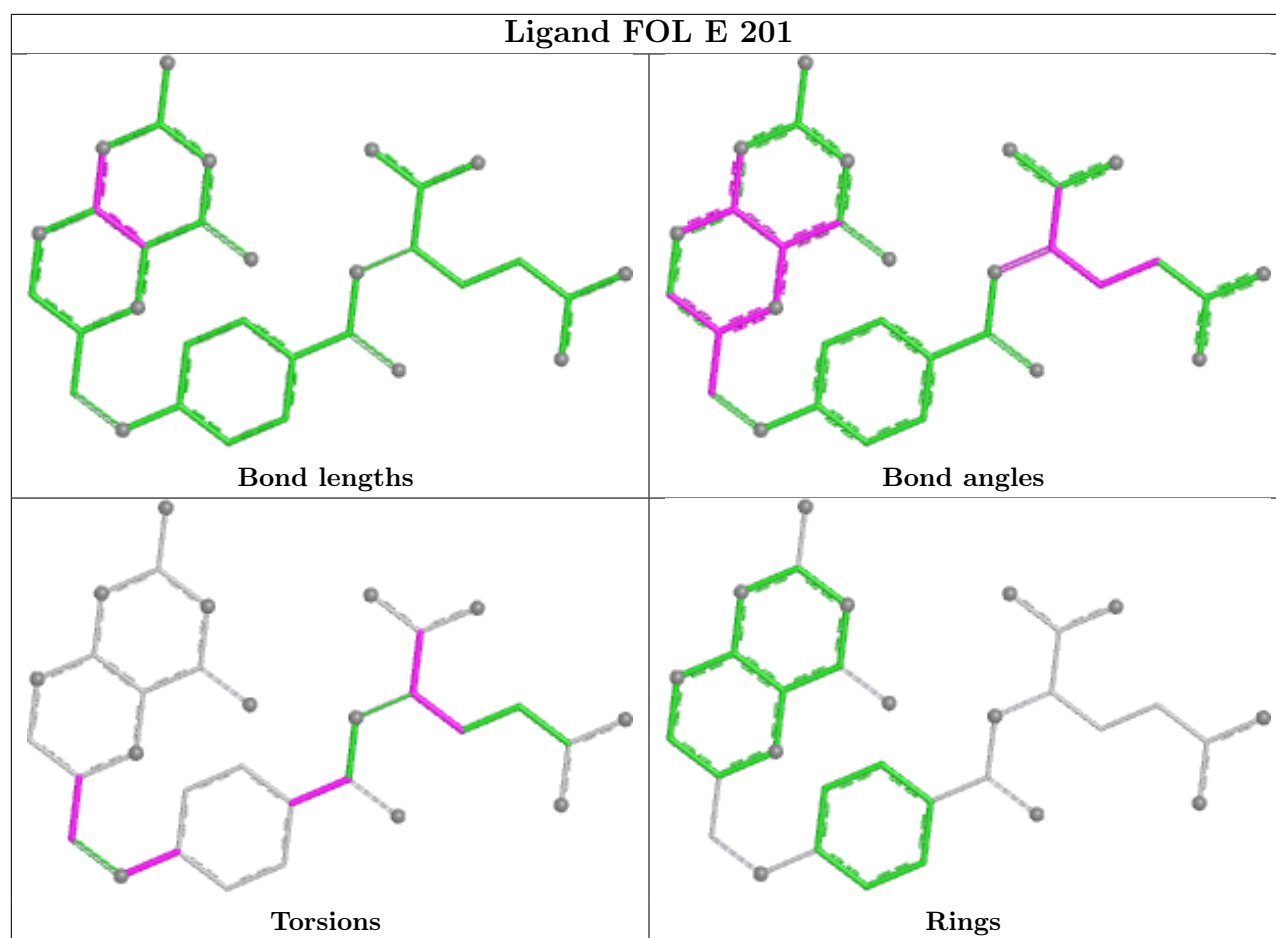


## Ligand FOL C 201



## Ligand FOL B 201





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 163/199 (81%)  | -1.06  | 0 100 100 | 51, 83, 134, 151      | 0     |
| 1   | B     | 168/199 (84%)  | -1.08  | 0 100 100 | 52, 81, 126, 169      | 0     |
| 1   | C     | 166/199 (83%)  | -1.10  | 0 100 100 | 24, 82, 128, 163      | 0     |
| 1   | D     | 166/199 (83%)  | -1.12  | 0 100 100 | 56, 84, 122, 138      | 0     |
| 1   | E     | 147/199 (73%)  | -1.01  | 0 100 100 | 25, 160, 191, 215     | 0     |
| 1   | F     | 150/199 (75%)  | -1.00  | 0 100 100 | 62, 146, 187, 233     | 0     |
| All | All   | 960/1194 (80%) | -1.07  | 0 100 100 | 24, 94, 176, 233      | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | FOL  | F     | 201 | 32/32 | 0.98 | 0.11 | 130,174,186,189            | 0     |

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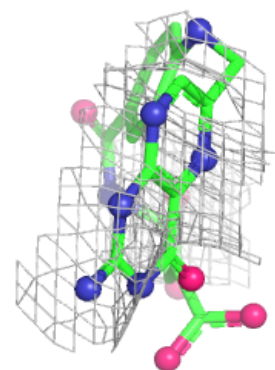
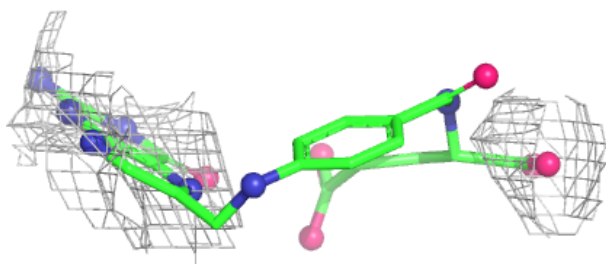
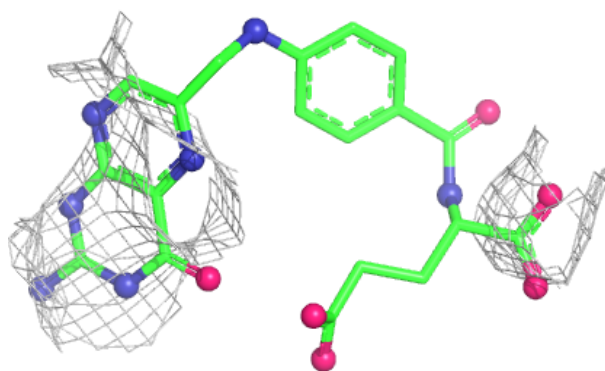
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | FOL  | B     | 201 | 32/32 | 0.99 | 0.09 | 75,99,164,170               | 0     |
| 2   | FOL  | C     | 201 | 32/32 | 0.99 | 0.09 | 71,104,159,185              | 0     |
| 2   | FOL  | D     | 201 | 32/32 | 0.99 | 0.09 | 88,116,160,163              | 0     |
| 2   | FOL  | E     | 201 | 32/32 | 0.99 | 0.09 | 127,158,201,207             | 0     |
| 2   | FOL  | A     | 201 | 32/32 | 0.99 | 0.07 | 69,98,137,146               | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

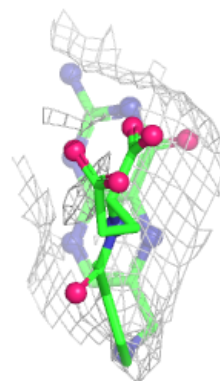
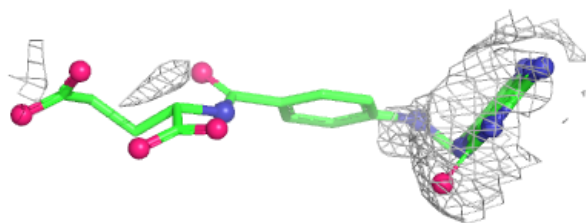
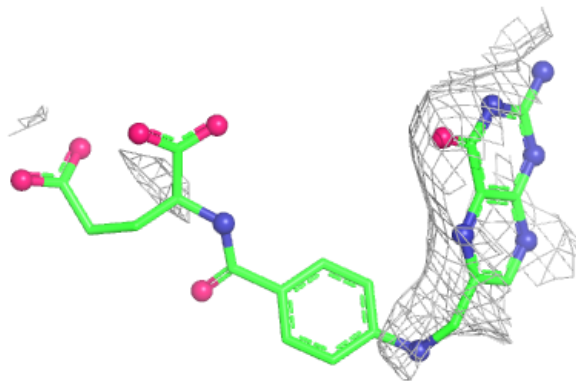
**Electron density around FOL F 201:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

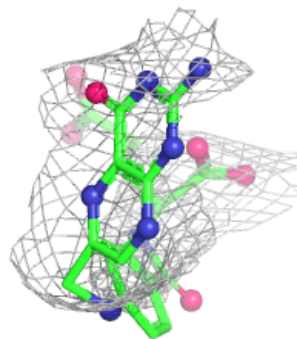
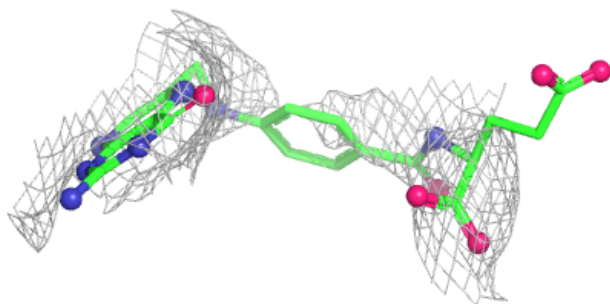
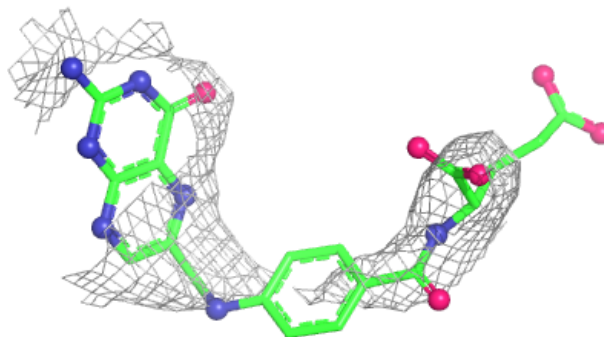


**Electron density around FOL B 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FOL C 201:**

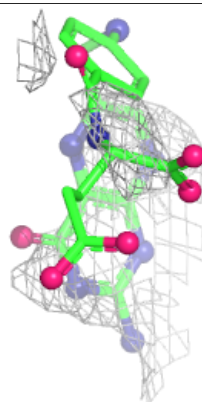
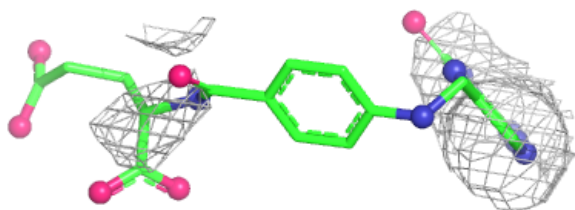
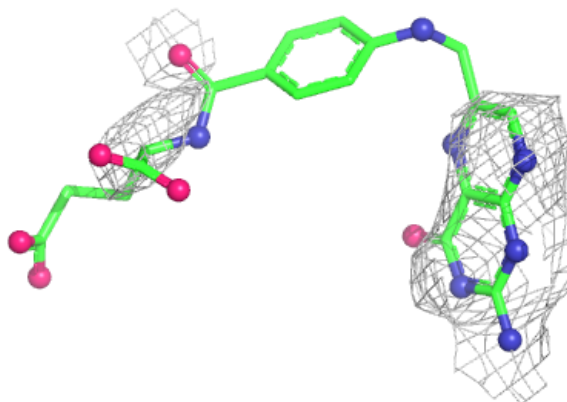
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



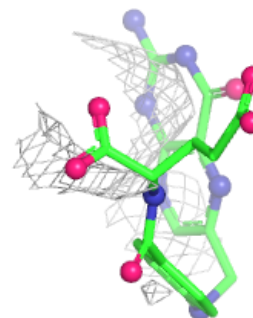
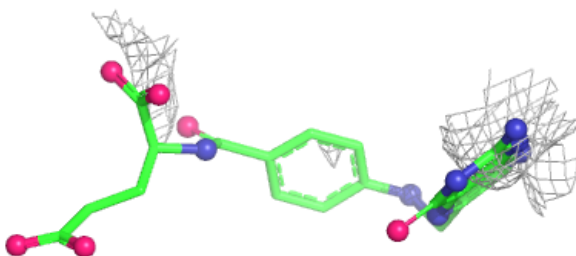
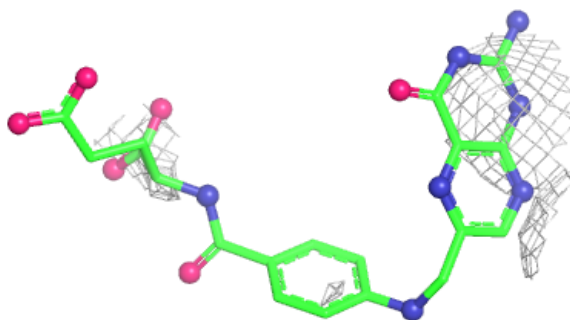


**Electron density around FOL D 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

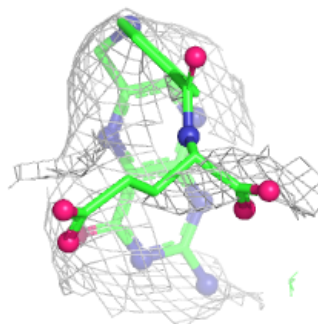
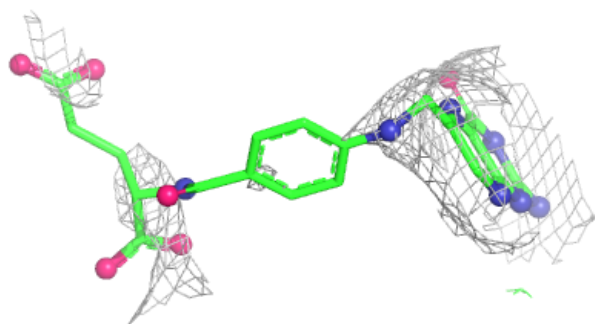
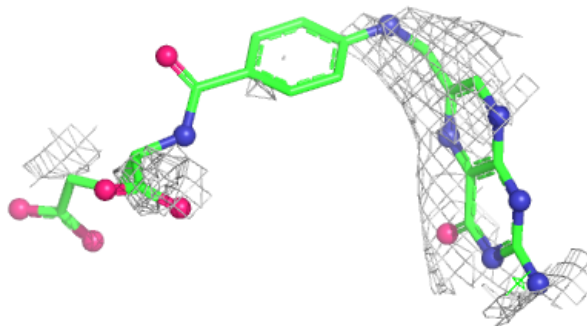
**Electron density around FOL E 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FOL A 201:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.