



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:25 PM UTC

PDB ID : 1K3F / pdb\_00001k3f  
Title : Uridine Phosphorylase from E. coli, Refined in the Monoclinic Crystal Lattice  
Authors : Morgunova, E.Yu.; Mikhailov, A.M.; Popov, A.N.; Blagova, E.V.; Smirnova, E.A.; Vainshtein, B.K.; Mao, C.; Armstrong, S.R.; Ealick, S.E.; Komissarov, A.A.; Linkova, E.V.; Burlakova, A.A.; Mironov, A.S.; Debabov, V.G.  
Deposited on : 2001-10-02  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

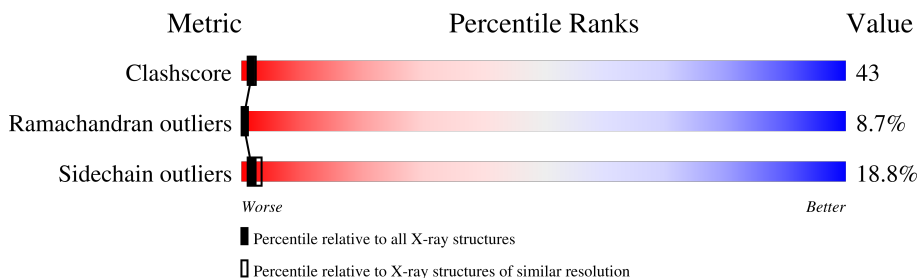
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 253    | <div> <div>38%</div> <div>43%</div> <div>15%</div> <div>.</div> </div> |
| 1   | B     | 253    | <div> <div>34%</div> <div>44%</div> <div>20%</div> <div>.</div> </div> |
| 1   | C     | 253    | <div> <div>34%</div> <div>46%</div> <div>17%</div> <div>.</div> </div> |
| 1   | D     | 253    | <div> <div>34%</div> <div>43%</div> <div>20%</div> <div>.</div> </div> |
| 1   | E     | 253    | <div> <div>35%</div> <div>43%</div> <div>20%</div> <div>.</div> </div> |
| 1   | F     | 253    | <div> <div>26%</div> <div>52%</div> <div>18%</div> <div>.</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11286 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 uridine phosphorylase.

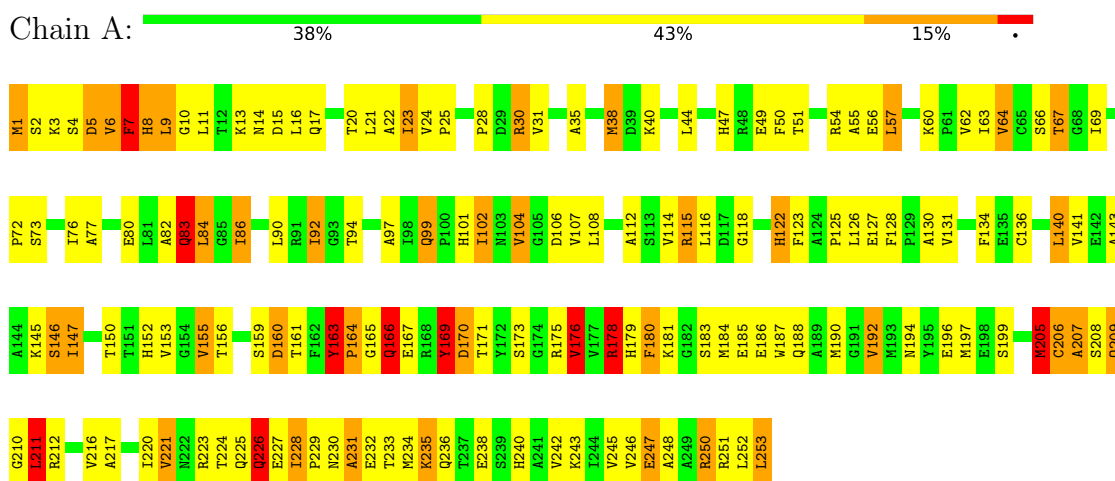
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1881  | 1180 | 322 | 367 | 12 |         |         |       |
| 1   | B     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1881  | 1180 | 322 | 367 | 12 |         |         |       |
| 1   | C     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1881  | 1180 | 322 | 367 | 12 |         |         |       |
| 1   | D     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1881  | 1180 | 322 | 367 | 12 |         |         |       |
| 1   | E     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1881  | 1180 | 322 | 367 | 12 |         |         |       |
| 1   | F     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1881  | 1180 | 322 | 367 | 12 |         |         |       |

### 3 Residue-property plots

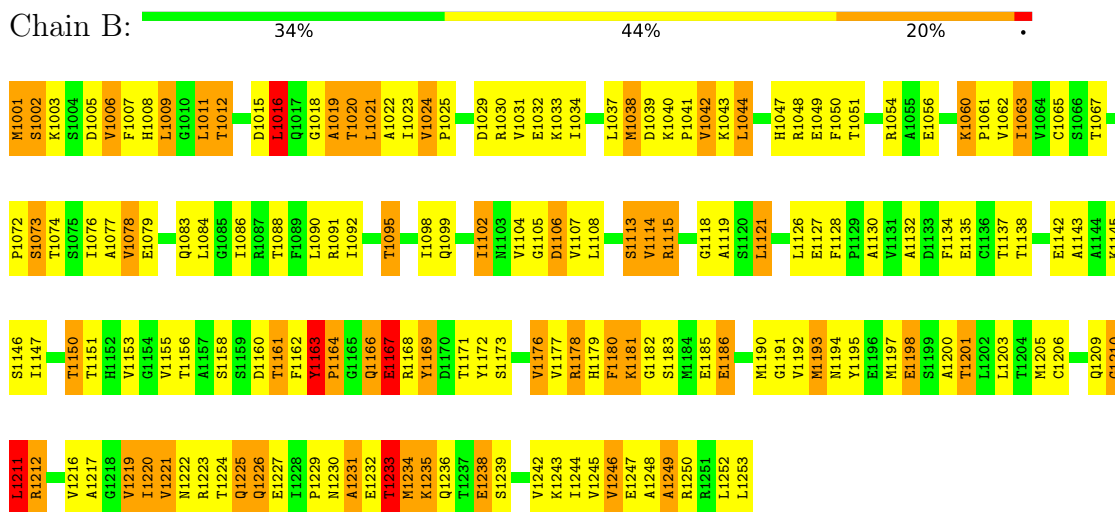
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: uridine phosphorylase

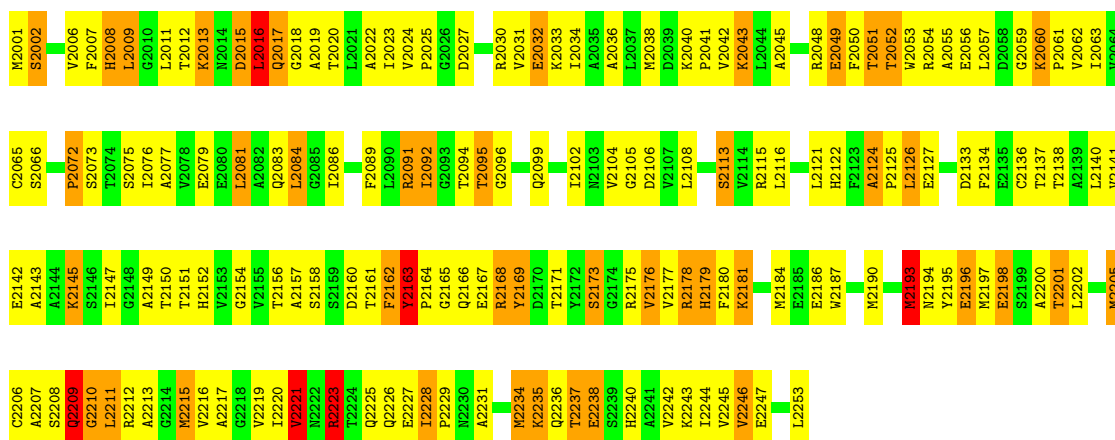


- Molecule 1: uridine phosphorylase



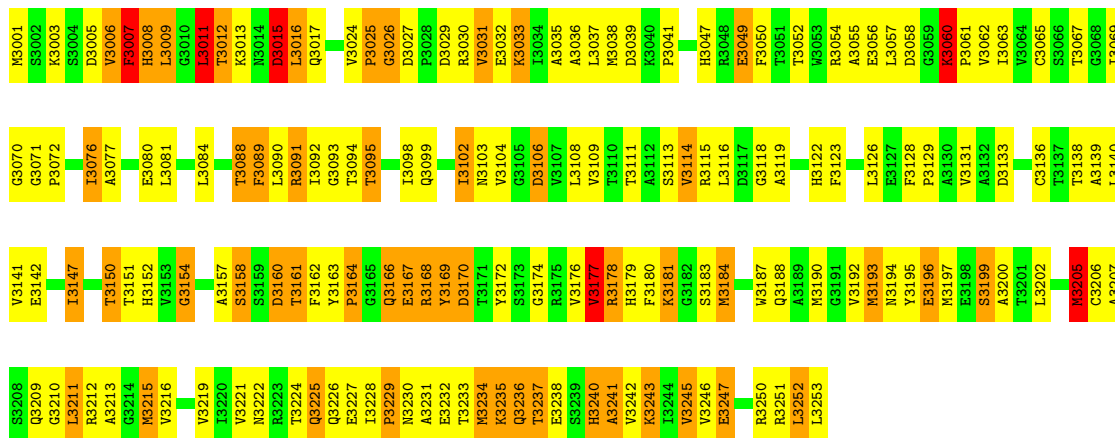
- Molecule 1: uridine phosphorylase





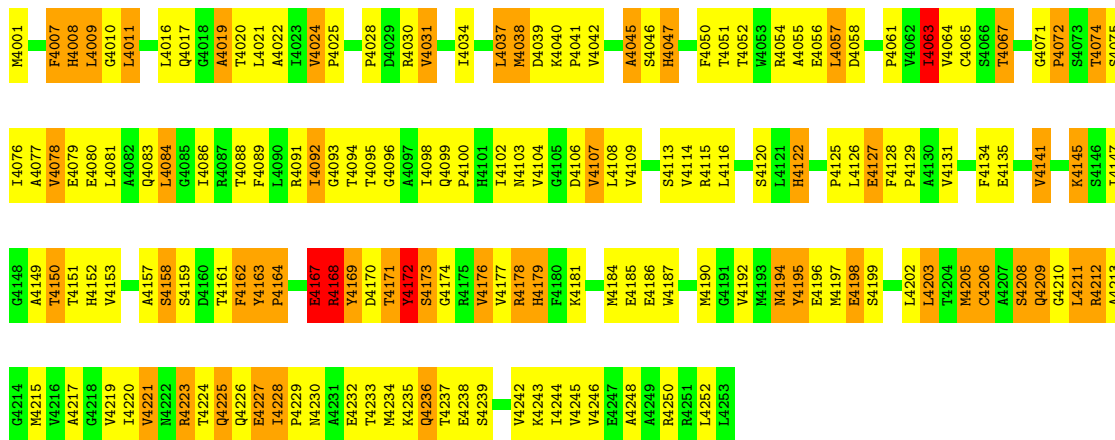
• Molecule 1: uridine phosphorylase

Chain D: 34% 43% 20% .

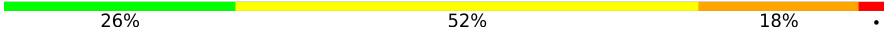


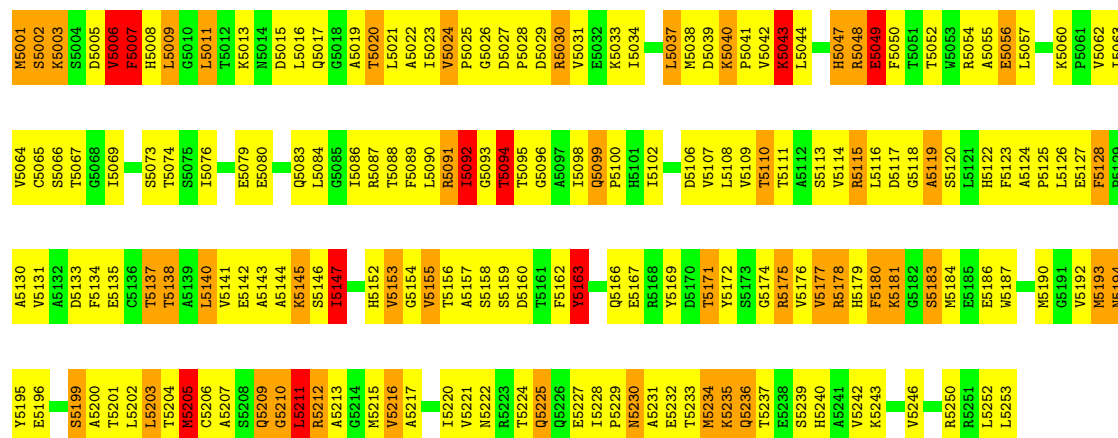
• Molecule 1: uridine phosphorylase

Chain E: 35% 43% 20% .



• Molecule 1: uridine phosphorylase

Chain F:  26% 52% 18%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                         | Source    |
|----------------------------------------------------------|-----------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 92.60Å 98.80Å 93.70Å<br>90.00° 120.20° 90.00° | Depositor |
| Resolution (Å)                                           | 6.00 – 2.50                                   | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (6.00-2.50)                   | Depositor |
| $R_{merge}$                                              | 0.10                                          | Depositor |
| $R_{sym}$                                                | (Not available)                               | Depositor |
| Refinement program                                       | X-PLOR 3.1                                    | Depositor |
| R, $R_{free}$                                            | 0.186 , (Not available)                       | Depositor |
| Estimated twinning fraction                              | No twinning to report.                        | Xtriage   |
| Total number of atoms                                    | 11286                                         | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 15.0                                          | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.89         | 1/1913 (0.1%)   | 1.36        | 24/2599 (0.9%)   |
| 1   | B     | 0.82         | 1/1913 (0.1%)   | 1.33        | 31/2599 (1.2%)   |
| 1   | C     | 0.89         | 2/1913 (0.1%)   | 1.32        | 17/2599 (0.7%)   |
| 1   | D     | 0.83         | 1/1913 (0.1%)   | 1.43        | 38/2599 (1.5%)   |
| 1   | E     | 0.87         | 1/1913 (0.1%)   | 1.34        | 17/2599 (0.7%)   |
| 1   | F     | 1.81         | 8/1913 (0.4%)   | 1.45        | 28/2599 (1.1%)   |
| All | All   | 1.08         | 14/11478 (0.1%) | 1.37        | 155/15594 (1.0%) |

All (14) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | F     | 5007 | PHE  | CD2-CE2 | 29.86 | 2.28        | 1.38     |
| 1   | F     | 5007 | PHE  | CD1-CE1 | 29.55 | 2.27        | 1.38     |
| 1   | F     | 5007 | PHE  | CE1-CZ  | 28.52 | 2.24        | 1.38     |
| 1   | F     | 5007 | PHE  | CE2-CZ  | 28.50 | 2.24        | 1.38     |
| 1   | F     | 5002 | SER  | N-CA    | 23.00 | 1.75        | 1.46     |
| 1   | F     | 5007 | PHE  | CG-CD2  | 21.08 | 1.83        | 1.38     |
| 1   | F     | 5007 | PHE  | CG-CD1  | 20.77 | 1.82        | 1.38     |
| 1   | F     | 5001 | MET  | C-N     | 11.34 | 1.49        | 1.33     |
| 1   | D     | 3215 | MET  | SD-CE   | 6.30  | 1.95        | 1.79     |
| 1   | C     | 2201 | THR  | CA-CB   | 6.05  | 1.62        | 1.53     |
| 1   | E     | 4024 | VAL  | CA-CB   | 6.02  | 1.59        | 1.54     |
| 1   | A     | 205  | MET  | CG-SD   | 5.67  | 1.95        | 1.80     |
| 1   | C     | 2193 | MET  | SD-CE   | -5.63 | 1.65        | 1.79     |
| 1   | B     | 1246 | VAL  | CA-CB   | 5.16  | 1.62        | 1.54     |

All (155) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | F     | 5001 | MET  | CA-C-N | 20.03 | 159.80      | 121.54   |
| 1   | F     | 5001 | MET  | C-N-CA | 20.03 | 159.80      | 121.54   |
| 1   | E     | 4170 | ASP  | N-CA-C | 11.71 | 127.87      | 110.30   |
| 1   | D     | 3007 | PHE  | N-CA-C | 11.22 | 124.36      | 108.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | D     | 3027 | ASP  | CA-C-N | 10.76 | 130.99      | 119.05   |
| 1   | D     | 3027 | ASP  | C-N-CA | 10.76 | 130.99      | 119.05   |
| 1   | C     | 2124 | ALA  | CA-C-N | 9.54  | 131.77      | 119.84   |
| 1   | C     | 2124 | ALA  | C-N-CA | 9.54  | 131.77      | 119.84   |
| 1   | F     | 5183 | SER  | N-CA-C | 9.26  | 124.12      | 113.01   |
| 1   | D     | 3011 | LEU  | N-CA-C | 9.14  | 120.69      | 108.07   |
| 1   | E     | 4024 | VAL  | CA-C-N | 9.01  | 130.62      | 120.98   |
| 1   | E     | 4024 | VAL  | C-N-CA | 9.01  | 130.62      | 120.98   |
| 1   | D     | 3167 | GLU  | N-CA-C | 8.88  | 123.61      | 110.46   |
| 1   | F     | 5205 | MET  | N-CA-C | -8.77 | 96.93       | 110.17   |
| 1   | D     | 3036 | ALA  | N-CA-C | -8.71 | 101.87      | 111.36   |
| 1   | C     | 2060 | LYS  | CA-C-N | 8.60  | 128.53      | 119.85   |
| 1   | C     | 2060 | LYS  | C-N-CA | 8.60  | 128.53      | 119.85   |
| 1   | D     | 3237 | THR  | N-CA-C | -8.50 | 101.23      | 111.69   |
| 1   | D     | 3031 | VAL  | N-CA-C | -8.48 | 103.03      | 110.74   |
| 1   | E     | 4127 | GLU  | N-CA-C | 8.31  | 120.34      | 111.28   |
| 1   | B     | 1180 | PHE  | N-CA-C | -8.16 | 101.62      | 112.72   |
| 1   | C     | 2246 | VAL  | N-CA-C | -8.16 | 102.48      | 110.72   |
| 1   | A     | 180  | PHE  | N-CA-C | -8.04 | 101.60      | 112.94   |
| 1   | A     | 210  | GLY  | N-CA-C | -7.92 | 102.88      | 115.08   |
| 1   | F     | 5177 | VAL  | N-CA-C | 7.82  | 119.84      | 108.58   |
| 1   | B     | 1198 | GLU  | N-CA-C | 7.72  | 122.80      | 112.30   |
| 1   | E     | 4024 | VAL  | N-CA-C | 7.65  | 115.73      | 108.15   |
| 1   | E     | 4057 | LEU  | N-CA-C | -7.65 | 94.97       | 108.13   |
| 1   | B     | 1115 | ARG  | N-CA-C | 7.59  | 121.00      | 109.62   |
| 1   | A     | 155  | VAL  | N-CA-C | 7.54  | 119.95      | 108.71   |
| 1   | B     | 1163 | TYR  | CA-C-N | 7.44  | 129.14      | 119.84   |
| 1   | B     | 1163 | TYR  | C-N-CA | 7.44  | 129.14      | 119.84   |
| 1   | A     | 104  | VAL  | N-CA-C | 7.40  | 120.10      | 109.51   |
| 1   | C     | 2175 | ARG  | N-CA-C | -7.34 | 101.49      | 110.88   |
| 1   | F     | 5180 | PHE  | N-CA-C | -7.31 | 106.29      | 114.62   |
| 1   | F     | 5160 | ASP  | N-CA-C | -7.28 | 98.85       | 110.14   |
| 1   | F     | 5119 | ALA  | N-CA-C | 7.26  | 120.24      | 111.82   |
| 1   | F     | 5110 | THR  | N-CA-C | 7.21  | 120.27      | 108.52   |
| 1   | E     | 4197 | MET  | N-CA-C | 7.18  | 124.38      | 113.61   |
| 1   | B     | 1114 | VAL  | N-CA-C | -7.13 | 99.48       | 108.89   |
| 1   | A     | 181  | LYS  | N-CA-C | 7.11  | 119.64      | 111.11   |
| 1   | A     | 10   | GLY  | N-CA-C | 7.10  | 125.90      | 112.62   |
| 1   | E     | 4078 | VAL  | N-CA-C | -7.09 | 103.42      | 110.30   |
| 1   | A     | 24   | VAL  | CA-C-N | -7.05 | 113.44      | 120.21   |
| 1   | A     | 24   | VAL  | C-N-CA | -7.05 | 113.44      | 120.21   |
| 1   | B     | 1191 | GLY  | N-CA-C | 7.05  | 124.70      | 115.40   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | D     | 3005 | ASP  | N-CA-C | -7.00 | 103.86      | 112.88   |
| 1   | B     | 1219 | VAL  | N-CA-C | 6.99  | 117.58      | 106.32   |
| 1   | D     | 3252 | LEU  | N-CA-C | 6.97  | 120.23      | 111.24   |
| 1   | B     | 1249 | ALA  | N-CA-C | -6.92 | 104.65      | 113.23   |
| 1   | E     | 4187 | TRP  | N-CA-C | -6.91 | 104.98      | 113.41   |
| 1   | F     | 5203 | LEU  | N-CA-C | 6.91  | 118.89      | 111.36   |
| 1   | D     | 3154 | GLY  | N-CA-C | 6.88  | 120.17      | 110.74   |
| 1   | B     | 1130 | ALA  | N-CA-C | -6.88 | 96.55       | 108.52   |
| 1   | E     | 4063 | ILE  | N-CA-C | 6.77  | 118.55      | 108.46   |
| 1   | E     | 4167 | GLU  | N-CA-C | -6.70 | 97.23       | 109.56   |
| 1   | B     | 1060 | LYS  | CA-C-N | 6.68  | 128.19      | 119.84   |
| 1   | B     | 1060 | LYS  | C-N-CA | 6.68  | 128.19      | 119.84   |
| 1   | A     | 243  | LYS  | N-CA-C | -6.67 | 104.08      | 111.36   |
| 1   | F     | 5212 | ARG  | N-CA-C | 6.66  | 120.90      | 110.17   |
| 1   | F     | 5095 | THR  | N-CA-C | 6.64  | 117.04      | 108.34   |
| 1   | B     | 1016 | LEU  | N-CA-C | -6.62 | 105.73      | 113.88   |
| 1   | B     | 1169 | TYR  | N-CA-C | -6.62 | 105.24      | 113.38   |
| 1   | F     | 5043 | LYS  | N-CA-C | -6.57 | 99.59       | 110.17   |
| 1   | E     | 4192 | VAL  | N-CA-C | -6.54 | 101.15      | 109.58   |
| 1   | A     | 99   | GLN  | CA-C-N | 6.48  | 126.24      | 119.05   |
| 1   | A     | 99   | GLN  | C-N-CA | 6.48  | 126.24      | 119.05   |
| 1   | B     | 1034 | ILE  | N-CA-C | -6.47 | 104.18      | 110.72   |
| 1   | A     | 3    | LYS  | N-CA-C | -6.46 | 102.51      | 111.81   |
| 1   | F     | 5154 | GLY  | N-CA-C | 6.45  | 121.53      | 111.08   |
| 1   | D     | 3199 | SER  | N-CA-C | 6.43  | 118.09      | 111.14   |
| 1   | D     | 3163 | TYR  | CA-C-N | 6.41  | 127.86      | 119.84   |
| 1   | D     | 3163 | TYR  | C-N-CA | 6.41  | 127.86      | 119.84   |
| 1   | D     | 3076 | ILE  | N-CA-C | -6.32 | 104.33      | 110.72   |
| 1   | E     | 4008 | HIS  | N-CA-C | 6.32  | 124.26      | 110.80   |
| 1   | B     | 1095 | THR  | N-CA-C | 6.32  | 118.11      | 108.07   |
| 1   | F     | 5147 | ILE  | N-CA-C | -6.28 | 106.68      | 112.96   |
| 1   | D     | 3158 | SER  | N-CA-C | 6.24  | 120.02      | 107.41   |
| 1   | C     | 2051 | THR  | N-CA-C | 6.23  | 118.85      | 108.20   |
| 1   | D     | 3131 | VAL  | N-CA-C | 6.22  | 117.44      | 108.48   |
| 1   | E     | 4158 | SER  | N-CA-C | 6.19  | 118.89      | 107.99   |
| 1   | C     | 2154 | GLY  | N-CA-C | 6.13  | 120.67      | 111.42   |
| 1   | D     | 3050 | PHE  | N-CA-C | 6.12  | 119.12      | 107.75   |
| 1   | A     | 67   | THR  | N-CA-C | 6.11  | 121.79      | 113.97   |
| 1   | D     | 3177 | VAL  | N-CA-C | 6.06  | 121.95      | 109.34   |
| 1   | F     | 5094 | THR  | N-CA-C | -6.06 | 99.12       | 109.24   |
| 1   | F     | 5052 | THR  | N-CA-C | 6.00  | 118.50      | 108.73   |
| 1   | F     | 5199 | SER  | N-CA-C | 5.98  | 117.49      | 110.97   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | D     | 3166 | GLN  | N-CA-C  | -5.98 | 98.12       | 108.52   |
| 1   | A     | 122  | HIS  | N-CA-C  | -5.87 | 105.88      | 113.16   |
| 1   | D     | 3015 | ASP  | N-CA-C  | -5.85 | 104.81      | 111.07   |
| 1   | C     | 2221 | VAL  | N-CA-C  | 5.85  | 116.79      | 108.42   |
| 1   | F     | 5135 | GLU  | N-CA-C  | 5.83  | 118.14      | 111.02   |
| 1   | B     | 1167 | GLU  | N-CA-C  | -5.80 | 98.45       | 110.80   |
| 1   | D     | 3168 | ARG  | N-CA-C  | -5.76 | 106.22      | 113.20   |
| 1   | F     | 5230 | ASN  | N-CA-C  | -5.75 | 106.08      | 112.57   |
| 1   | B     | 1024 | VAL  | CA-C-N  | 5.75  | 127.02      | 119.84   |
| 1   | B     | 1024 | VAL  | C-N-CA  | 5.75  | 127.02      | 119.84   |
| 1   | D     | 3193 | MET  | N-CA-C  | 5.73  | 119.93      | 111.04   |
| 1   | F     | 5237 | THR  | N-CA-C  | -5.73 | 104.67      | 111.03   |
| 1   | C     | 2027 | ASP  | N-CA-C  | 5.67  | 117.75      | 109.71   |
| 1   | A     | 188  | GLN  | N-CA-C  | -5.65 | 105.03      | 111.07   |
| 1   | A     | 69   | ILE  | N-CA-C  | 5.64  | 117.30      | 109.80   |
| 1   | E     | 4107 | VAL  | N-CA-C  | 5.61  | 115.74      | 107.15   |
| 1   | C     | 2023 | ILE  | N-CA-C  | -5.59 | 99.70       | 107.80   |
| 1   | F     | 5190 | MET  | N-CA-C  | -5.57 | 106.48      | 113.72   |
| 1   | C     | 2198 | GLU  | N-CA-C  | 5.56  | 120.95      | 113.72   |
| 1   | B     | 1113 | SER  | N-CA-C  | 5.56  | 118.46      | 109.40   |
| 1   | E     | 4122 | HIS  | N-CA-C  | -5.55 | 106.00      | 112.89   |
| 1   | B     | 1248 | ALA  | N-CA-C  | 5.54  | 120.10      | 113.23   |
| 1   | F     | 5092 | ILE  | CB-CA-C | -5.53 | 102.45      | 110.63   |
| 1   | A     | 83   | GLN  | N-CA-C  | -5.49 | 105.21      | 111.14   |
| 1   | F     | 5236 | GLN  | N-CA-C  | 5.44  | 119.17      | 112.54   |
| 1   | D     | 3205 | MET  | N-CA-C  | -5.42 | 106.16      | 112.89   |
| 1   | F     | 5128 | PHE  | N-CA-C  | 5.41  | 117.46      | 109.50   |
| 1   | D     | 3060 | LYS  | CA-C-N  | 5.41  | 125.58      | 119.90   |
| 1   | D     | 3060 | LYS  | C-N-CA  | 5.41  | 125.58      | 119.90   |
| 1   | F     | 5098 | ILE  | N-CA-C  | -5.40 | 106.16      | 111.88   |
| 1   | B     | 1128 | PHE  | CA-C-N  | 5.35  | 125.61      | 119.83   |
| 1   | B     | 1128 | PHE  | C-N-CA  | 5.35  | 125.61      | 119.83   |
| 1   | C     | 2181 | LYS  | N-CA-C  | 5.35  | 116.97      | 111.03   |
| 1   | D     | 3089 | PHE  | N-CA-C  | 5.34  | 117.66      | 109.07   |
| 1   | C     | 2113 | SER  | N-CA-C  | 5.32  | 118.23      | 109.72   |
| 1   | C     | 2193 | MET  | N-CA-C  | 5.32  | 118.23      | 111.69   |
| 1   | B     | 1150 | THR  | N-CA-C  | 5.31  | 118.25      | 108.58   |
| 1   | B     | 1153 | VAL  | N-CA-C  | -5.30 | 100.85      | 108.48   |
| 1   | D     | 3150 | THR  | N-CA-C  | -5.29 | 101.54      | 109.15   |
| 1   | D     | 3245 | VAL  | CB-CA-C | -5.23 | 105.17      | 112.02   |
| 1   | B     | 1246 | VAL  | N-CA-C  | -5.21 | 106.06      | 111.58   |
| 1   | D     | 3241 | ALA  | N-CA-C  | 5.21  | 117.70      | 111.71   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | F     | 5210 | GLY  | N-CA-C | -5.21 | 107.18      | 115.66   |
| 1   | D     | 3024 | VAL  | CA-C-N | 5.19  | 126.33      | 119.84   |
| 1   | D     | 3024 | VAL  | C-N-CA | 5.19  | 126.33      | 119.84   |
| 1   | A     | 28   | PRO  | N-CA-C | -5.17 | 101.81      | 112.47   |
| 1   | C     | 2063 | ILE  | N-CA-C | 5.17  | 115.54      | 107.99   |
| 1   | B     | 1195 | TYR  | N-CA-C | -5.17 | 102.55      | 110.14   |
| 1   | B     | 1073 | SER  | N-CA-C | -5.15 | 105.36      | 111.69   |
| 1   | D     | 3190 | MET  | N-CA-C | -5.15 | 107.16      | 112.93   |
| 1   | B     | 1051 | THR  | N-CA-C | -5.15 | 102.14      | 110.32   |
| 1   | A     | 250  | ARG  | N-CA-C | -5.14 | 105.75      | 111.36   |
| 1   | F     | 5024 | VAL  | N-CA-C | 5.13  | 119.97      | 108.88   |
| 1   | D     | 3174 | GLY  | N-CA-C | -5.13 | 101.03      | 113.18   |
| 1   | D     | 3114 | VAL  | N-CA-C | -5.12 | 102.12      | 108.89   |
| 1   | E     | 4159 | SER  | N-CA-C | -5.10 | 103.66      | 110.55   |
| 1   | D     | 3102 | ILE  | N-CA-C | 5.10  | 114.61      | 107.37   |
| 1   | B     | 1238 | GLU  | N-CA-C | -5.09 | 105.73      | 111.28   |
| 1   | D     | 3235 | LYS  | N-CA-C | -5.08 | 105.92      | 111.82   |
| 1   | B     | 1193 | MET  | N-CA-C | 5.07  | 119.42      | 112.68   |
| 1   | A     | 131  | VAL  | N-CA-C | 5.06  | 116.59      | 108.89   |
| 1   | C     | 2145 | LYS  | N-CA-C | -5.05 | 105.87      | 112.23   |
| 1   | A     | 209  | GLN  | N-CA-C | -5.05 | 100.84      | 108.46   |
| 1   | A     | 23   | ILE  | N-CA-C | -5.04 | 100.51      | 108.23   |
| 1   | A     | 192  | VAL  | N-CA-C | -5.04 | 101.20      | 108.87   |
| 1   | A     | 160  | ASP  | N-CA-C | -5.04 | 107.09      | 113.18   |
| 1   | D     | 3006 | VAL  | N-CA-C | 5.03  | 119.80      | 109.34   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1881  | 0        | 1871     | 160     | 0            |
| 1   | B     | 1881  | 0        | 1868     | 157     | 0            |
| 1   | C     | 1881  | 0        | 1868     | 188     | 0            |
| 1   | D     | 1881  | 0        | 1868     | 151     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 1881  | 0        | 1868     | 157     | 0            |
| 1   | F     | 1881  | 0        | 1868     | 222     | 0            |
| All | All   | 11286 | 0        | 11211    | 965     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (965) 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:F:5007:PHE:CD1  | 1:F:5007:PHE:CG   | 1.82                     | 1.67              |
| 1:F:5007:PHE:CG   | 1:F:5007:PHE:CD2  | 1.83                     | 1.60              |
| 1:F:5002:SER:N    | 1:F:5002:SER:CA   | 1.75                     | 1.48              |
| 1:F:5007:PHE:CZ   | 1:F:5007:PHE:CE1  | 2.24                     | 1.26              |
| 1:F:5007:PHE:CZ   | 1:F:5007:PHE:CE2  | 2.24                     | 1.25              |
| 1:F:5002:SER:N    | 1:F:5007:PHE:CE1  | 2.07                     | 1.22              |
| 1:F:5007:PHE:CD2  | 1:F:5007:PHE:CE2  | 2.28                     | 1.22              |
| 1:F:5007:PHE:CD1  | 1:F:5007:PHE:CE1  | 2.27                     | 1.22              |
| 1:F:5002:SER:N    | 1:F:5007:PHE:CZ   | 2.08                     | 1.22              |
| 1:F:5002:SER:N    | 1:F:5007:PHE:CE2  | 2.09                     | 1.20              |
| 1:F:5002:SER:HA   | 1:F:5007:PHE:CD2  | 1.75                     | 1.19              |
| 1:F:5002:SER:N    | 1:F:5007:PHE:CD1  | 2.10                     | 1.19              |
| 1:A:225:GLN:HB2   | 1:D:3001:MET:SD   | 1.86                     | 1.15              |
| 1:D:3228:ILE:HG12 | 1:D:3229:PRO:HA   | 1.17                     | 1.14              |
| 1:F:5002:SER:N    | 1:F:5007:PHE:CD2  | 2.16                     | 1.12              |
| 1:F:5205:MET:SD   | 1:F:5205:MET:N    | 2.21                     | 1.12              |
| 1:C:2229:PRO:HG2  | 1:C:2234:MET:HG2  | 1.22                     | 1.12              |
| 1:A:1:MET:SD      | 1:D:3229:PRO:HD3  | 1.94                     | 1.08              |
| 1:D:3234:MET:SD   | 1:D:3234:MET:N    | 2.26                     | 1.08              |
| 1:F:5002:SER:N    | 1:F:5007:PHE:CG   | 2.21                     | 1.08              |
| 1:A:228:ILE:HB    | 1:A:229:PRO:HA    | 1.41                     | 1.03              |
| 1:F:5002:SER:CA   | 1:F:5007:PHE:CD2  | 2.45                     | 1.00              |
| 1:A:178:ARG:HH22  | 1:B:1186:GLU:HB3  | 1.27                     | 0.98              |
| 1:A:167:GLU:HB3   | 1:A:184:MET:HE2   | 1.45                     | 0.97              |
| 1:F:5123:PHE:HD1  | 1:F:5205:MET:HE3  | 1.30                     | 0.96              |
| 1:C:2211:LEU:HG   | 1:C:2212:ARG:H    | 1.31                     | 0.96              |
| 1:C:2220:ILE:HG13 | 1:C:2221:VAL:HG23 | 1.47                     | 0.96              |
| 1:D:3108:LEU:HB3  | 1:D:3193:MET:HE3  | 1.47                     | 0.95              |
| 1:C:2001:MET:N    | 1:E:4223:ARG:HA   | 1.81                     | 0.95              |
| 1:F:5201:THR:HG23 | 1:F:5205:MET:HE2  | 1.49                     | 0.94              |
| 1:A:9:LEU:HG      | 1:A:50:PHE:CD1    | 2.03                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:220:ILE:HG13  | 1:A:221:VAL:HG22  | 1.51                     | 0.92              |
| 1:A:9:LEU:HG      | 1:A:50:PHE:CE1    | 2.04                     | 0.91              |
| 1:F:5001:MET:C    | 1:F:5007:PHE:CD2  | 2.48                     | 0.91              |
| 1:C:2137:THR:O    | 1:C:2141:VAL:HG13 | 1.71                     | 0.91              |
| 1:F:5201:THR:O    | 1:F:5205:MET:SD   | 2.28                     | 0.91              |
| 1:F:5130:ALA:HB1  | 1:F:5203:LEU:HB2  | 1.53                     | 0.91              |
| 1:C:2167:GLU:HA   | 1:C:2184:MET:HE2  | 1.53                     | 0.90              |
| 1:D:3017:GLN:CD   | 1:D:3054:ARG:HD2  | 1.97                     | 0.90              |
| 1:F:5109:VAL:HG13 | 1:F:5140:LEU:HD12 | 1.52                     | 0.90              |
| 1:C:2126:LEU:HD23 | 1:F:5126:LEU:HD23 | 1.53                     | 0.89              |
| 1:F:5123:PHE:CD1  | 1:F:5205:MET:HE3  | 2.07                     | 0.89              |
| 1:C:2105:GLY:HA2  | 1:C:2237:THR:OG1  | 1.73                     | 0.88              |
| 1:D:3039:ASP:HB2  | 1:D:3056:GLU:HB3  | 1.54                     | 0.87              |
| 1:E:4178:ARG:HA   | 1:E:4181:LYS:HE2  | 1.55                     | 0.87              |
| 1:A:31:VAL:HG13   | 1:A:64:VAL:HG22   | 1.57                     | 0.86              |
| 1:C:2205:MET:SD   | 1:C:2205:MET:C    | 2.59                     | 0.86              |
| 1:E:4176:VAL:HG12 | 1:E:4177:VAL:H    | 1.41                     | 0.86              |
| 1:F:5091:ARG:HG2  | 1:F:5215:MET:HG3  | 1.57                     | 0.86              |
| 1:F:5002:SER:CA   | 1:F:5007:PHE:CG   | 2.59                     | 0.85              |
| 1:F:5022:ALA:HB2  | 1:F:5086:ILE:HD13 | 1.58                     | 0.85              |
| 1:B:1134:PHE:O    | 1:B:1138:THR:HG23 | 1.75                     | 0.84              |
| 1:C:2178:ARG:CZ   | 1:E:4125:PRO:HG3  | 2.07                     | 0.84              |
| 1:D:3233:THR:OG1  | 1:D:3234:MET:SD   | 2.35                     | 0.84              |
| 1:F:5141:VAL:O    | 1:F:5145:LYS:HG2  | 1.77                     | 0.84              |
| 1:F:5001:MET:C    | 1:F:5007:PHE:CG   | 2.55                     | 0.84              |
| 1:F:5100:PRO:HB3  | 1:F:5224:THR:HG21 | 1.59                     | 0.84              |
| 1:F:5002:SER:CA   | 1:F:5007:PHE:CE2  | 2.60                     | 0.83              |
| 1:F:5001:MET:C    | 1:F:5007:PHE:CE2  | 2.55                     | 0.83              |
| 1:F:5001:MET:O    | 1:F:5007:PHE:CD2  | 2.32                     | 0.82              |
| 1:F:5001:MET:HA   | 1:F:5007:PHE:CE1  | 2.13                     | 0.82              |
| 1:F:5120:SER:HA   | 1:F:5205:MET:HE1  | 1.59                     | 0.82              |
| 1:E:4104:VAL:HG21 | 1:E:4229:PRO:HG3  | 1.61                     | 0.82              |
| 1:A:225:GLN:CB    | 1:D:3001:MET:SD   | 2.68                     | 0.81              |
| 1:A:125:PRO:HB3   | 1:D:3178:ARG:HG2  | 1.63                     | 0.81              |
| 1:D:3038:MET:SD   | 1:D:3062:VAL:HG21 | 2.20                     | 0.81              |
| 1:B:1243:LYS:O    | 1:B:1247:GLU:HG2  | 1.81                     | 0.81              |
| 1:D:3241:ALA:O    | 1:D:3245:VAL:HG23 | 1.81                     | 0.80              |
| 1:E:4212:ARG:HH11 | 1:E:4252:LEU:HD23 | 1.46                     | 0.80              |
| 1:F:5001:MET:C    | 1:F:5007:PHE:CD1  | 2.60                     | 0.80              |
| 1:D:3211:LEU:HG   | 1:D:3212:ARG:H    | 1.47                     | 0.80              |
| 1:A:228:ILE:HB    | 1:A:229:PRO:CA    | 2.12                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2211:LEU:HG   | 1:C:2212:ARG:N    | 1.96                     | 0.80              |
| 1:D:3016:LEU:HD13 | 1:D:3063:ILE:HG13 | 1.65                     | 0.79              |
| 1:D:3180:PHE:HD2  | 1:D:3181:LYS:H    | 1.31                     | 0.79              |
| 1:B:1002:SER:HA   | 1:B:1008:HIS:HA   | 1.64                     | 0.78              |
| 1:C:2017:GLN:OE1  | 1:C:2061:PRO:HG3  | 1.83                     | 0.78              |
| 1:E:4167:GLU:HG3  | 1:E:4184:MET:HG3  | 1.65                     | 0.78              |
| 1:B:1063:ILE:HD11 | 1:B:1065:CYS:HB2  | 1.64                     | 0.78              |
| 1:B:1235:LYS:H    | 1:B:1235:LYS:HD3  | 1.49                     | 0.78              |
| 1:F:5114:VAL:HG22 | 1:F:5157:ALA:HA   | 1.65                     | 0.78              |
| 1:F:5204:THR:C    | 1:F:5205:MET:SD   | 2.68                     | 0.77              |
| 1:B:1158:SER:HB3  | 1:B:1200:ALA:HB2  | 1.65                     | 0.77              |
| 1:D:3009:LEU:HD12 | 1:D:3047:HIS:HB3  | 1.66                     | 0.77              |
| 1:F:5040:LYS:N    | 1:F:5041:PRO:HD3  | 1.98                     | 0.77              |
| 1:C:2002:SER:HB2  | 1:E:4226:GLN:HE21 | 1.49                     | 0.76              |
| 1:A:226:GLN:CA    | 1:D:3001:MET:HB2  | 2.15                     | 0.76              |
| 1:F:5002:SER:HB2  | 1:F:5007:PHE:CZ   | 2.20                     | 0.76              |
| 1:A:11:LEU:HD13   | 1:A:15:ASP:HB2    | 1.67                     | 0.76              |
| 1:D:3161:THR:HG22 | 1:D:3162:PHE:H    | 1.51                     | 0.76              |
| 1:C:2173:SER:OG   | 1:C:2176:VAL:HA   | 1.85                     | 0.75              |
| 1:A:242:VAL:HA    | 1:A:245:VAL:HG12  | 1.67                     | 0.75              |
| 1:D:3030:ARG:HH21 | 1:D:3238:GLU:HG3  | 1.50                     | 0.75              |
| 1:F:5120:SER:HA   | 1:F:5205:MET:CE   | 2.17                     | 0.75              |
| 1:C:2011:LEU:HD21 | 1:C:2052:THR:HG21 | 1.67                     | 0.74              |
| 1:C:2016:LEU:HD23 | 1:C:2016:LEU:H    | 1.50                     | 0.74              |
| 1:D:3012:THR:O    | 1:D:3015:ASP:HB2  | 1.88                     | 0.74              |
| 1:C:2038:MET:HE2  | 1:C:2246:VAL:HG13 | 1.70                     | 0.74              |
| 1:A:136:CYS:O     | 1:A:140:LEU:HD13  | 1.88                     | 0.74              |
| 1:C:2223:ARG:H    | 1:C:2223:ARG:HD2  | 1.53                     | 0.73              |
| 1:B:1074:THR:HG22 | 1:B:1078:VAL:HG21 | 1.70                     | 0.73              |
| 1:E:4210:GLY:O    | 1:E:4212:ARG:N    | 2.22                     | 0.73              |
| 1:F:5002:SER:C    | 1:F:5007:PHE:CD1  | 2.66                     | 0.73              |
| 1:C:2179:HIS:CD2  | 1:C:2179:HIS:H    | 2.05                     | 0.72              |
| 1:E:4011:LEU:HB3  | 1:E:4084:LEU:HD21 | 1.69                     | 0.72              |
| 1:E:4078:VAL:HG11 | 1:E:4205:MET:SD   | 2.30                     | 0.72              |
| 1:B:1044:LEU:HD22 | 1:B:1054:ARG:HB2  | 1.71                     | 0.72              |
| 1:F:5236:GLN:HA   | 1:F:5239:SER:OG   | 1.89                     | 0.72              |
| 1:C:2025:PRO:HD2  | 1:C:2065:CYS:O    | 1.90                     | 0.71              |
| 1:D:3026:GLY:HA2  | 1:D:3067:THR:OG1  | 1.90                     | 0.71              |
| 1:D:3038:MET:SD   | 1:D:3062:VAL:CG2  | 2.79                     | 0.71              |
| 1:C:2167:GLU:CG   | 1:C:2223:ARG:HG2  | 2.21                     | 0.71              |
| 1:D:3123:PHE:CD2  | 1:D:3205:MET:SD   | 2.84                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3238:GLU:O    | 1:D:3242:VAL:HG23 | 1.89                     | 0.71              |
| 1:C:2104:VAL:HG11 | 1:C:2229:PRO:HB3  | 1.73                     | 0.71              |
| 1:F:5037:LEU:HD13 | 1:F:5246:VAL:HG21 | 1.73                     | 0.71              |
| 1:D:3017:GLN:NE2  | 1:D:3054:ARG:HD2  | 2.05                     | 0.71              |
| 1:A:226:GLN:HA    | 1:D:3001:MET:HB2  | 1.71                     | 0.70              |
| 1:B:1025:PRO:HD2  | 1:B:1065:CYS:O    | 1.91                     | 0.70              |
| 1:A:178:ARG:NH2   | 1:B:1186:GLU:HB3  | 2.04                     | 0.70              |
| 1:D:3030:ARG:NH2  | 1:D:3238:GLU:HG3  | 2.06                     | 0.70              |
| 1:D:3228:ILE:CG1  | 1:D:3229:PRO:HA   | 2.10                     | 0.70              |
| 1:C:2235:LYS:HA   | 1:C:2238:GLU:HG3  | 1.73                     | 0.70              |
| 1:D:3123:PHE:CE2  | 1:D:3205:MET:SD   | 2.85                     | 0.70              |
| 1:C:2177:VAL:HB   | 1:C:2181:LYS:HD3  | 1.73                     | 0.70              |
| 1:D:3247:GLU:O    | 1:D:3250:ARG:HG2  | 1.92                     | 0.70              |
| 1:E:4072:PRO:O    | 1:E:4076:ILE:HG13 | 1.91                     | 0.70              |
| 1:F:5201:THR:CG2  | 1:F:5205:MET:HE2  | 2.21                     | 0.70              |
| 1:A:190:MET:HE1   | 1:E:4125:PRO:HD3  | 1.72                     | 0.70              |
| 1:A:226:GLN:HA    | 1:D:3001:MET:CB   | 2.20                     | 0.70              |
| 1:D:3038:MET:HB2  | 1:D:3055:ALA:HB1  | 1.74                     | 0.70              |
| 1:E:4102:ILE:HG21 | 1:E:4108:LEU:HD21 | 1.72                     | 0.70              |
| 1:F:5002:SER:CA   | 1:F:5007:PHE:CD1  | 2.73                     | 0.70              |
| 1:F:5163:TYR:HD1  | 1:F:5163:TYR:H    | 1.40                     | 0.69              |
| 1:F:5001:MET:CA   | 1:F:5007:PHE:CE1  | 2.75                     | 0.69              |
| 1:A:167:GLU:OE1   | 1:A:223:ARG:HD3   | 1.93                     | 0.69              |
| 1:B:1242:VAL:O    | 1:B:1245:VAL:HG12 | 1.93                     | 0.69              |
| 1:F:5205:MET:O    | 1:F:5206:CYS:HB2  | 1.92                     | 0.69              |
| 1:C:2207:ALA:N    | 1:C:2211:LEU:HD13 | 2.08                     | 0.69              |
| 1:D:3008:HIS:HB3  | 1:D:3080:GLU:OE2  | 1.93                     | 0.69              |
| 1:D:3091:ARG:HB3  | 1:D:3215:MET:HG3  | 1.74                     | 0.69              |
| 1:F:5025:PRO:HD2  | 1:F:5065:CYS:O    | 1.93                     | 0.69              |
| 1:F:5119:ALA:HB3  | 1:F:5201:THR:OG1  | 1.93                     | 0.69              |
| 1:C:2176:VAL:HG23 | 1:C:2177:VAL:H    | 1.58                     | 0.68              |
| 1:A:23:ILE:HG22   | 1:A:25:PRO:HD3    | 1.75                     | 0.68              |
| 1:B:1012:THR:HG23 | 1:B:1015:ASP:OD1  | 1.93                     | 0.68              |
| 1:D:3077:ALA:O    | 1:D:3081:LEU:HD13 | 1.93                     | 0.68              |
| 1:B:1115:ARG:HH21 | 1:B:1121:LEU:HD22 | 1.59                     | 0.68              |
| 1:D:3038:MET:HB3  | 1:D:3056:GLU:O    | 1.93                     | 0.68              |
| 1:B:1176:VAL:HG23 | 1:B:1177:VAL:H    | 1.58                     | 0.68              |
| 1:C:2136:CYS:O    | 1:C:2140:LEU:HD12 | 1.94                     | 0.68              |
| 1:F:5240:HIS:HA   | 1:F:5243:LYS:HE2  | 1.76                     | 0.68              |
| 1:E:4089:PHE:O    | 1:E:4213:ALA:HA   | 1.93                     | 0.68              |
| 1:C:2178:ARG:HB3  | 1:C:2179:HIS:HD2  | 1.58                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3136:CYS:O    | 1:D:3140:LEU:HG   | 1.94                     | 0.68              |
| 1:F:5001:MET:C    | 1:F:5007:PHE:CZ   | 2.72                     | 0.68              |
| 1:D:3162:PHE:O    | 1:D:3164:PRO:HD3  | 1.93                     | 0.68              |
| 1:C:2167:GLU:HG2  | 1:C:2223:ARG:HG2  | 1.73                     | 0.67              |
| 1:F:5007:PHE:CD2  | 1:F:5007:PHE:O    | 2.48                     | 0.67              |
| 1:C:2104:VAL:HG11 | 1:C:2229:PRO:HG3  | 1.75                     | 0.67              |
| 1:C:2115:ARG:O    | 1:C:2116:LEU:HD23 | 1.95                     | 0.67              |
| 1:C:2210:GLY:O    | 1:C:2211:LEU:HB3  | 1.92                     | 0.67              |
| 1:F:5114:VAL:HG23 | 1:F:5116:LEU:HG   | 1.77                     | 0.67              |
| 1:A:1:MET:SD      | 1:D:3229:PRO:CD   | 2.79                     | 0.67              |
| 1:B:1108:LEU:HB3  | 1:B:1193:MET:HE3  | 1.77                     | 0.67              |
| 1:C:2043:LYS:HE2  | 1:C:2053:TRP:NE1  | 2.10                     | 0.67              |
| 1:B:1003:LYS:CB   | 1:B:1007:PHE:HB2  | 2.25                     | 0.66              |
| 1:D:3103:ASN:O    | 1:D:3106:ASP:HB2  | 1.94                     | 0.66              |
| 1:F:5002:SER:CB   | 1:F:5007:PHE:CZ   | 2.77                     | 0.66              |
| 1:C:2031:VAL:HG21 | 1:C:2066:SER:HB2  | 1.76                     | 0.66              |
| 1:E:4039:ASP:HB2  | 1:E:4056:GLU:HB2  | 1.77                     | 0.66              |
| 1:F:5091:ARG:HG2  | 1:F:5215:MET:CG   | 2.25                     | 0.66              |
| 1:B:1234:MET:HE3  | 1:B:1235:LYS:HE2  | 1.78                     | 0.66              |
| 1:D:3029:ASP:O    | 1:D:3033:LYS:HG2  | 1.95                     | 0.66              |
| 1:D:3109:VAL:O    | 1:D:3193:MET:HE1  | 1.96                     | 0.66              |
| 1:E:4212:ARG:NH1  | 1:E:4252:LEU:HD23 | 2.09                     | 0.66              |
| 1:E:4145:LYS:HE2  | 1:E:4145:LYS:HA   | 1.78                     | 0.65              |
| 1:F:5236:GLN:HA   | 1:F:5239:SER:HG   | 1.61                     | 0.65              |
| 1:C:2141:VAL:HG21 | 1:F:5134:PHE:CE1  | 2.32                     | 0.65              |
| 1:D:3235:LYS:HD2  | 1:D:3235:LYS:O    | 1.96                     | 0.65              |
| 1:F:5140:LEU:HD13 | 1:F:5216:VAL:HB   | 1.78                     | 0.65              |
| 1:C:2024:VAL:O    | 1:C:2091:ARG:HG3  | 1.97                     | 0.65              |
| 1:C:2079:GLU:O    | 1:C:2083:GLN:HG2  | 1.96                     | 0.65              |
| 1:E:4171:THR:O    | 1:E:4172:TYR:HB2  | 1.95                     | 0.65              |
| 1:A:225:GLN:C     | 1:D:3001:MET:SD   | 2.80                     | 0.65              |
| 1:B:1210:GLY:O    | 1:B:1211:LEU:HB2  | 1.97                     | 0.65              |
| 1:D:3183:SER:HA   | 1:D:3187:TRP:HD1  | 1.62                     | 0.65              |
| 1:F:5183:SER:HA   | 1:F:5186:GLU:HG3  | 1.78                     | 0.65              |
| 1:C:2099:GLN:HB2  | 1:C:2102:ILE:HD12 | 1.77                     | 0.65              |
| 1:C:2178:ARG:NH2  | 1:E:4125:PRO:HG3  | 2.12                     | 0.65              |
| 1:D:3106:ASP:OD2  | 1:D:3150:THR:HB   | 1.96                     | 0.65              |
| 1:B:1072:PRO:O    | 1:B:1076:ILE:HG13 | 1.97                     | 0.64              |
| 1:C:2179:HIS:H    | 1:C:2179:HIS:HD2  | 1.43                     | 0.64              |
| 1:F:5111:THR:HG23 | 1:F:5153:VAL:HG12 | 1.79                     | 0.64              |
| 1:B:1104:VAL:HG13 | 1:B:1220:ILE:HA   | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:5001:MET:C    | 1:F:5007:PHE:CE1  | 2.74                     | 0.64              |
| 1:C:2206:CYS:O    | 1:C:2211:LEU:HB2  | 1.97                     | 0.64              |
| 1:D:3138:THR:HA   | 1:D:3141:VAL:HG22 | 1.77                     | 0.64              |
| 1:E:4067:THR:HG22 | 1:E:4077:ALA:HB3  | 1.80                     | 0.64              |
| 1:F:5212:ARG:NH1  | 1:F:5252:LEU:HD22 | 2.12                     | 0.64              |
| 1:B:1121:LEU:O    | 1:F:5177:VAL:HG11 | 1.98                     | 0.64              |
| 1:E:4034:ILE:HG12 | 1:E:4242:VAL:HG13 | 1.80                     | 0.64              |
| 1:F:5011:LEU:HD11 | 1:F:5016:LEU:HD21 | 1.79                     | 0.64              |
| 1:D:3161:THR:HG22 | 1:D:3162:PHE:N    | 2.12                     | 0.64              |
| 1:D:3178:ARG:HG3  | 1:D:3179:HIS:ND1  | 2.12                     | 0.63              |
| 1:F:5022:ALA:HB2  | 1:F:5086:ILE:CD1  | 2.28                     | 0.63              |
| 1:F:5030:ARG:HA   | 1:F:5033:LYS:HE3  | 1.80                     | 0.63              |
| 1:A:11:LEU:HD11   | 1:A:16:LEU:HD23   | 1.81                     | 0.63              |
| 1:D:3025:PRO:HD2  | 1:D:3065:CYS:O    | 1.98                     | 0.63              |
| 1:F:5002:SER:HA   | 1:F:5007:PHE:CG   | 2.33                     | 0.63              |
| 1:C:2104:VAL:HG11 | 1:C:2229:PRO:CB   | 2.28                     | 0.63              |
| 1:C:2167:GLU:HA   | 1:C:2184:MET:CE   | 2.28                     | 0.63              |
| 1:A:72:PRO:HB2    | 1:D:3069:ILE:HG22 | 1.81                     | 0.63              |
| 1:B:1001:MET:HG3  | 1:B:1009:LEU:HD23 | 1.79                     | 0.63              |
| 1:B:1022:ALA:HB2  | 1:B:1086:ILE:HG21 | 1.81                     | 0.63              |
| 1:B:1178:ARG:NH2  | 1:B:1179:HIS:HB3  | 2.14                     | 0.63              |
| 1:E:4202:LEU:O    | 1:E:4205:MET:O    | 2.16                     | 0.63              |
| 1:F:5042:VAL:HG21 | 1:F:5054:ARG:HH21 | 1.63                     | 0.63              |
| 1:F:5209:GLN:HG3  | 1:F:5209:GLN:O    | 1.99                     | 0.63              |
| 1:C:2126:LEU:HD23 | 1:F:5126:LEU:CD2  | 2.28                     | 0.63              |
| 1:E:4096:GLY:HA3  | 1:E:4221:VAL:HG12 | 1.81                     | 0.63              |
| 1:F:5034:ILE:O    | 1:F:5037:LEU:HD12 | 1.98                     | 0.62              |
| 1:B:1209:GLN:O    | 1:B:1211:LEU:N    | 2.32                     | 0.62              |
| 1:D:3007:PHE:O    | 1:D:3009:LEU:N    | 2.32                     | 0.62              |
| 1:D:3091:ARG:HG2  | 1:D:3215:MET:HG3  | 1.80                     | 0.62              |
| 1:E:4058:ASP:CG   | 1:E:4250:ARG:HD2  | 2.24                     | 0.62              |
| 1:F:5155:VAL:O    | 1:F:5192:VAL:HG13 | 1.99                     | 0.62              |
| 1:F:5002:SER:N    | 1:F:5002:SER:HA   | 2.06                     | 0.62              |
| 1:C:2223:ARG:HD2  | 1:C:2223:ARG:N    | 2.14                     | 0.62              |
| 1:A:14:ASN:O      | 1:A:17:GLN:HG2    | 1.99                     | 0.62              |
| 1:B:1226:GLN:HE21 | 1:B:1226:GLN:HA   | 1.63                     | 0.62              |
| 1:E:4040:LYS:N    | 1:E:4041:PRO:HD3  | 2.13                     | 0.62              |
| 1:D:3147:ILE:HD11 | 1:D:3243:LYS:HD2  | 1.79                     | 0.62              |
| 1:A:108:LEU:HA    | 1:A:152:HIS:O     | 1.99                     | 0.62              |
| 1:C:2041:PRO:HA   | 1:C:2054:ARG:O    | 1.99                     | 0.62              |
| 1:D:3183:SER:HB3  | 1:D:3195:TYR:OH   | 1.99                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:5123:PHE:CD1  | 1:F:5205:MET:HG3  | 2.34                     | 0.62              |
| 1:F:5007:PHE:O    | 1:F:5007:PHE:HD2  | 1.80                     | 0.62              |
| 1:D:3037:LEU:HD23 | 1:D:3246:VAL:HG21 | 1.81                     | 0.61              |
| 1:E:4094:THR:HB   | 1:E:4220:ILE:CG2  | 2.30                     | 0.61              |
| 1:A:83:GLN:HG3    | 1:D:3172:TYR:CZ   | 2.35                     | 0.61              |
| 1:B:1060:LYS:HG3  | 1:B:1253:LEU:HB3  | 1.83                     | 0.61              |
| 1:F:5204:THR:HB   | 1:F:5205:MET:SD   | 2.40                     | 0.61              |
| 1:B:1016:LEU:HD23 | 1:B:1084:LEU:HD13 | 1.82                     | 0.61              |
| 1:A:147:ILE:HG22  | 1:A:147:ILE:O     | 2.00                     | 0.61              |
| 1:A:225:GLN:HB2   | 1:D:3001:MET:CE   | 2.29                     | 0.61              |
| 1:F:5013:LYS:HA   | 1:F:5084:LEU:HD22 | 1.80                     | 0.61              |
| 1:B:1163:TYR:N    | 1:B:1163:TYR:CD1  | 2.68                     | 0.61              |
| 1:B:1233:THR:HA   | 1:B:1236:GLN:HE21 | 1.65                     | 0.61              |
| 1:F:5002:SER:CA   | 1:F:5002:SER:H    | 2.03                     | 0.61              |
| 1:C:2051:THR:H    | 1:C:2066:SER:HB3  | 1.66                     | 0.60              |
| 1:C:2205:MET:SD   | 1:C:2205:MET:O    | 2.58                     | 0.60              |
| 1:E:4235:LYS:CG   | 1:E:4236:GLN:H    | 2.14                     | 0.60              |
| 1:B:1008:HIS:CD2  | 1:B:1076:ILE:HG21 | 2.36                     | 0.60              |
| 1:B:1177:VAL:CG1  | 1:B:1180:PHE:HB2  | 2.31                     | 0.60              |
| 1:C:2234:MET:O    | 1:C:2237:THR:HB   | 2.01                     | 0.60              |
| 1:B:1113:SER:OG   | 1:B:1203:LEU:HD12 | 2.02                     | 0.60              |
| 1:B:1158:SER:CB   | 1:B:1200:ALA:HB2  | 2.32                     | 0.60              |
| 1:E:4238:GLU:O    | 1:E:4242:VAL:HG23 | 2.02                     | 0.60              |
| 1:A:163:TYR:CE2   | 1:A:223:ARG:NH1   | 2.69                     | 0.60              |
| 1:B:1132:ALA:HB2  | 1:B:1203:LEU:HD22 | 1.84                     | 0.59              |
| 1:B:1156:THR:HG23 | 1:B:1194:ASN:OD1  | 2.02                     | 0.59              |
| 1:C:2060:LYS:HB2  | 1:C:2253:LEU:HD13 | 1.84                     | 0.59              |
| 1:B:1019:ALA:HB1  | 1:B:1086:ILE:HD12 | 1.84                     | 0.59              |
| 1:B:1180:PHE:HA   | 1:B:1183:SER:HB3  | 1.83                     | 0.59              |
| 1:C:2104:VAL:HG11 | 1:C:2229:PRO:CG   | 2.31                     | 0.59              |
| 1:C:2106:ASP:OD1  | 1:C:2152:HIS:HE1  | 1.85                     | 0.59              |
| 1:C:2158:SER:HA   | 1:C:2196:GLU:O    | 2.01                     | 0.59              |
| 1:F:5019:ALA:O    | 1:F:5020:THR:HB   | 2.02                     | 0.59              |
| 1:B:1190:MET:HG2  | 1:D:3128:PHE:CE2  | 2.37                     | 0.59              |
| 1:E:4016:LEU:N    | 1:E:4016:LEU:HD22 | 2.18                     | 0.59              |
| 1:D:3006:VAL:HG23 | 1:D:3007:PHE:H    | 1.67                     | 0.59              |
| 1:A:112:ALA:HB1   | 1:A:130:ALA:O     | 2.03                     | 0.59              |
| 1:B:1205:MET:O    | 1:B:1209:GLN:HG3  | 2.01                     | 0.59              |
| 1:B:1238:GLU:O    | 1:B:1242:VAL:HG22 | 2.03                     | 0.59              |
| 1:E:4162:PHE:C    | 1:E:4164:PRO:HD3  | 2.28                     | 0.59              |
| 1:D:3207:ALA:HA   | 1:D:3211:LEU:HD22 | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:5042:VAL:HG12 | 1:F:5043:LYS:O    | 2.03                     | 0.59              |
| 1:E:4141:VAL:HG22 | 1:E:4151:THR:HG21 | 1.85                     | 0.58              |
| 1:D:3016:LEU:HA   | 1:D:3063:ILE:HD11 | 1.85                     | 0.58              |
| 1:E:4104:VAL:HG12 | 1:E:4233:THR:HG21 | 1.85                     | 0.58              |
| 1:E:4078:VAL:HB   | 1:E:4205:MET:SD   | 2.44                     | 0.58              |
| 1:E:4248:ALA:O    | 1:E:4252:LEU:HD12 | 2.04                     | 0.58              |
| 1:B:1005:ASP:HB2  | 1:B:1007:PHE:CE2  | 2.38                     | 0.58              |
| 1:B:1135:GLU:HB3  | 1:B:1212:ARG:HH11 | 1.69                     | 0.58              |
| 1:E:4104:VAL:HA   | 1:E:4219:VAL:HG12 | 1.85                     | 0.58              |
| 1:E:4078:VAL:CG1  | 1:E:4205:MET:SD   | 2.92                     | 0.58              |
| 1:F:5183:SER:HA   | 1:F:5186:GLU:CG   | 2.33                     | 0.58              |
| 1:A:196:GLU:HG3   | 1:A:197:MET:H     | 1.69                     | 0.58              |
| 1:F:5024:VAL:HB   | 1:F:5067:THR:HG23 | 1.84                     | 0.58              |
| 1:A:114:VAL:HG22  | 1:E:4129:PRO:HD3  | 1.86                     | 0.57              |
| 1:A:143:ALA:O     | 1:A:147:ILE:HG12  | 2.04                     | 0.57              |
| 1:E:4232:GLU:O    | 1:E:4235:LYS:HG2  | 2.04                     | 0.57              |
| 1:E:4235:LYS:HG3  | 1:E:4236:GLN:H    | 1.69                     | 0.57              |
| 1:B:1077:ALA:O    | 1:B:1078:VAL:HG23 | 2.04                     | 0.57              |
| 1:B:1162:PHE:HB2  | 1:F:5076:ILE:HD11 | 1.86                     | 0.57              |
| 1:F:5002:SER:CA   | 1:F:5007:PHE:CZ   | 2.87                     | 0.57              |
| 1:F:5230:ASN:O    | 1:F:5232:GLU:HG3  | 2.04                     | 0.57              |
| 1:C:2091:ARG:O    | 1:C:2216:VAL:HG12 | 2.04                     | 0.57              |
| 1:F:5011:LEU:HD12 | 1:F:5015:ASP:HB2  | 1.86                     | 0.57              |
| 1:F:5233:THR:OG1  | 1:F:5234:MET:HE2  | 2.05                     | 0.57              |
| 1:C:2242:VAL:O    | 1:C:2246:VAL:HG23 | 2.04                     | 0.57              |
| 1:F:5222:ASN:HB3  | 1:F:5225:GLN:OE1  | 2.04                     | 0.57              |
| 1:A:167:GLU:CB    | 1:A:184:MET:HE2   | 2.28                     | 0.57              |
| 1:D:3006:VAL:HG23 | 1:D:3007:PHE:N    | 2.20                     | 0.57              |
| 1:A:11:LEU:CD1    | 1:A:15:ASP:HB2    | 2.35                     | 0.57              |
| 1:A:207:ALA:HA    | 1:A:211:LEU:HB3   | 1.87                     | 0.57              |
| 1:C:2034:ILE:HG12 | 1:C:2242:VAL:HG13 | 1.87                     | 0.57              |
| 1:C:2206:CYS:HB3  | 1:C:2211:LEU:HA   | 1.87                     | 0.57              |
| 1:B:1234:MET:HB2  | 1:B:1235:LYS:HD3  | 1.85                     | 0.57              |
| 1:C:2158:SER:OG   | 1:C:2200:ALA:HB2  | 2.05                     | 0.56              |
| 1:C:2178:ARG:HE   | 1:C:2179:HIS:CD2  | 2.22                     | 0.56              |
| 1:E:4219:VAL:O    | 1:E:4237:THR:HG21 | 2.05                     | 0.56              |
| 1:A:11:LEU:HD23   | 1:A:11:LEU:H      | 1.70                     | 0.56              |
| 1:A:114:VAL:HG11  | 1:A:187:TRP:CZ3   | 2.39                     | 0.56              |
| 1:A:225:GLN:CA    | 1:D:3001:MET:SD   | 2.93                     | 0.56              |
| 1:C:2208:SER:O    | 1:C:2209:GLN:HB3  | 2.05                     | 0.56              |
| 1:E:4086:ILE:HD12 | 1:E:4086:ILE:H    | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:4172:TYR:HD2  | 1:E:4173:SER:H    | 1.53                     | 0.56              |
| 1:F:5002:SER:CB   | 1:F:5007:PHE:CE2  | 2.89                     | 0.56              |
| 1:A:35:ALA:HB2    | 1:A:64:VAL:HG11   | 1.86                     | 0.56              |
| 1:A:205:MET:C     | 1:A:205:MET:SD    | 2.88                     | 0.56              |
| 1:E:4009:LEU:HD22 | 1:E:4080:GLU:HB2  | 1.88                     | 0.56              |
| 1:E:4209:GLN:C    | 1:E:4211:LEU:H    | 2.14                     | 0.56              |
| 1:A:238:GLU:O     | 1:A:242:VAL:HG23  | 2.06                     | 0.56              |
| 1:B:1023:ILE:HD12 | 1:B:1023:ILE:N    | 2.21                     | 0.56              |
| 1:D:3102:ILE:O    | 1:D:3222:ASN:ND2  | 2.38                     | 0.56              |
| 1:E:4038:MET:HE2  | 1:E:4246:VAL:HG13 | 1.87                     | 0.56              |
| 1:E:4094:THR:HB   | 1:E:4220:ILE:HG23 | 1.86                     | 0.56              |
| 1:E:4098:ILE:O    | 1:E:4224:THR:HG21 | 2.06                     | 0.56              |
| 1:B:1119:ALA:HB3  | 1:B:1201:THR:OG1  | 2.06                     | 0.56              |
| 1:C:2001:MET:SD   | 1:C:2001:MET:C    | 2.89                     | 0.56              |
| 1:D:3142:GLU:HB3  | 1:D:3251:ARG:NH1  | 2.21                     | 0.56              |
| 1:F:5007:PHE:CD1  | 1:F:5007:PHE:CB   | 2.81                     | 0.56              |
| 1:F:5106:ASP:OD1  | 1:F:5152:HIS:HE1  | 1.89                     | 0.56              |
| 1:C:2091:ARG:HD3  | 1:C:2202:LEU:HD22 | 1.89                     | 0.55              |
| 1:F:5039:ASP:C    | 1:F:5041:PRO:HD3  | 2.31                     | 0.55              |
| 1:B:1235:LYS:H    | 1:B:1235:LYS:CD   | 2.12                     | 0.55              |
| 1:D:3076:ILE:O    | 1:D:3080:GLU:HG2  | 2.05                     | 0.55              |
| 1:E:4042:VAL:HG22 | 1:E:4054:ARG:HB3  | 1.87                     | 0.55              |
| 1:F:5040:LYS:N    | 1:F:5041:PRO:CD   | 2.69                     | 0.55              |
| 1:F:5115:ARG:NH1  | 1:F:5128:PHE:HB3  | 2.20                     | 0.55              |
| 1:F:5179:HIS:O    | 1:F:5180:PHE:HD2  | 1.90                     | 0.55              |
| 1:C:2163:TYR:CD1  | 1:C:2163:TYR:N    | 2.72                     | 0.55              |
| 1:B:1049:GLU:HG3  | 1:F:5049:GLU:OE2  | 2.07                     | 0.55              |
| 1:B:1220:ILE:HD13 | 1:B:1220:ILE:H    | 1.71                     | 0.55              |
| 1:B:1016:LEU:HD11 | 1:B:1086:ILE:HD11 | 1.87                     | 0.55              |
| 1:E:4149:ALA:O    | 1:E:4151:THR:N    | 2.39                     | 0.55              |
| 1:A:233:THR:O     | 1:A:236:GLN:HB3   | 2.06                     | 0.55              |
| 1:E:4079:GLU:O    | 1:E:4083:GLN:HG3  | 2.07                     | 0.55              |
| 1:E:4186:GLU:O    | 1:E:4190:MET:HG3  | 2.07                     | 0.55              |
| 1:F:5002:SER:OG   | 1:F:5007:PHE:CE2  | 2.59                     | 0.55              |
| 1:F:5009:LEU:HB3  | 1:F:5047:HIS:O    | 2.06                     | 0.55              |
| 1:F:5205:MET:O    | 1:F:5207:ALA:N    | 2.37                     | 0.55              |
| 1:F:5242:VAL:O    | 1:F:5246:VAL:HG23 | 2.07                     | 0.55              |
| 1:B:1126:LEU:HD23 | 1:D:3126:LEU:HD23 | 1.87                     | 0.55              |
| 1:C:2032:GLU:HG2  | 1:C:2033:LYS:N    | 2.22                     | 0.55              |
| 1:B:1155:VAL:HG23 | 1:B:1192:VAL:HG22 | 1.89                     | 0.55              |
| 1:B:1163:TYR:N    | 1:B:1163:TYR:HD1  | 2.04                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2226:GLN:C    | 1:C:2228:ILE:H    | 2.15                     | 0.55              |
| 1:D:3033:LYS:HD2  | 1:D:3033:LYS:N    | 2.22                     | 0.55              |
| 1:C:2076:ILE:HA   | 1:C:2079:GLU:HG2  | 1.89                     | 0.54              |
| 1:F:5023:ILE:HG22 | 1:F:5092:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:233:THR:HG23  | 1:A:236:GLN:CD    | 2.33                     | 0.54              |
| 1:D:3055:ALA:HB3  | 1:D:3062:VAL:HG23 | 1.88                     | 0.54              |
| 1:A:6:VAL:O       | 1:A:8:HIS:N       | 2.39                     | 0.54              |
| 1:A:49:GLU:HG3    | 1:D:3049:GLU:HG3  | 1.88                     | 0.54              |
| 1:A:196:GLU:CG    | 1:A:197:MET:H     | 2.20                     | 0.54              |
| 1:A:247:GLU:O     | 1:A:250:ARG:HG2   | 2.08                     | 0.54              |
| 1:C:2099:GLN:HB2  | 1:C:2102:ILE:CD1  | 2.38                     | 0.54              |
| 1:A:1:MET:HG2     | 1:A:2:SER:N       | 2.21                     | 0.54              |
| 1:C:2017:GLN:CD   | 1:C:2018:GLY:N    | 2.66                     | 0.54              |
| 1:D:3035:ALA:O    | 1:D:3041:PRO:HB3  | 2.08                     | 0.54              |
| 1:F:5235:LYS:NZ   | 1:F:5239:SER:OG   | 2.41                     | 0.54              |
| 1:A:16:LEU:HD11   | 1:A:84:LEU:HB3    | 1.90                     | 0.54              |
| 1:A:56:GLU:HB2    | 1:A:60:LYS:O      | 2.08                     | 0.54              |
| 1:D:3058:ASP:O    | 1:D:3060:LYS:HD3  | 2.08                     | 0.54              |
| 1:E:4031:VAL:HB   | 1:E:4064:VAL:HG12 | 1.90                     | 0.54              |
| 1:A:141:VAL:HG11  | 1:E:4134:PHE:CE1  | 2.43                     | 0.54              |
| 1:E:4037:LEU:HD12 | 1:E:4037:LEU:H    | 1.73                     | 0.54              |
| 1:F:5001:MET:CA   | 1:F:5007:PHE:CZ   | 2.91                     | 0.54              |
| 1:F:5016:LEU:HD11 | 1:F:5084:LEU:HD13 | 1.89                     | 0.54              |
| 1:A:183:SER:O     | 1:A:187:TRP:CD1   | 2.61                     | 0.54              |
| 1:C:2229:PRO:CG   | 1:C:2234:MET:HG2  | 2.16                     | 0.54              |
| 1:B:1032:GLU:HG3  | 1:B:1033:LYS:N    | 2.22                     | 0.54              |
| 1:E:4212:ARG:HH11 | 1:E:4252:LEU:CD2  | 2.20                     | 0.54              |
| 1:F:5230:ASN:O    | 1:F:5232:GLU:N    | 2.41                     | 0.54              |
| 1:A:235:LYS:O     | 1:A:238:GLU:HB3   | 2.09                     | 0.53              |
| 1:A:8:HIS:CG      | 1:A:9:LEU:HD22    | 2.42                     | 0.53              |
| 1:D:3168:ARG:CZ   | 1:D:3168:ARG:HB3  | 2.36                     | 0.53              |
| 1:E:4168:ARG:O    | 1:E:4168:ARG:NE   | 2.41                     | 0.53              |
| 1:A:161:THR:O     | 1:A:163:TYR:N     | 2.41                     | 0.53              |
| 1:B:1155:VAL:CG2  | 1:B:1192:VAL:HG22 | 2.38                     | 0.53              |
| 1:B:1212:ARG:NH1  | 1:B:1252:LEU:HG   | 2.24                     | 0.53              |
| 1:D:3089:PHE:O    | 1:D:3213:ALA:HA   | 2.09                     | 0.53              |
| 1:A:6:VAL:O       | 1:A:8:HIS:HB2     | 2.08                     | 0.53              |
| 1:A:9:LEU:HA      | 1:A:47:HIS:ND1    | 2.24                     | 0.53              |
| 1:B:1106:ASP:HB3  | 1:B:1150:THR:HB   | 1.91                     | 0.53              |
| 1:C:2076:ILE:O    | 1:C:2079:GLU:HG2  | 2.08                     | 0.53              |
| 1:F:5023:ILE:CG2  | 1:F:5092:ILE:HD11 | 2.38                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1161:THR:O    | 1:B:1197:MET:HE3  | 2.09                     | 0.53              |
| 1:C:2238:GLU:O    | 1:C:2242:VAL:HG23 | 2.08                     | 0.53              |
| 1:D:3133:ASP:HB2  | 1:D:3211:LEU:HG   | 1.90                     | 0.53              |
| 1:F:5037:LEU:HD11 | 1:F:5242:VAL:HG12 | 1.89                     | 0.53              |
| 1:A:112:ALA:CB    | 1:E:4131:VAL:HG11 | 2.38                     | 0.53              |
| 1:C:2056:GLU:HG2  | 1:C:2057:LEU:N    | 2.24                     | 0.53              |
| 1:C:2116:LEU:HD23 | 1:F:5127:GLU:HG2  | 1.90                     | 0.53              |
| 1:C:2225:GLN:O    | 1:C:2228:ILE:HG22 | 2.09                     | 0.53              |
| 1:E:4019:ALA:C    | 1:E:4021:LEU:H    | 2.17                     | 0.53              |
| 1:E:4038:MET:HE2  | 1:E:4246:VAL:CG1  | 2.39                     | 0.53              |
| 1:E:4176:VAL:HG12 | 1:E:4177:VAL:N    | 2.17                     | 0.53              |
| 1:A:97:ALA:HA     | 1:A:194:ASN:HB3   | 1.91                     | 0.53              |
| 1:C:2140:LEU:HD22 | 1:C:2216:VAL:HB   | 1.91                     | 0.53              |
| 1:A:38:MET:HB2    | 1:A:55:ALA:HB1    | 1.90                     | 0.53              |
| 1:B:1143:ALA:O    | 1:B:1146:SER:HB3  | 2.09                     | 0.53              |
| 1:A:67:THR:HG22   | 1:A:77:ALA:CB     | 2.38                     | 0.53              |
| 1:C:2231:ALA:HA   | 1:C:2234:MET:HG3  | 1.90                     | 0.53              |
| 1:C:2216:VAL:HG11 | 1:C:2245:VAL:HB   | 1.92                     | 0.52              |
| 1:D:3106:ASP:O    | 1:D:3219:VAL:HB   | 2.08                     | 0.52              |
| 1:E:4071:GLY:HA2  | 1:E:4074:THR:HB   | 1.91                     | 0.52              |
| 1:D:3160:ASP:HA   | 1:D:3197:MET:HG3  | 1.91                     | 0.52              |
| 1:F:5001:MET:HA   | 1:F:5007:PHE:CZ   | 2.45                     | 0.52              |
| 1:C:2094:THR:HB   | 1:C:2220:ILE:HG23 | 1.91                     | 0.52              |
| 1:A:38:MET:CB     | 1:A:55:ALA:HB1    | 2.40                     | 0.52              |
| 1:A:211:LEU:HD23  | 1:A:211:LEU:H     | 1.75                     | 0.52              |
| 1:D:3025:PRO:HG3  | 1:D:3031:VAL:HG22 | 1.91                     | 0.52              |
| 1:E:4028:PRO:HB3  | 1:E:4051:THR:HG21 | 1.91                     | 0.52              |
| 1:E:4178:ARG:O    | 1:E:4181:LYS:HG2  | 2.09                     | 0.52              |
| 1:B:1114:VAL:HA   | 1:D:3129:PRO:HD3  | 1.91                     | 0.52              |
| 1:B:1178:ARG:HH21 | 1:B:1179:HIS:HB3  | 1.73                     | 0.52              |
| 1:F:5002:SER:CA   | 1:F:5007:PHE:CE1  | 2.92                     | 0.52              |
| 1:F:5011:LEU:HD23 | 1:F:5011:LEU:N    | 2.25                     | 0.52              |
| 1:F:5102:ILE:HG12 | 1:F:5152:HIS:CE1  | 2.45                     | 0.52              |
| 1:B:1003:LYS:CB   | 1:B:1007:PHE:HD2  | 2.23                     | 0.52              |
| 1:E:4038:MET:HB3  | 1:E:4055:ALA:HB1  | 1.90                     | 0.52              |
| 1:E:4210:GLY:O    | 1:E:4211:LEU:C    | 2.53                     | 0.52              |
| 1:A:62:VAL:CG2    | 1:A:253:LEU:HD21  | 2.38                     | 0.52              |
| 1:C:2176:VAL:HG23 | 1:C:2177:VAL:N    | 2.23                     | 0.52              |
| 1:D:3092:ILE:HD12 | 1:D:3093:GLY:H    | 1.75                     | 0.52              |
| 1:F:5021:LEU:HG   | 1:F:5022:ALA:N    | 2.24                     | 0.52              |
| 1:F:5057:LEU:HD11 | 1:F:5250:ARG:NH1  | 2.25                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:5163:TYR:CD1  | 1:F:5163:TYR:N    | 2.77                     | 0.52              |
| 1:A:226:GLN:HA    | 1:D:3001:MET:HB3  | 1.90                     | 0.52              |
| 1:A:248:ALA:O     | 1:A:252:LEU:HD23  | 2.10                     | 0.52              |
| 1:C:2043:LYS:NZ   | 1:C:2052:THR:O    | 2.40                     | 0.52              |
| 1:D:3057:LEU:O    | 1:D:3060:LYS:HB2  | 2.10                     | 0.52              |
| 1:E:4057:LEU:HD11 | 1:E:4250:ARG:HB2  | 1.92                     | 0.52              |
| 1:F:5002:SER:C    | 1:F:5007:PHE:CG   | 2.87                     | 0.52              |
| 1:B:1039:ASP:N    | 1:B:1056:GLU:O    | 2.43                     | 0.52              |
| 1:C:2096:GLY:HA2  | 1:C:2221:VAL:O    | 2.10                     | 0.52              |
| 1:F:5024:VAL:HG23 | 1:F:5024:VAL:O    | 2.10                     | 0.52              |
| 1:A:2:SER:C       | 1:A:4:SER:H       | 2.17                     | 0.52              |
| 1:C:2115:ARG:HH21 | 1:C:2121:LEU:HD12 | 1.74                     | 0.52              |
| 1:D:3091:ARG:CG   | 1:D:3215:MET:HG3  | 2.40                     | 0.52              |
| 1:E:4158:SER:HA   | 1:E:4196:GLU:O    | 2.09                     | 0.52              |
| 1:F:5201:THR:HA   | 1:F:5205:MET:CE   | 2.40                     | 0.52              |
| 1:B:1038:MET:CE   | 1:B:1246:VAL:HG12 | 2.40                     | 0.51              |
| 1:D:3243:LYS:O    | 1:D:3247:GLU:HB2  | 2.10                     | 0.51              |
| 1:A:114:VAL:HG13  | 1:E:4128:PHE:HA   | 1.90                     | 0.51              |
| 1:B:1074:THR:CG2  | 1:B:1078:VAL:HG21 | 2.38                     | 0.51              |
| 1:B:1163:TYR:HB3  | 1:B:1223:ARG:NH2  | 2.25                     | 0.51              |
| 1:C:2019:ALA:O    | 1:C:2020:THR:HB   | 2.09                     | 0.51              |
| 1:D:3139:ALA:CB   | 1:D:3252:LEU:HD21 | 2.40                     | 0.51              |
| 1:D:3176:VAL:HG22 | 1:D:3177:VAL:HG22 | 1.92                     | 0.51              |
| 1:E:4206:CYS:O    | 1:E:4208:SER:N    | 2.42                     | 0.51              |
| 1:F:5091:ARG:HG2  | 1:F:5215:MET:SD   | 2.50                     | 0.51              |
| 1:A:1:MET:N       | 1:D:3228:ILE:HG22 | 2.25                     | 0.51              |
| 1:B:1104:VAL:HG12 | 1:B:1233:THR:HG21 | 1.93                     | 0.51              |
| 1:C:2089:PHE:O    | 1:C:2213:ALA:HA   | 2.09                     | 0.51              |
| 1:E:4078:VAL:CB   | 1:E:4205:MET:SD   | 2.99                     | 0.51              |
| 1:F:5002:SER:HA   | 1:F:5007:PHE:CE2  | 2.42                     | 0.51              |
| 1:B:1177:VAL:HG11 | 1:B:1180:PHE:HB2  | 1.92                     | 0.51              |
| 1:E:4024:VAL:HG23 | 1:E:4024:VAL:O    | 2.10                     | 0.51              |
| 1:E:4028:PRO:HA   | 1:E:4031:VAL:HG13 | 1.92                     | 0.51              |
| 1:F:5022:ALA:HA   | 1:F:5063:ILE:O    | 2.11                     | 0.51              |
| 1:F:5055:ALA:C    | 1:F:5056:GLU:HG2  | 2.35                     | 0.51              |
| 1:B:1161:THR:OG1  | 1:F:5122:HIS:HD2  | 1.93                     | 0.51              |
| 1:C:2011:LEU:HB2  | 1:C:2084:LEU:HD21 | 1.93                     | 0.51              |
| 1:C:2156:THR:HG23 | 1:C:2194:ASN:OD1  | 2.11                     | 0.51              |
| 1:E:4128:PHE:CG   | 1:E:4129:PRO:HD2  | 2.46                     | 0.51              |
| 1:B:1001:MET:HG3  | 1:B:1009:LEU:CD2  | 2.41                     | 0.51              |
| 1:B:1147:ILE:HD11 | 1:B:1244:ILE:HD11 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2007:PHE:O    | 1:C:2008:HIS:HB2  | 2.10                     | 0.51              |
| 1:E:4209:GLN:C    | 1:E:4211:LEU:N    | 2.68                     | 0.51              |
| 1:B:1249:ALA:O    | 1:B:1253:LEU:HG   | 2.10                     | 0.51              |
| 1:A:227:GLU:N     | 1:D:3001:MET:HB2  | 2.26                     | 0.51              |
| 1:B:1098:ILE:HG12 | 1:B:1193:MET:O    | 2.10                     | 0.51              |
| 1:C:2054:ARG:HG2  | 1:C:2055:ALA:N    | 2.26                     | 0.51              |
| 1:E:4007:PHE:CG   | 1:E:4008:HIS:N    | 2.72                     | 0.51              |
| 1:A:6:VAL:HG13    | 1:A:7:PHE:N       | 2.26                     | 0.50              |
| 1:A:206:CYS:O     | 1:A:208:SER:N     | 2.44                     | 0.50              |
| 1:B:1115:ARG:NH2  | 1:B:1121:LEU:HD22 | 2.23                     | 0.50              |
| 1:B:1162:PHE:CZ   | 1:F:5008:HIS:HD2  | 2.29                     | 0.50              |
| 1:F:5113:SER:HA   | 1:F:5156:THR:O    | 2.11                     | 0.50              |
| 1:F:5142:GLU:O    | 1:F:5145:LYS:HB2  | 2.11                     | 0.50              |
| 1:B:1009:LEU:HD22 | 1:B:1047:HIS:HB3  | 1.93                     | 0.50              |
| 1:C:2104:VAL:CG2  | 1:C:2228:ILE:HG13 | 2.41                     | 0.50              |
| 1:E:4164:PRO:HB3  | 1:E:4171:THR:HB   | 1.93                     | 0.50              |
| 1:A:108:LEU:HD23  | 1:A:152:HIS:HB2   | 1.93                     | 0.50              |
| 1:C:2001:MET:HB3  | 1:E:4223:ARG:HD2  | 1.92                     | 0.50              |
| 1:E:4225:GLN:O    | 1:E:4227:GLU:HG3  | 2.11                     | 0.50              |
| 1:B:1076:ILE:HD13 | 1:F:5162:PHE:HE1  | 1.75                     | 0.50              |
| 1:C:2015:ASP:C    | 1:C:2017:GLN:H    | 2.20                     | 0.50              |
| 1:C:2036:ALA:C    | 1:C:2038:MET:H    | 2.20                     | 0.50              |
| 1:C:2240:HIS:HA   | 1:C:2243:LYS:HZ3  | 1.76                     | 0.50              |
| 1:F:5025:PRO:O    | 1:F:5066:SER:HA   | 2.12                     | 0.50              |
| 1:F:5110:THR:HG21 | 1:F:5156:THR:HB   | 1.94                     | 0.50              |
| 1:A:62:VAL:HG22   | 1:A:253:LEU:HD21  | 1.94                     | 0.50              |
| 1:A:126:LEU:HD21  | 1:E:4127:GLU:HG2  | 1.94                     | 0.50              |
| 1:D:3207:ALA:N    | 1:D:3211:LEU:HD13 | 2.26                     | 0.50              |
| 1:E:4091:ARG:NH2  | 1:E:4198:GLU:HG3  | 2.26                     | 0.50              |
| 1:A:167:GLU:CD    | 1:A:223:ARG:HD3   | 2.37                     | 0.50              |
| 1:B:1022:ALA:CB   | 1:B:1086:ILE:HG21 | 2.40                     | 0.50              |
| 1:C:2095:THR:HG21 | 1:C:2194:ASN:ND2  | 2.26                     | 0.50              |
| 1:E:4226:GLN:O    | 1:E:4227:GLU:HB3  | 2.12                     | 0.50              |
| 1:F:5087:ARG:CB   | 1:F:5211:LEU:HD13 | 2.42                     | 0.50              |
| 1:A:107:VAL:HA    | 1:A:217:ALA:O     | 2.12                     | 0.50              |
| 1:F:5024:VAL:HG22 | 1:F:5090:LEU:O    | 2.12                     | 0.50              |
| 1:C:2208:SER:O    | 1:C:2209:GLN:CB   | 2.60                     | 0.50              |
| 1:D:3226:GLN:HG3  | 1:D:3227:GLU:N    | 2.27                     | 0.50              |
| 1:E:4008:HIS:CE1  | 1:E:4076:ILE:HG21 | 2.47                     | 0.50              |
| 1:E:4223:ARG:HD3  | 1:E:4223:ARG:H    | 1.77                     | 0.50              |
| 1:F:5025:PRO:HB3  | 1:F:5092:ILE:HD12 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1118:GLY:HA3  | 1:F:5118:GLY:HA3  | 1.93                     | 0.49              |
| 1:D:3136:CYS:SG   | 1:D:3212:ARG:HA   | 2.52                     | 0.49              |
| 1:A:6:VAL:O       | 1:A:7:PHE:C       | 2.55                     | 0.49              |
| 1:B:1074:THR:O    | 1:B:1078:VAL:HG23 | 2.12                     | 0.49              |
| 1:D:3091:ARG:CB   | 1:D:3215:MET:HG3  | 2.39                     | 0.49              |
| 1:F:5057:LEU:HB3  | 1:F:5253:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:21:LEU:HD21   | 1:A:90:LEU:HD23   | 1.93                     | 0.49              |
| 1:F:5029:ASP:O    | 1:F:5031:VAL:N    | 2.46                     | 0.49              |
| 1:F:5096:GLY:HA2  | 1:F:5221:VAL:O    | 2.12                     | 0.49              |
| 1:C:2001:MET:N    | 1:E:4226:GLN:HB2  | 2.27                     | 0.49              |
| 1:C:2009:LEU:HB3  | 1:C:2011:LEU:HD23 | 1.93                     | 0.49              |
| 1:C:2149:ALA:O    | 1:C:2151:THR:N    | 2.45                     | 0.49              |
| 1:C:2152:HIS:HB3  | 1:C:2193:MET:HE1  | 1.94                     | 0.49              |
| 1:E:4102:ILE:CG2  | 1:E:4108:LEU:HD21 | 2.41                     | 0.49              |
| 1:A:140:LEU:HD12  | 1:A:248:ALA:CB    | 2.43                     | 0.49              |
| 1:A:206:CYS:C     | 1:A:211:LEU:HA    | 2.38                     | 0.49              |
| 1:A:233:THR:HG23  | 1:A:236:GLN:OE1   | 2.13                     | 0.49              |
| 1:C:2001:MET:HG2  | 1:E:4221:VAL:HG21 | 1.92                     | 0.49              |
| 1:C:2062:VAL:CG1  | 1:C:2253:LEU:HD11 | 2.42                     | 0.49              |
| 1:C:2062:VAL:HG13 | 1:C:2253:LEU:HD11 | 1.94                     | 0.49              |
| 1:D:3095:THR:O    | 1:D:3219:VAL:HA   | 2.12                     | 0.49              |
| 1:D:3230:ASN:HD22 | 1:D:3233:THR:HG23 | 1.77                     | 0.49              |
| 1:B:1167:GLU:HG2  | 1:B:1168:ARG:N    | 2.27                     | 0.49              |
| 1:C:2017:GLN:CD   | 1:C:2018:GLY:H    | 2.19                     | 0.49              |
| 1:C:2206:CYS:SG   | 1:C:2213:ALA:HB2  | 2.52                     | 0.49              |
| 1:C:2207:ALA:HA   | 1:C:2211:LEU:HD22 | 1.93                     | 0.49              |
| 1:C:2240:HIS:O    | 1:C:2244:ILE:HG13 | 2.13                     | 0.49              |
| 1:D:3114:VAL:HB   | 1:D:3157:ALA:HA   | 1.94                     | 0.49              |
| 1:D:3216:VAL:HG11 | 1:D:3245:VAL:HG22 | 1.94                     | 0.49              |
| 1:E:4028:PRO:HB3  | 1:E:4051:THR:CG2  | 2.43                     | 0.49              |
| 1:A:38:MET:CE     | 1:A:246:VAL:HG22  | 2.42                     | 0.49              |
| 1:A:140:LEU:HD12  | 1:A:248:ALA:HB1   | 1.95                     | 0.49              |
| 1:B:1001:MET:SD   | 1:B:1002:SER:N    | 2.86                     | 0.49              |
| 1:F:5008:HIS:CE1  | 1:F:5076:ILE:HG21 | 2.48                     | 0.49              |
| 1:D:3228:ILE:HG12 | 1:D:3229:PRO:CA   | 2.12                     | 0.49              |
| 1:E:4205:MET:O    | 1:E:4206:CYS:CB   | 2.60                     | 0.49              |
| 1:F:5163:TYR:HD1  | 1:F:5163:TYR:N    | 2.06                     | 0.49              |
| 1:C:2104:VAL:HG21 | 1:C:2228:ILE:HG13 | 1.93                     | 0.49              |
| 1:D:3038:MET:CB   | 1:D:3055:ALA:HB1  | 2.43                     | 0.49              |
| 1:D:3041:PRO:HA   | 1:D:3054:ARG:O    | 2.13                     | 0.49              |
| 1:F:5115:ARG:HH12 | 1:F:5128:PHE:HB3  | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:11:LEU:HD11   | 1:A:16:LEU:CD2    | 2.43                     | 0.49              |
| 1:A:101:HIS:H     | 1:A:101:HIS:CD2   | 2.31                     | 0.49              |
| 1:A:140:LEU:CD1   | 1:A:140:LEU:N     | 2.76                     | 0.49              |
| 1:B:1098:ILE:N    | 1:B:1193:MET:O    | 2.39                     | 0.49              |
| 1:C:2007:PHE:O    | 1:C:2008:HIS:CB   | 2.61                     | 0.49              |
| 1:F:5037:LEU:HD11 | 1:F:5242:VAL:CG1  | 2.43                     | 0.49              |
| 1:A:165:GLY:HA2   | 1:A:183:SER:OG    | 2.13                     | 0.48              |
| 1:A:211:LEU:O     | 1:A:212:ARG:HB2   | 2.13                     | 0.48              |
| 1:B:1022:ALA:HA   | 1:B:1063:ILE:O    | 2.12                     | 0.48              |
| 1:C:2190:MET:HE1  | 1:F:5124:ALA:HA   | 1.95                     | 0.48              |
| 1:E:4050:PHE:HE1  | 1:E:4067:THR:O    | 1.95                     | 0.48              |
| 1:E:4211:LEU:O    | 1:E:4212:ARG:HG2  | 2.12                     | 0.48              |
| 1:F:5177:VAL:HG21 | 1:F:5179:HIS:NE2  | 2.28                     | 0.48              |
| 1:B:1178:ARG:HD3  | 1:F:5124:ALA:C    | 2.38                     | 0.48              |
| 1:B:1206:CYS:O    | 1:B:1211:LEU:HA   | 2.13                     | 0.48              |
| 1:C:2108:LEU:HD12 | 1:C:2217:ALA:HB3  | 1.94                     | 0.48              |
| 1:C:2187:TRP:CH2  | 1:F:5125:PRO:HG2  | 2.48                     | 0.48              |
| 1:E:4093:GLY:O    | 1:E:4217:ALA:HA   | 2.13                     | 0.48              |
| 1:F:5107:VAL:O    | 1:F:5108:LEU:HD23 | 2.13                     | 0.48              |
| 1:A:73:SER:HA     | 1:A:76:ILE:HD12   | 1.95                     | 0.48              |
| 1:A:226:GLN:C     | 1:D:3001:MET:HB2  | 2.39                     | 0.48              |
| 1:D:3088:THR:HB   | 1:D:3212:ARG:HB3  | 1.94                     | 0.48              |
| 1:C:2001:MET:SD   | 1:C:2001:MET:O    | 2.71                     | 0.48              |
| 1:C:2125:PRO:O    | 1:C:2127:GLU:N    | 2.46                     | 0.48              |
| 1:C:2206:CYS:HB3  | 1:C:2211:LEU:HD12 | 1.94                     | 0.48              |
| 1:C:2207:ALA:CA   | 1:C:2211:LEU:HD13 | 2.43                     | 0.48              |
| 1:E:4235:LYS:CG   | 1:E:4236:GLN:N    | 2.75                     | 0.48              |
| 1:C:2011:LEU:HD12 | 1:C:2016:LEU:HD22 | 1.95                     | 0.48              |
| 1:C:2043:LYS:NZ   | 1:C:2045:ALA:O    | 2.44                     | 0.48              |
| 1:C:2190:MET:HE2  | 1:F:5123:PHE:O    | 2.13                     | 0.48              |
| 1:C:2236:GLN:O    | 1:C:2240:HIS:CD2  | 2.67                     | 0.48              |
| 1:D:3210:GLY:O    | 1:D:3211:LEU:O    | 2.31                     | 0.48              |
| 1:B:1018:GLY:O    | 1:B:1061:PRO:HG2  | 2.14                     | 0.48              |
| 1:C:2206:CYS:C    | 1:C:2211:LEU:HB2  | 2.39                     | 0.48              |
| 1:E:4022:ALA:HA   | 1:E:4063:ILE:O    | 2.13                     | 0.48              |
| 1:E:4034:ILE:HD11 | 1:E:4092:ILE:HD13 | 1.96                     | 0.48              |
| 1:D:3104:VAL:HA   | 1:D:3219:VAL:HG12 | 1.96                     | 0.48              |
| 1:D:3228:ILE:HD11 | 1:D:3234:MET:HE2  | 1.94                     | 0.48              |
| 1:E:4235:LYS:HG3  | 1:E:4236:GLN:N    | 2.28                     | 0.48              |
| 1:C:2228:ILE:HD12 | 1:C:2229:PRO:HA   | 1.96                     | 0.48              |
| 1:F:5001:MET:O    | 1:F:5007:PHE:CG   | 2.67                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:5133:ASP:O    | 1:F:5137:THR:OG1  | 2.23                     | 0.48              |
| 1:A:165:GLY:HA2   | 1:A:180:PHE:O     | 2.14                     | 0.47              |
| 1:A:235:LYS:H     | 1:A:235:LYS:HD2   | 1.79                     | 0.47              |
| 1:D:3038:MET:SD   | 1:D:3062:VAL:HG23 | 2.53                     | 0.47              |
| 1:D:3108:LEU:HD22 | 1:D:3152:HIS:HB2  | 1.96                     | 0.47              |
| 1:E:4016:LEU:HD12 | 1:E:4063:ILE:HD13 | 1.96                     | 0.47              |
| 1:E:4242:VAL:O    | 1:E:4246:VAL:HG23 | 2.14                     | 0.47              |
| 1:F:5116:LEU:O    | 1:F:5159:SER:HA   | 2.13                     | 0.47              |
| 1:B:1047:HIS:O    | 1:B:1049:GLU:N    | 2.48                     | 0.47              |
| 1:D:3232:GLU:O    | 1:D:3236:GLN:N    | 2.44                     | 0.47              |
| 1:F:5193:MET:O    | 1:F:5194:ASN:OD1  | 2.32                     | 0.47              |
| 1:A:206:CYS:O     | 1:A:211:LEU:HB3   | 2.15                     | 0.47              |
| 1:F:5013:LYS:CA   | 1:F:5084:LEU:HD22 | 2.45                     | 0.47              |
| 1:A:106:ASP:OD1   | 1:A:150:THR:HB    | 2.13                     | 0.47              |
| 1:A:125:PRO:HB2   | 1:A:127:GLU:CD    | 2.39                     | 0.47              |
| 1:B:1163:TYR:HB3  | 1:B:1223:ARG:HH22 | 1.78                     | 0.47              |
| 1:B:1212:ARG:HH12 | 1:B:1252:LEU:HG   | 1.79                     | 0.47              |
| 1:F:5158:SER:HB2  | 1:F:5199:SER:OG   | 2.14                     | 0.47              |
| 1:B:1166:GLN:HB3  | 1:B:1177:VAL:HG21 | 1.96                     | 0.47              |
| 1:C:2091:ARG:HB3  | 1:C:2215:MET:HG3  | 1.97                     | 0.47              |
| 1:C:2138:THR:O    | 1:C:2142:GLU:HG2  | 2.15                     | 0.47              |
| 1:D:3108:LEU:HD13 | 1:D:3193:MET:HB3  | 1.96                     | 0.47              |
| 1:D:3196:GLU:HG3  | 1:D:3199:SER:OG   | 2.14                     | 0.47              |
| 1:D:3211:LEU:CG   | 1:D:3212:ARG:H    | 2.13                     | 0.47              |
| 1:E:4010:GLY:O    | 1:E:4011:LEU:HD22 | 2.15                     | 0.47              |
| 1:E:4039:ASP:O    | 1:E:4056:GLU:HG2  | 2.13                     | 0.47              |
| 1:E:4228:ILE:O    | 1:E:4230:ASN:N    | 2.48                     | 0.47              |
| 1:A:21:LEU:HD23   | 1:A:22:ALA:N      | 2.30                     | 0.47              |
| 1:A:141:VAL:HG11  | 1:E:4134:PHE:HE1  | 1.78                     | 0.47              |
| 1:F:5175:ARG:O    | 1:F:5176:VAL:HG23 | 2.14                     | 0.47              |
| 1:F:5005:ASP:O    | 1:F:5006:VAL:HB   | 2.15                     | 0.47              |
| 1:F:5178:ARG:HA   | 1:F:5181:LYS:HB3  | 1.97                     | 0.47              |
| 1:C:2091:ARG:NH1  | 1:C:2198:GLU:HB2  | 2.29                     | 0.47              |
| 1:E:4046:SER:OG   | 1:E:4047:HIS:N    | 2.47                     | 0.47              |
| 1:A:51:THR:H      | 1:A:66:SER:HG     | 1.62                     | 0.47              |
| 1:E:4016:LEU:HD12 | 1:E:4063:ILE:HG21 | 1.96                     | 0.47              |
| 1:A:20:THR:HA     | 1:A:86:ILE:HA     | 1.96                     | 0.47              |
| 1:A:22:ALA:HB2    | 1:A:86:ILE:HG12   | 1.96                     | 0.47              |
| 1:A:163:TYR:CD2   | 1:A:223:ARG:NH1   | 2.83                     | 0.47              |
| 1:B:1209:GLN:C    | 1:B:1211:LEU:N    | 2.73                     | 0.47              |
| 1:E:4037:LEU:O    | 1:E:4038:MET:HG3  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:9:LEU:HD22    | 1:A:9:LEU:H       | 1.80                     | 0.46              |
| 1:B:1167:GLU:CG   | 1:B:1168:ARG:N    | 2.78                     | 0.46              |
| 1:E:4178:ARG:HG3  | 1:E:4179:HIS:N    | 2.29                     | 0.46              |
| 1:A:134:PHE:CE1   | 1:E:4141:VAL:HG11 | 2.50                     | 0.46              |
| 1:C:2168:ARG:O    | 1:C:2171:THR:HG23 | 2.15                     | 0.46              |
| 1:D:3032:GLU:HG3  | 1:D:3033:LYS:HD2  | 1.97                     | 0.46              |
| 1:D:3092:ILE:HB   | 1:D:3245:VAL:HG21 | 1.96                     | 0.46              |
| 1:E:4024:VAL:O    | 1:E:4091:ARG:HG3  | 2.14                     | 0.46              |
| 1:E:4094:THR:HB   | 1:E:4220:ILE:HG21 | 1.97                     | 0.46              |
| 1:A:115:ARG:C     | 1:A:116:LEU:HD23  | 2.39                     | 0.46              |
| 1:B:1009:LEU:HD22 | 1:B:1047:HIS:CB   | 2.45                     | 0.46              |
| 1:B:1182:GLY:O    | 1:B:1185:GLU:HG2  | 2.15                     | 0.46              |
| 1:E:4100:PRO:HB3  | 1:E:4224:THR:HB   | 1.96                     | 0.46              |
| 1:F:5211:LEU:HB3  | 1:F:5212:ARG:H    | 1.67                     | 0.46              |
| 1:A:167:GLU:OE2   | 1:A:223:ARG:NH2   | 2.48                     | 0.46              |
| 1:B:1230:ASN:O    | 1:B:1231:ALA:HB3  | 2.15                     | 0.46              |
| 1:F:5050:PHE:HA   | 1:F:5066:SER:OG   | 2.14                     | 0.46              |
| 1:C:2196:GLU:HG2  | 1:C:2197:MET:H    | 1.80                     | 0.46              |
| 1:F:5056:GLU:HA   | 1:F:5060:LYS:O    | 2.15                     | 0.46              |
| 1:F:5107:VAL:C    | 1:F:5108:LEU:HD23 | 2.40                     | 0.46              |
| 1:A:38:MET:HE1    | 1:A:246:VAL:HG22  | 1.96                     | 0.46              |
| 1:D:3016:LEU:O    | 1:D:3017:GLN:HG2  | 2.16                     | 0.46              |
| 1:F:5138:THR:O    | 1:F:5141:VAL:HG22 | 2.15                     | 0.46              |
| 1:A:2:SER:HA      | 1:A:5:ASP:OD1     | 2.16                     | 0.46              |
| 1:A:38:MET:HG3    | 1:A:57:LEU:HD13   | 1.98                     | 0.46              |
| 1:D:3158:SER:HB3  | 1:D:3200:ALA:HB2  | 1.98                     | 0.46              |
| 1:E:4194:ASN:N    | 1:E:4194:ASN:HD22 | 2.14                     | 0.46              |
| 1:F:5146:SER:C    | 1:F:5147:ILE:HD13 | 2.41                     | 0.46              |
| 1:A:82:ALA:HA     | 1:A:86:ILE:O      | 2.16                     | 0.46              |
| 1:B:1077:ALA:O    | 1:B:1078:VAL:CG2  | 2.64                     | 0.46              |
| 1:B:1246:VAL:O    | 1:B:1250:ARG:HB2  | 2.15                     | 0.46              |
| 1:C:2001:MET:HA   | 1:E:4221:VAL:HG22 | 1.97                     | 0.46              |
| 1:F:5048:ARG:O    | 1:F:5050:PHE:N    | 2.44                     | 0.46              |
| 1:F:5073:SER:O    | 1:F:5074:THR:C    | 2.59                     | 0.46              |
| 1:F:5206:CYS:HA   | 1:F:5210:GLY:HA3  | 1.98                     | 0.46              |
| 1:A:163:TYR:N     | 1:A:163:TYR:CD1   | 2.84                     | 0.46              |
| 1:B:1015:ASP:O    | 1:B:1044:LEU:HD21 | 2.16                     | 0.46              |
| 1:B:1067:THR:O    | 1:B:1073:SER:HB2  | 2.15                     | 0.46              |
| 1:B:1099:GLN:HB2  | 1:B:1102:ILE:HG13 | 1.97                     | 0.46              |
| 1:B:1226:GLN:HE21 | 1:B:1226:GLN:CA   | 2.28                     | 0.46              |
| 1:B:1024:VAL:HG23 | 1:B:1024:VAL:O    | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1104:VAL:HG13 | 1:B:1219:VAL:O    | 2.15                     | 0.45              |
| 1:B:1166:GLN:O    | 1:B:1167:GLU:HB3  | 2.16                     | 0.45              |
| 1:C:2163:TYR:HE1  | 1:C:2197:MET:HG3  | 1.81                     | 0.45              |
| 1:C:2209:GLN:O    | 1:C:2211:LEU:N    | 2.48                     | 0.45              |
| 1:A:1:MET:H1      | 1:D:3228:ILE:HG22 | 1.81                     | 0.45              |
| 1:A:224:THR:O     | 1:A:225:GLN:CD    | 2.59                     | 0.45              |
| 1:B:1079:GLU:O    | 1:B:1083:GLN:HG3  | 2.16                     | 0.45              |
| 1:C:2165:GLY:HA2  | 1:C:2180:PHE:O    | 2.16                     | 0.45              |
| 1:D:3119:ALA:O    | 1:D:3122:HIS:HB2  | 2.17                     | 0.45              |
| 1:F:5094:THR:HB   | 1:F:5220:ILE:HD13 | 1.97                     | 0.45              |
| 1:B:1102:ILE:O    | 1:B:1222:ASN:ND2  | 2.49                     | 0.45              |
| 1:B:1161:THR:OG1  | 1:F:5122:HIS:CD2  | 2.68                     | 0.45              |
| 1:D:3009:LEU:HD12 | 1:D:3047:HIS:CB   | 2.41                     | 0.45              |
| 1:D:3099:GLN:HE22 | 1:D:3188:GLN:HA   | 1.81                     | 0.45              |
| 1:A:208:SER:HA    | 1:E:4190:MET:O    | 2.16                     | 0.45              |
| 1:C:2065:CYS:SG   | 1:C:2066:SER:N    | 2.90                     | 0.45              |
| 1:C:2077:ALA:O    | 1:C:2081:LEU:HB2  | 2.17                     | 0.45              |
| 1:F:5240:HIS:HD2  | 1:F:5243:LYS:NZ   | 2.14                     | 0.45              |
| 1:A:115:ARG:NH1   | 1:A:128:PHE:O     | 2.50                     | 0.45              |
| 1:C:2161:THR:O    | 1:C:2163:TYR:N    | 2.50                     | 0.45              |
| 1:C:2072:PRO:O    | 1:C:2076:ILE:HG13 | 2.17                     | 0.45              |
| 1:C:2211:LEU:CG   | 1:C:2212:ARG:N    | 2.68                     | 0.45              |
| 1:E:4104:VAL:CG1  | 1:E:4233:THR:HG21 | 2.47                     | 0.45              |
| 1:F:5171:THR:HG23 | 1:F:5176:VAL:HG21 | 1.99                     | 0.45              |
| 1:B:1095:THR:HG21 | 1:B:1194:ASN:HD22 | 1.81                     | 0.45              |
| 1:C:2122:HIS:HA   | 1:E:4177:VAL:HG23 | 1.98                     | 0.45              |
| 1:E:4163:TYR:O    | 1:E:4169:TYR:HB3  | 2.16                     | 0.45              |
| 1:F:5187:TRP:HA   | 1:F:5187:TRP:CE3  | 2.52                     | 0.45              |
| 1:F:5236:GLN:HA   | 1:F:5239:SER:CB   | 2.47                     | 0.45              |
| 1:A:180:PHE:CE1   | 1:D:3122:HIS:HA   | 2.52                     | 0.45              |
| 1:A:206:CYS:C     | 1:A:211:LEU:HB3   | 2.41                     | 0.45              |
| 1:F:5016:LEU:CD1  | 1:F:5084:LEU:HB3  | 2.47                     | 0.45              |
| 1:B:1150:THR:HG22 | 1:B:1150:THR:O    | 2.17                     | 0.45              |
| 1:E:4113:SER:OG   | 1:E:4203:LEU:HD23 | 2.16                     | 0.45              |
| 1:F:5031:VAL:HG13 | 1:F:5064:VAL:CG1  | 2.47                     | 0.45              |
| 1:F:5089:PHE:O    | 1:F:5213:ALA:HA   | 2.17                     | 0.45              |
| 1:F:5123:PHE:CE1  | 1:F:5205:MET:HG3  | 2.51                     | 0.45              |
| 1:C:2022:ALA:CB   | 1:C:2086:ILE:HG21 | 2.47                     | 0.45              |
| 1:D:3183:SER:HA   | 1:D:3187:TRP:CD1  | 2.46                     | 0.45              |
| 1:E:4195:TYR:O    | 1:E:4196:GLU:HG2  | 2.17                     | 0.45              |
| 1:F:5143:ALA:C    | 1:F:5145:LYS:H    | 2.23                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2095:THR:HG21 | 1:C:2194:ASN:HD22 | 1.82                     | 0.44              |
| 1:C:2133:ASP:CB   | 1:C:2212:ARG:HA   | 2.47                     | 0.44              |
| 1:D:3178:ARG:HG3  | 1:D:3179:HIS:CE1  | 2.51                     | 0.44              |
| 1:D:3237:THR:HA   | 1:D:3240:HIS:HB2  | 1.99                     | 0.44              |
| 1:E:4091:ARG:HB3  | 1:E:4215:MET:HG3  | 1.98                     | 0.44              |
| 1:E:4212:ARG:HD2  | 1:E:4212:ARG:HA   | 1.72                     | 0.44              |
| 1:A:44:LEU:HD11   | 1:A:54:ARG:HB2    | 2.00                     | 0.44              |
| 1:A:92:ILE:HG13   | 1:A:216:VAL:HB    | 1.99                     | 0.44              |
| 1:C:2169:TYR:C    | 1:C:2171:THR:N    | 2.74                     | 0.44              |
| 1:C:2240:HIS:CD2  | 1:C:2240:HIS:H    | 2.35                     | 0.44              |
| 1:D:3154:GLY:HA3  | 1:D:3193:MET:SD   | 2.57                     | 0.44              |
| 1:E:4010:GLY:O    | 1:E:4045:ALA:HB3  | 2.17                     | 0.44              |
| 1:A:141:VAL:O     | 1:A:145:LYS:HG2   | 2.17                     | 0.44              |
| 1:C:2205:MET:SD   | 1:C:2206:CYS:N    | 2.91                     | 0.44              |
| 1:E:4051:THR:O    | 1:E:4065:CYS:SG   | 2.74                     | 0.44              |
| 1:A:170:ASP:HB2   | 1:A:171:THR:H     | 1.58                     | 0.44              |
| 1:E:4127:GLU:H    | 1:E:4127:GLU:HG3  | 1.59                     | 0.44              |
| 1:B:1038:MET:HB3  | 1:B:1039:ASP:H    | 1.45                     | 0.44              |
| 1:B:1145:LYS:HA   | 1:B:1145:LYS:HD3  | 1.69                     | 0.44              |
| 1:B:1190:MET:HE3  | 1:B:1190:MET:HB2  | 1.86                     | 0.44              |
| 1:B:1225:GLN:HA   | 1:B:1225:GLN:OE1  | 2.17                     | 0.44              |
| 1:C:2157:ALA:O    | 1:C:2195:TYR:HA   | 2.17                     | 0.44              |
| 1:A:126:LEU:O     | 1:A:126:LEU:HG    | 2.16                     | 0.44              |
| 1:B:1054:ARG:O    | 1:B:1054:ARG:HG2  | 2.17                     | 0.44              |
| 1:B:1179:HIS:C    | 1:B:1181:LYS:H    | 2.25                     | 0.44              |
| 1:C:2001:MET:HB3  | 1:E:4223:ARG:HB3  | 1.99                     | 0.44              |
| 1:D:3084:LEU:HD23 | 1:D:3084:LEU:HA   | 1.74                     | 0.44              |
| 1:E:4211:LEU:O    | 1:E:4212:ARG:CG   | 2.66                     | 0.44              |
| 1:F:5031:VAL:HG13 | 1:F:5064:VAL:HG12 | 1.99                     | 0.44              |
| 1:F:5140:LEU:HD11 | 1:F:5216:VAL:HG12 | 1.99                     | 0.44              |
| 1:F:5243:LYS:HE2  | 1:F:5243:LYS:HB2  | 1.75                     | 0.44              |
| 1:B:1022:ALA:C    | 1:B:1023:ILE:HD12 | 2.43                     | 0.44              |
| 1:B:1040:LYS:N    | 1:B:1041:PRO:CD   | 2.80                     | 0.44              |
| 1:B:1235:LYS:HD3  | 1:B:1235:LYS:N    | 2.25                     | 0.44              |
| 1:C:2226:GLN:O    | 1:C:2228:ILE:N    | 2.50                     | 0.44              |
| 1:E:4106:ASP:HB3  | 1:E:4152:HIS:CD2  | 2.53                     | 0.44              |
| 1:E:4226:GLN:O    | 1:E:4227:GLU:CB   | 2.64                     | 0.44              |
| 1:A:123:PHE:CD2   | 1:A:205:MET:HG2   | 2.52                     | 0.44              |
| 1:B:1077:ALA:C    | 1:B:1078:VAL:HG23 | 2.42                     | 0.44              |
| 1:B:1220:ILE:HG12 | 1:B:1221:VAL:HG22 | 2.00                     | 0.44              |
| 1:E:4205:MET:O    | 1:E:4206:CYS:HB2  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:5166:GLN:O    | 1:F:5184:MET:HE1  | 2.17                     | 0.44              |
| 1:F:5184:MET:HA   | 1:F:5195:TYR:OH   | 2.18                     | 0.44              |
| 1:F:5199:SER:O    | 1:F:5203:LEU:HG   | 2.18                     | 0.44              |
| 1:A:72:PRO:HD3    | 1:D:3072:PRO:HG2  | 2.00                     | 0.44              |
| 1:C:2092:ILE:HA   | 1:C:2216:VAL:O    | 2.18                     | 0.44              |
| 1:D:3233:THR:O    | 1:D:3237:THR:N    | 2.49                     | 0.44              |
| 1:F:5093:GLY:O    | 1:F:5217:ALA:HA   | 2.18                     | 0.44              |
| 1:F:5096:GLY:O    | 1:F:5194:ASN:HB2  | 2.17                     | 0.44              |
| 1:B:1001:MET:SD   | 1:B:1009:LEU:HD23 | 2.58                     | 0.43              |
| 1:C:2048:ARG:C    | 1:C:2050:PHE:H    | 2.26                     | 0.43              |
| 1:C:2122:HIS:ND1  | 1:E:4161:THR:OG1  | 2.51                     | 0.43              |
| 1:A:30:ARG:HH11   | 1:A:238:GLU:CD    | 2.26                     | 0.43              |
| 1:D:3092:ILE:HA   | 1:D:3216:VAL:O    | 2.17                     | 0.43              |
| 1:D:3228:ILE:HD11 | 1:D:3234:MET:CE   | 2.48                     | 0.43              |
| 1:E:4096:GLY:O    | 1:E:4194:ASN:HB2  | 2.18                     | 0.43              |
| 1:C:2009:LEU:CD2  | 1:C:2050:PHE:HB3  | 2.48                     | 0.43              |
| 1:C:2012:THR:O    | 1:C:2013:LYS:CB   | 2.67                     | 0.43              |
| 1:C:2173:SER:OG   | 1:C:2176:VAL:CA   | 2.62                     | 0.43              |
| 1:E:4091:ARG:CZ   | 1:E:4198:GLU:HG3  | 2.49                     | 0.43              |
| 1:F:5140:LEU:CD1  | 1:F:5216:VAL:HB   | 2.46                     | 0.43              |
| 1:A:8:HIS:CD2     | 1:A:9:LEU:HD22    | 2.54                     | 0.43              |
| 1:A:122:HIS:O     | 1:D:3176:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:1216:VAL:HG22 | 1:B:1217:ALA:H    | 1.82                     | 0.43              |
| 1:B:1239:SER:O    | 1:B:1243:LYS:HG3  | 2.18                     | 0.43              |
| 1:C:2016:LEU:HD23 | 1:C:2016:LEU:N    | 2.26                     | 0.43              |
| 1:C:2177:VAL:CB   | 1:C:2181:LYS:HD3  | 2.47                     | 0.43              |
| 1:E:4017:GLN:O    | 1:E:4061:PRO:HG3  | 2.18                     | 0.43              |
| 1:E:4095:THR:HG22 | 1:E:4217:ALA:HB1  | 1.99                     | 0.43              |
| 1:C:2167:GLU:O    | 1:C:2168:ARG:HB2  | 2.19                     | 0.43              |
| 1:C:2209:GLN:O    | 1:C:2209:GLN:HG3  | 2.19                     | 0.43              |
| 1:D:3092:ILE:HD12 | 1:D:3093:GLY:N    | 2.33                     | 0.43              |
| 1:F:5144:ALA:C    | 1:F:5145:LYS:HE3  | 2.43                     | 0.43              |
| 1:A:146:SER:O     | 1:A:147:ILE:HG12  | 2.19                     | 0.43              |
| 1:A:163:TYR:HA    | 1:A:164:PRO:HD3   | 1.86                     | 0.43              |
| 1:A:178:ARG:C     | 1:A:180:PHE:H     | 2.25                     | 0.43              |
| 1:D:3071:GLY:N    | 1:D:3072:PRO:CD   | 2.81                     | 0.43              |
| 1:D:3099:GLN:HG2  | 1:D:3192:VAL:O    | 2.18                     | 0.43              |
| 1:D:3206:CYS:HB3  | 1:D:3211:LEU:HD12 | 2.00                     | 0.43              |
| 1:F:5178:ARG:HA   | 1:F:5181:LYS:CB   | 2.49                     | 0.43              |
| 1:A:102:ILE:O     | 1:A:106:ASP:OD2   | 2.37                     | 0.43              |
| 1:A:196:GLU:CG    | 1:A:197:MET:N     | 2.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2015:ASP:O    | 1:C:2017:GLN:N    | 2.52                     | 0.43              |
| 1:E:4025:PRO:HB3  | 1:E:4030:ARG:CD   | 2.49                     | 0.43              |
| 1:F:5015:ASP:HB3  | 1:F:5044:LEU:HD13 | 2.01                     | 0.43              |
| 1:F:5228:ILE:CG2  | 1:F:5229:PRO:HA   | 2.49                     | 0.43              |
| 1:C:2015:ASP:C    | 1:C:2017:GLN:N    | 2.77                     | 0.43              |
| 1:C:2076:ILE:HA   | 1:C:2079:GLU:OE2  | 2.19                     | 0.43              |
| 1:A:147:ILE:O     | 1:A:147:ILE:CG2   | 2.65                     | 0.43              |
| 1:B:1042:VAL:HG22 | 1:B:1043:LYS:O    | 2.18                     | 0.43              |
| 1:E:4161:THR:CG2  | 1:E:4164:PRO:HG3  | 2.49                     | 0.43              |
| 1:F:5013:LYS:HD2  | 1:F:5084:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:2:SER:C       | 1:A:4:SER:N       | 2.77                     | 0.43              |
| 1:A:169:TYR:O     | 1:A:170:ASP:CB    | 2.67                     | 0.43              |
| 1:C:2009:LEU:HD23 | 1:C:2050:PHE:CD1  | 2.53                     | 0.43              |
| 1:E:4063:ILE:HD11 | 1:E:4081:LEU:HD22 | 2.00                     | 0.43              |
| 1:F:5147:ILE:HD13 | 1:F:5147:ILE:N    | 2.34                     | 0.43              |
| 1:A:38:MET:CG     | 1:A:57:LEU:HD13   | 2.49                     | 0.42              |
| 1:B:1226:GLN:HA   | 1:B:1226:GLN:NE2  | 2.31                     | 0.42              |
| 1:F:5021:LEU:HD12 | 1:F:5088:THR:HB   | 1.99                     | 0.42              |
| 1:B:1029:ASP:O    | 1:B:1032:GLU:HG2  | 2.19                     | 0.42              |
| 1:B:1201:THR:O    | 1:B:1205:MET:HE2  | 2.19                     | 0.42              |
| 1:D:3009:LEU:HD12 | 1:D:3047:HIS:CG   | 2.54                     | 0.42              |
| 1:E:4107:VAL:HG11 | 1:E:4244:ILE:HD13 | 2.01                     | 0.42              |
| 1:F:5203:LEU:N    | 1:F:5203:LEU:HD23 | 2.33                     | 0.42              |
| 1:A:57:LEU:CD2    | 1:A:250:ARG:HB3   | 2.49                     | 0.42              |
| 1:A:116:LEU:HB2   | 1:A:159:SER:HA    | 2.01                     | 0.42              |
| 1:B:1001:MET:O    | 1:B:1002:SER:HB2  | 2.18                     | 0.42              |
| 1:C:2176:VAL:HG23 | 1:C:2177:VAL:O    | 2.20                     | 0.42              |
| 1:D:3167:GLU:HG3  | 1:D:3169:TYR:CB   | 2.50                     | 0.42              |
| 1:E:4114:VAL:HG12 | 1:E:4116:LEU:HG   | 2.01                     | 0.42              |
| 1:A:112:ALA:HB2   | 1:E:4131:VAL:HG11 | 2.00                     | 0.42              |
| 1:B:1209:GLN:OE1  | 1:F:5174:GLY:HA3  | 2.19                     | 0.42              |
| 1:C:2060:LYS:HD2  | 1:C:2253:LEU:HB3  | 2.02                     | 0.42              |
| 1:D:3211:LEU:CG   | 1:D:3212:ARG:N    | 2.78                     | 0.42              |
| 1:B:1050:PHE:CE2  | 1:B:1077:ALA:HB2  | 2.54                     | 0.42              |
| 1:C:2178:ARG:HB3  | 1:C:2179:HIS:H    | 1.53                     | 0.42              |
| 1:C:2226:GLN:C    | 1:C:2228:ILE:N    | 2.77                     | 0.42              |
| 1:E:4232:GLU:O    | 1:E:4232:GLU:HG3  | 2.19                     | 0.42              |
| 1:F:5127:GLU:H    | 1:F:5127:GLU:CD   | 2.27                     | 0.42              |
| 1:B:1008:HIS:CD2  | 1:B:1076:ILE:CG2  | 3.01                     | 0.42              |
| 1:C:2040:LYS:N    | 1:C:2041:PRO:CD   | 2.83                     | 0.42              |
| 1:C:2196:GLU:HG2  | 1:C:2197:MET:N    | 2.35                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:2228:ILE:HA   | 1:C:2229:PRO:HA  | 1.62                     | 0.42              |
| 1:D:3114:VAL:HG12 | 1:D:3116:LEU:HG  | 2.01                     | 0.42              |
| 1:D:3161:THR:CG2  | 1:D:3162:PHE:H   | 2.21                     | 0.42              |
| 1:E:4184:MET:HE3  | 1:E:4185:GLU:HG2 | 2.01                     | 0.42              |
| 1:F:5079:GLU:O    | 1:F:5083:GLN:HG3 | 2.20                     | 0.42              |
| 1:F:5167:GLU:C    | 1:F:5169:TYR:H   | 2.27                     | 0.42              |
| 1:B:1166:GLN:HG3  | 1:B:1167:GLU:N   | 2.34                     | 0.42              |
| 1:B:1216:VAL:HG22 | 1:B:1217:ALA:N   | 2.35                     | 0.42              |
| 1:C:2113:SER:HA   | 1:C:2156:THR:O   | 2.20                     | 0.42              |
| 1:C:2134:PHE:HZ   | 1:F:5138:THR:HA  | 1.84                     | 0.42              |
| 1:D:3060:LYS:HA   | 1:D:3061:PRO:HD2 | 1.85                     | 0.42              |
| 1:F:5003:LYS:N    | 1:F:5007:PHE:CD1 | 2.87                     | 0.42              |
| 1:A:211:LEU:O     | 1:A:212:ARG:O    | 2.38                     | 0.42              |
| 1:B:1030:ARG:O    | 1:B:1031:VAL:C   | 2.62                     | 0.42              |
| 1:D:3011:LEU:HD12 | 1:D:3011:LEU:N   | 2.35                     | 0.42              |
| 1:A:9:LEU:HD23    | 1:A:76:ILE:HG21  | 2.01                     | 0.42              |
| 1:C:2180:PHE:CE1  | 1:E:4122:HIS:HA  | 2.54                     | 0.42              |
| 1:D:3013:LYS:O    | 1:D:3016:LEU:HB2 | 2.20                     | 0.42              |
| 1:D:3167:GLU:H    | 1:D:3167:GLU:HG2 | 1.74                     | 0.42              |
| 1:E:4104:VAL:HG13 | 1:E:4219:VAL:O   | 2.20                     | 0.42              |
| 1:F:5026:GLY:O    | 1:F:5066:SER:HB2 | 2.19                     | 0.42              |
| 1:A:125:PRO:HB2   | 1:A:127:GLU:OE1  | 2.20                     | 0.42              |
| 1:C:2179:HIS:CD2  | 1:C:2179:HIS:N   | 2.81                     | 0.42              |
| 1:E:4067:THR:HG22 | 1:E:4077:ALA:CB  | 2.49                     | 0.42              |
| 1:E:4116:LEU:HB2  | 1:E:4158:SER:O   | 2.20                     | 0.42              |
| 1:F:5240:HIS:HD2  | 1:F:5243:LYS:HZ1 | 1.68                     | 0.42              |
| 1:A:7:PHE:N       | 1:A:7:PHE:CD2    | 2.85                     | 0.41              |
| 1:A:9:LEU:HA      | 1:A:47:HIS:CE1   | 2.55                     | 0.41              |
| 1:A:175:ARG:C     | 1:A:176:VAL:HG23 | 2.45                     | 0.41              |
| 1:D:3099:GLN:NE2  | 1:D:3188:GLN:HA  | 2.35                     | 0.41              |
| 1:E:4219:VAL:HG13 | 1:E:4221:VAL:O   | 2.20                     | 0.41              |
| 1:F:5011:LEU:HD11 | 1:F:5016:LEU:CD2 | 2.48                     | 0.41              |
| 1:A:99:GLN:NE2    | 1:A:192:VAL:O    | 2.52                     | 0.41              |
| 1:C:2105:GLY:HA2  | 1:C:2237:THR:HG1 | 1.82                     | 0.41              |
| 1:F:5158:SER:HB3  | 1:F:5200:ALA:HB2 | 2.00                     | 0.41              |
| 1:F:5206:CYS:HA   | 1:F:5210:GLY:C   | 2.45                     | 0.41              |
| 1:A:230:ASN:O     | 1:A:231:ALA:HB3  | 2.20                     | 0.41              |
| 1:B:1006:VAL:O    | 1:B:1007:PHE:C   | 2.63                     | 0.41              |
| 1:B:1009:LEU:HD22 | 1:B:1047:HIS:CG  | 2.55                     | 0.41              |
| 1:B:1106:ASP:HB2  | 1:B:1150:THR:O   | 2.21                     | 0.41              |
| 1:C:2133:ASP:HB3  | 1:C:2136:CYS:HB2 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3037:LEU:CD2  | 1:D:3246:VAL:HG21 | 2.49                     | 0.41              |
| 1:F:5027:ASP:HA   | 1:F:5028:PRO:HD3  | 1.91                     | 0.41              |
| 1:F:5117:ASP:OD2  | 1:F:5120:SER:OG   | 2.36                     | 0.41              |
| 1:A:25:PRO:O      | 1:A:66:SER:HA     | 2.21                     | 0.41              |
| 1:A:234:MET:HE3   | 1:A:234:MET:HB2   | 1.92                     | 0.41              |
| 1:B:1001:MET:CG   | 1:B:1009:LEU:HD23 | 2.48                     | 0.41              |
| 1:D:3167:GLU:HG3  | 1:D:3169:TYR:HB2  | 2.01                     | 0.41              |
| 1:E:4099:GLN:HB2  | 1:E:4102:ILE:HD12 | 2.01                     | 0.41              |
| 1:A:206:CYS:HB3   | 1:A:211:LEU:HA    | 2.02                     | 0.41              |
| 1:C:2115:ARG:NH2  | 1:C:2124:ALA:O    | 2.52                     | 0.41              |
| 1:D:3160:ASP:O    | 1:D:3161:THR:OG1  | 2.21                     | 0.41              |
| 1:E:4075:SER:O    | 1:E:4205:MET:HE1  | 2.20                     | 0.41              |
| 1:E:4157:ALA:O    | 1:E:4195:TYR:CD1  | 2.73                     | 0.41              |
| 1:F:5034:ILE:CD1  | 1:F:5092:ILE:CD1  | 2.98                     | 0.41              |
| 1:F:5038:MET:HG2  | 1:F:5057:LEU:HD13 | 2.02                     | 0.41              |
| 1:F:5183:SER:O    | 1:F:5186:GLU:HB2  | 2.20                     | 0.41              |
| 1:F:5205:MET:C    | 1:F:5207:ALA:N    | 2.78                     | 0.41              |
| 1:B:1086:ILE:HD12 | 1:B:1086:ILE:N    | 2.35                     | 0.41              |
| 1:B:1239:SER:HA   | 1:B:1242:VAL:HG22 | 2.02                     | 0.41              |
| 1:E:4039:ASP:O    | 1:E:4056:GLU:N    | 2.48                     | 0.41              |
| 1:F:5013:LYS:HD2  | 1:F:5084:LEU:CD2  | 2.51                     | 0.41              |
| 1:A:155:VAL:HG12  | 1:A:192:VAL:HG22  | 2.02                     | 0.41              |
| 1:A:247:GLU:HA    | 1:A:250:ARG:HG2   | 2.03                     | 0.41              |
| 1:B:1021:LEU:O    | 1:B:1063:ILE:HG23 | 2.21                     | 0.41              |
| 1:B:1205:MET:HG2  | 1:B:1209:GLN:NE2  | 2.35                     | 0.41              |
| 1:C:2056:GLU:CD   | 1:C:2059:GLY:H    | 2.29                     | 0.41              |
| 1:D:3177:VAL:HB   | 1:D:3178:ARG:H    | 1.66                     | 0.41              |
| 1:A:165:GLY:O     | 1:A:166:GLN:CB    | 2.68                     | 0.41              |
| 1:B:1142:GLU:O    | 1:B:1146:SER:HB2  | 2.21                     | 0.41              |
| 1:B:1209:GLN:OE1  | 1:F:5172:TYR:HE2  | 2.02                     | 0.41              |
| 1:C:2050:PHE:N    | 1:C:2050:PHE:CD2  | 2.88                     | 0.41              |
| 1:F:5099:GLN:HB2  | 1:F:5102:ILE:HD12 | 2.02                     | 0.41              |
| 1:B:1239:SER:HA   | 1:B:1242:VAL:CG2  | 2.51                     | 0.41              |
| 1:C:2133:ASP:HB2  | 1:C:2212:ARG:HA   | 2.02                     | 0.41              |
| 1:C:2167:GLU:HG2  | 1:C:2223:ARG:CG   | 2.48                     | 0.41              |
| 1:C:2240:HIS:HA   | 1:C:2243:LYS:NZ   | 2.35                     | 0.41              |
| 1:D:3091:ARG:HG3  | 1:D:3092:ILE:N    | 2.36                     | 0.41              |
| 1:E:4243:LYS:HD2  | 1:E:4243:LYS:HA   | 1.83                     | 0.41              |
| 1:F:5034:ILE:HD11 | 1:F:5092:ILE:CD1  | 2.51                     | 0.41              |
| 1:F:5120:SER:CA   | 1:F:5205:MET:HE1  | 2.41                     | 0.41              |
| 1:F:5206:CYS:HA   | 1:F:5210:GLY:CA   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1209:GLN:O    | 1:B:1210:GLY:C    | 2.62                     | 0.41              |
| 1:C:2048:ARG:C    | 1:C:2049:GLU:HG2  | 2.46                     | 0.41              |
| 1:C:2207:ALA:HA   | 1:C:2211:LEU:HD13 | 2.02                     | 0.41              |
| 1:E:4011:LEU:HD12 | 1:E:4016:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:238:GLU:C     | 1:A:240:HIS:H     | 2.29                     | 0.40              |
| 1:B:1164:PRO:C    | 1:B:1166:GLN:H    | 2.28                     | 0.40              |
| 1:B:1172:TYR:HE1  | 1:F:5209:GLN:O    | 2.04                     | 0.40              |
| 1:C:2011:LEU:HD21 | 1:C:2052:THR:CG2  | 2.45                     | 0.40              |
| 1:D:3225:GLN:OE1  | 1:D:3226:GLN:N    | 2.53                     | 0.40              |
| 1:F:5013:LYS:HD2  | 1:F:5084:LEU:HA   | 2.02                     | 0.40              |
| 1:A:247:GLU:O     | 1:A:251:ARG:HG3   | 2.22                     | 0.40              |
| 1:B:1019:ALA:O    | 1:B:1020:THR:HB   | 2.21                     | 0.40              |
| 1:C:2048:ARG:O    | 1:C:2049:GLU:HG2  | 2.22                     | 0.40              |
| 1:C:2122:HIS:CG   | 1:E:4161:THR:OG1  | 2.74                     | 0.40              |
| 1:C:2143:ALA:HB1  | 1:C:2247:GLU:HG3  | 2.03                     | 0.40              |
| 1:C:2234:MET:HB3  | 1:C:2234:MET:HE3  | 1.69                     | 0.40              |
| 1:D:3070:GLY:HA2  | 1:D:3197:MET:HG2  | 2.02                     | 0.40              |
| 1:E:4074:THR:OG1  | 1:E:4198:GLU:HB3  | 2.21                     | 0.40              |
| 1:B:1063:ILE:O    | 1:B:1063:ILE:HG13 | 2.20                     | 0.40              |
| 1:C:2024:VAL:O    | 1:C:2024:VAL:HG23 | 2.22                     | 0.40              |
| 1:F:5109:VAL:HB   | 1:F:5153:VAL:HG13 | 2.03                     | 0.40              |
| 1:F:5204:THR:CA   | 1:F:5205:MET:SD   | 3.09                     | 0.40              |
| 1:B:1008:HIS:HD2  | 1:B:1076:ILE:CG2  | 2.35                     | 0.40              |
| 1:C:2011:LEU:CD2  | 1:C:2011:LEU:H    | 2.35                     | 0.40              |
| 1:C:2220:ILE:O    | 1:C:2229:PRO:HD3  | 2.21                     | 0.40              |
| 1:E:4042:VAL:O    | 1:E:4042:VAL:HG23 | 2.21                     | 0.40              |
| 1:F:5228:ILE:HG23 | 1:F:5229:PRO:HA   | 2.04                     | 0.40              |
| 1:A:209:GLN:HA    | 1:A:211:LEU:HD23  | 2.04                     | 0.40              |
| 1:B:1105:GLY:N    | 1:B:1219:VAL:O    | 2.55                     | 0.40              |
| 1:B:1106:ASP:OD2  | 1:B:1106:ASP:N    | 2.53                     | 0.40              |
| 1:E:4020:THR:O    | 1:E:4088:THR:N    | 2.49                     | 0.40              |
| 1:E:4115:ARG:HH22 | 1:E:4125:PRO:C    | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | A     | 251/253 (99%)   | 189 (75%)  | 37 (15%)  | 25 (10%) | 0           | 0 |
| 1   | B     | 251/253 (99%)   | 180 (72%)  | 47 (19%)  | 24 (10%) | 0           | 0 |
| 1   | C     | 251/253 (99%)   | 193 (77%)  | 35 (14%)  | 23 (9%)  | 0           | 0 |
| 1   | D     | 251/253 (99%)   | 194 (77%)  | 40 (16%)  | 17 (7%)  | 1           | 1 |
| 1   | E     | 251/253 (99%)   | 187 (74%)  | 41 (16%)  | 23 (9%)  | 0           | 0 |
| 1   | F     | 251/253 (99%)   | 193 (77%)  | 39 (16%)  | 19 (8%)  | 1           | 0 |
| All | All   | 1506/1518 (99%) | 1136 (75%) | 239 (16%) | 131 (9%) | 0           | 0 |

All (131) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 6    | VAL  |
| 1   | A     | 7    | PHE  |
| 1   | A     | 13   | LYS  |
| 1   | A     | 30   | ARG  |
| 1   | A     | 163  | TYR  |
| 1   | A     | 164  | PRO  |
| 1   | A     | 166  | GLN  |
| 1   | A     | 178  | ARG  |
| 1   | A     | 211  | LEU  |
| 1   | A     | 228  | ILE  |
| 1   | B     | 1002 | SER  |
| 1   | B     | 1164 | PRO  |
| 1   | B     | 1167 | GLU  |
| 1   | B     | 1176 | VAL  |
| 1   | B     | 1178 | ARG  |
| 1   | B     | 1212 | ARG  |
| 1   | B     | 1225 | GLN  |
| 1   | B     | 1227 | GLU  |
| 1   | B     | 1229 | PRO  |
| 1   | B     | 1232 | GLU  |
| 1   | C     | 2008 | HIS  |
| 1   | C     | 2126 | LEU  |
| 1   | C     | 2162 | PHE  |
| 1   | C     | 2166 | GLN  |
| 1   | C     | 2168 | ARG  |
| 1   | C     | 2209 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2211 | LEU  |
| 1   | D     | 3008 | HIS  |
| 1   | D     | 3025 | PRO  |
| 1   | D     | 3115 | ARG  |
| 1   | D     | 3164 | PRO  |
| 1   | D     | 3177 | VAL  |
| 1   | D     | 3181 | LYS  |
| 1   | D     | 3184 | MET  |
| 1   | D     | 3211 | LEU  |
| 1   | D     | 3231 | ALA  |
| 1   | E     | 4150 | THR  |
| 1   | E     | 4162 | PHE  |
| 1   | E     | 4172 | TYR  |
| 1   | E     | 4206 | CYS  |
| 1   | E     | 4211 | LEU  |
| 1   | F     | 5227 | GLU  |
| 1   | F     | 5231 | ALA  |
| 1   | F     | 5234 | MET  |
| 1   | A     | 115  | ARG  |
| 1   | A     | 147  | ILE  |
| 1   | A     | 170  | ASP  |
| 1   | A     | 173  | SER  |
| 1   | A     | 176  | VAL  |
| 1   | A     | 226  | GLN  |
| 1   | A     | 231  | ALA  |
| 1   | B     | 1009 | LEU  |
| 1   | B     | 1019 | ALA  |
| 1   | B     | 1020 | THR  |
| 1   | B     | 1037 | LEU  |
| 1   | B     | 1048 | ARG  |
| 1   | B     | 1078 | VAL  |
| 1   | B     | 1210 | GLY  |
| 1   | B     | 1211 | LEU  |
| 1   | C     | 2016 | LEU  |
| 1   | C     | 2150 | THR  |
| 1   | C     | 2164 | PRO  |
| 1   | C     | 2176 | VAL  |
| 1   | C     | 2178 | ARG  |
| 1   | C     | 2223 | ARG  |
| 1   | D     | 3003 | LYS  |
| 1   | D     | 3160 | ASP  |
| 1   | D     | 3161 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3170 | ASP  |
| 1   | E     | 4007 | PHE  |
| 1   | E     | 4045 | ALA  |
| 1   | E     | 4168 | ARG  |
| 1   | E     | 4171 | THR  |
| 1   | E     | 4176 | VAL  |
| 1   | E     | 4179 | HIS  |
| 1   | E     | 4208 | SER  |
| 1   | E     | 4209 | GLN  |
| 1   | E     | 4227 | GLU  |
| 1   | E     | 4234 | MET  |
| 1   | F     | 5003 | LYS  |
| 1   | F     | 5030 | ARG  |
| 1   | F     | 5047 | HIS  |
| 1   | F     | 5049 | GLU  |
| 1   | F     | 5175 | ARG  |
| 1   | A     | 5    | ASP  |
| 1   | A     | 169  | TYR  |
| 1   | A     | 179  | HIS  |
| 1   | A     | 207  | ALA  |
| 1   | B     | 1011 | LEU  |
| 1   | B     | 1233 | THR  |
| 1   | B     | 1234 | MET  |
| 1   | C     | 2015 | ASP  |
| 1   | C     | 2017 | GLN  |
| 1   | C     | 2227 | GLU  |
| 1   | D     | 3026 | GLY  |
| 1   | D     | 3225 | GLN  |
| 1   | E     | 4019 | ALA  |
| 1   | E     | 4164 | PRO  |
| 1   | E     | 4173 | SER  |
| 1   | E     | 4178 | ARG  |
| 1   | E     | 4212 | ARG  |
| 1   | F     | 5017 | GLN  |
| 1   | F     | 5048 | ARG  |
| 1   | F     | 5163 | TYR  |
| 1   | F     | 5209 | GLN  |
| 1   | A     | 118  | GLY  |
| 1   | A     | 206  | CYS  |
| 1   | C     | 2030 | ARG  |
| 1   | C     | 2049 | GLU  |
| 1   | C     | 2210 | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 4163 | TYR  |
| 1   | F     | 5009 | LEU  |
| 1   | F     | 5020 | THR  |
| 1   | F     | 5171 | THR  |
| 1   | F     | 5211 | LEU  |
| 1   | A     | 186  | GLU  |
| 1   | B     | 1231 | ALA  |
| 1   | C     | 2009 | LEU  |
| 1   | D     | 3009 | LEU  |
| 1   | E     | 4038 | MET  |
| 1   | F     | 5115 | ARG  |
| 1   | B     | 1121 | LEU  |
| 1   | C     | 2219 | VAL  |
| 1   | A     | 102  | ILE  |
| 1   | C     | 2147 | ILE  |
| 1   | C     | 2163 | TYR  |
| 1   | F     | 5040 | LYS  |
| 1   | E     | 4174 | GLY  |
| 1   | B     | 1006 | VAL  |
| 1   | F     | 5006 | VAL  |
| 1   | D     | 3118 | GLY  |

### 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     | 200/204 (98%)   | 164 (82%) | 36 (18%)  | 2           | 3 |
| 1   | B     | 200/204 (98%)   | 161 (80%) | 39 (20%)  | 1           | 2 |
| 1   | C     | 200/204 (98%)   | 163 (82%) | 37 (18%)  | 1           | 3 |
| 1   | D     | 200/204 (98%)   | 161 (80%) | 39 (20%)  | 1           | 2 |
| 1   | E     | 200/204 (98%)   | 160 (80%) | 40 (20%)  | 1           | 2 |
| 1   | F     | 200/204 (98%)   | 166 (83%) | 34 (17%)  | 2           | 4 |
| All | All   | 1200/1224 (98%) | 975 (81%) | 225 (19%) | 1           | 3 |



All (225) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1    | MET  |
| 1   | A     | 7    | PHE  |
| 1   | A     | 8    | HIS  |
| 1   | A     | 9    | LEU  |
| 1   | A     | 38   | MET  |
| 1   | A     | 40   | LYS  |
| 1   | A     | 57   | LEU  |
| 1   | A     | 63   | ILE  |
| 1   | A     | 64   | VAL  |
| 1   | A     | 80   | GLU  |
| 1   | A     | 83   | GLN  |
| 1   | A     | 84   | LEU  |
| 1   | A     | 86   | ILE  |
| 1   | A     | 92   | ILE  |
| 1   | A     | 94   | THR  |
| 1   | A     | 104  | VAL  |
| 1   | A     | 140  | LEU  |
| 1   | A     | 146  | SER  |
| 1   | A     | 153  | VAL  |
| 1   | A     | 156  | THR  |
| 1   | A     | 160  | ASP  |
| 1   | A     | 163  | TYR  |
| 1   | A     | 166  | GLN  |
| 1   | A     | 169  | TYR  |
| 1   | A     | 176  | VAL  |
| 1   | A     | 178  | ARG  |
| 1   | A     | 185  | GLU  |
| 1   | A     | 199  | SER  |
| 1   | A     | 205  | MET  |
| 1   | A     | 211  | LEU  |
| 1   | A     | 221  | VAL  |
| 1   | A     | 226  | GLN  |
| 1   | A     | 232  | GLU  |
| 1   | A     | 235  | LYS  |
| 1   | A     | 247  | GLU  |
| 1   | A     | 253  | LEU  |
| 1   | B     | 1001 | MET  |
| 1   | B     | 1011 | LEU  |
| 1   | B     | 1012 | THR  |
| 1   | B     | 1016 | LEU  |
| 1   | B     | 1021 | LEU  |
| 1   | B     | 1038 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1042 | VAL  |
| 1   | B     | 1044 | LEU  |
| 1   | B     | 1062 | VAL  |
| 1   | B     | 1063 | ILE  |
| 1   | B     | 1088 | THR  |
| 1   | B     | 1090 | LEU  |
| 1   | B     | 1091 | ARG  |
| 1   | B     | 1092 | ILE  |
| 1   | B     | 1102 | ILE  |
| 1   | B     | 1106 | ASP  |
| 1   | B     | 1107 | VAL  |
| 1   | B     | 1127 | GLU  |
| 1   | B     | 1137 | THR  |
| 1   | B     | 1151 | THR  |
| 1   | B     | 1160 | ASP  |
| 1   | B     | 1161 | THR  |
| 1   | B     | 1163 | TYR  |
| 1   | B     | 1166 | GLN  |
| 1   | B     | 1167 | GLU  |
| 1   | B     | 1169 | TYR  |
| 1   | B     | 1171 | THR  |
| 1   | B     | 1173 | SER  |
| 1   | B     | 1181 | LYS  |
| 1   | B     | 1186 | GLU  |
| 1   | B     | 1198 | GLU  |
| 1   | B     | 1201 | THR  |
| 1   | B     | 1211 | LEU  |
| 1   | B     | 1220 | ILE  |
| 1   | B     | 1221 | VAL  |
| 1   | B     | 1224 | THR  |
| 1   | B     | 1226 | GLN  |
| 1   | B     | 1233 | THR  |
| 1   | B     | 1235 | LYS  |
| 1   | C     | 2002 | SER  |
| 1   | C     | 2006 | VAL  |
| 1   | C     | 2013 | LYS  |
| 1   | C     | 2016 | LEU  |
| 1   | C     | 2032 | GLU  |
| 1   | C     | 2042 | VAL  |
| 1   | C     | 2043 | LYS  |
| 1   | C     | 2052 | THR  |
| 1   | C     | 2072 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2073 | SER  |
| 1   | C     | 2075 | SER  |
| 1   | C     | 2081 | LEU  |
| 1   | C     | 2084 | LEU  |
| 1   | C     | 2091 | ARG  |
| 1   | C     | 2092 | ILE  |
| 1   | C     | 2095 | THR  |
| 1   | C     | 2145 | LYS  |
| 1   | C     | 2160 | ASP  |
| 1   | C     | 2162 | PHE  |
| 1   | C     | 2163 | TYR  |
| 1   | C     | 2169 | TYR  |
| 1   | C     | 2173 | SER  |
| 1   | C     | 2179 | HIS  |
| 1   | C     | 2186 | GLU  |
| 1   | C     | 2193 | MET  |
| 1   | C     | 2196 | GLU  |
| 1   | C     | 2201 | THR  |
| 1   | C     | 2205 | MET  |
| 1   | C     | 2209 | GLN  |
| 1   | C     | 2215 | MET  |
| 1   | C     | 2221 | VAL  |
| 1   | C     | 2223 | ARG  |
| 1   | C     | 2228 | ILE  |
| 1   | C     | 2234 | MET  |
| 1   | C     | 2235 | LYS  |
| 1   | C     | 2237 | THR  |
| 1   | C     | 2238 | GLU  |
| 1   | D     | 3007 | PHE  |
| 1   | D     | 3011 | LEU  |
| 1   | D     | 3012 | THR  |
| 1   | D     | 3015 | ASP  |
| 1   | D     | 3016 | LEU  |
| 1   | D     | 3033 | LYS  |
| 1   | D     | 3049 | GLU  |
| 1   | D     | 3052 | THR  |
| 1   | D     | 3060 | LYS  |
| 1   | D     | 3088 | THR  |
| 1   | D     | 3090 | LEU  |
| 1   | D     | 3091 | ARG  |
| 1   | D     | 3094 | THR  |
| 1   | D     | 3095 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3098 | ILE  |
| 1   | D     | 3106 | ASP  |
| 1   | D     | 3111 | THR  |
| 1   | D     | 3113 | SER  |
| 1   | D     | 3147 | ILE  |
| 1   | D     | 3151 | THR  |
| 1   | D     | 3166 | GLN  |
| 1   | D     | 3169 | TYR  |
| 1   | D     | 3170 | ASP  |
| 1   | D     | 3178 | ARG  |
| 1   | D     | 3184 | MET  |
| 1   | D     | 3194 | ASN  |
| 1   | D     | 3196 | GLU  |
| 1   | D     | 3202 | LEU  |
| 1   | D     | 3205 | MET  |
| 1   | D     | 3209 | GLN  |
| 1   | D     | 3221 | VAL  |
| 1   | D     | 3224 | THR  |
| 1   | D     | 3229 | PRO  |
| 1   | D     | 3234 | MET  |
| 1   | D     | 3236 | GLN  |
| 1   | D     | 3240 | HIS  |
| 1   | D     | 3243 | LYS  |
| 1   | D     | 3247 | GLU  |
| 1   | D     | 3253 | LEU  |
| 1   | E     | 4001 | MET  |
| 1   | E     | 4009 | LEU  |
| 1   | E     | 4011 | LEU  |
| 1   | E     | 4031 | VAL  |
| 1   | E     | 4037 | LEU  |
| 1   | E     | 4047 | HIS  |
| 1   | E     | 4052 | THR  |
| 1   | E     | 4063 | ILE  |
| 1   | E     | 4067 | THR  |
| 1   | E     | 4072 | PRO  |
| 1   | E     | 4074 | THR  |
| 1   | E     | 4084 | LEU  |
| 1   | E     | 4092 | ILE  |
| 1   | E     | 4103 | ASN  |
| 1   | E     | 4109 | VAL  |
| 1   | E     | 4120 | SER  |
| 1   | E     | 4126 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 4135 | GLU  |
| 1   | E     | 4141 | VAL  |
| 1   | E     | 4145 | LYS  |
| 1   | E     | 4147 | ILE  |
| 1   | E     | 4150 | THR  |
| 1   | E     | 4153 | VAL  |
| 1   | E     | 4167 | GLU  |
| 1   | E     | 4168 | ARG  |
| 1   | E     | 4169 | TYR  |
| 1   | E     | 4172 | TYR  |
| 1   | E     | 4194 | ASN  |
| 1   | E     | 4195 | TYR  |
| 1   | E     | 4198 | GLU  |
| 1   | E     | 4199 | SER  |
| 1   | E     | 4203 | LEU  |
| 1   | E     | 4205 | MET  |
| 1   | E     | 4221 | VAL  |
| 1   | E     | 4223 | ARG  |
| 1   | E     | 4225 | GLN  |
| 1   | E     | 4228 | ILE  |
| 1   | E     | 4236 | GLN  |
| 1   | E     | 4239 | SER  |
| 1   | E     | 4245 | VAL  |
| 1   | F     | 5006 | VAL  |
| 1   | F     | 5007 | PHE  |
| 1   | F     | 5011 | LEU  |
| 1   | F     | 5037 | LEU  |
| 1   | F     | 5043 | LYS  |
| 1   | F     | 5049 | GLU  |
| 1   | F     | 5056 | GLU  |
| 1   | F     | 5062 | VAL  |
| 1   | F     | 5069 | ILE  |
| 1   | F     | 5080 | GLU  |
| 1   | F     | 5091 | ARG  |
| 1   | F     | 5092 | ILE  |
| 1   | F     | 5094 | THR  |
| 1   | F     | 5099 | GLN  |
| 1   | F     | 5131 | VAL  |
| 1   | F     | 5137 | THR  |
| 1   | F     | 5138 | THR  |
| 1   | F     | 5140 | LEU  |
| 1   | F     | 5145 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 5147 | ILE  |
| 1   | F     | 5153 | VAL  |
| 1   | F     | 5155 | VAL  |
| 1   | F     | 5163 | TYR  |
| 1   | F     | 5178 | ARG  |
| 1   | F     | 5181 | LYS  |
| 1   | F     | 5193 | MET  |
| 1   | F     | 5194 | ASN  |
| 1   | F     | 5196 | GLU  |
| 1   | F     | 5202 | LEU  |
| 1   | F     | 5205 | MET  |
| 1   | F     | 5211 | LEU  |
| 1   | F     | 5216 | VAL  |
| 1   | F     | 5225 | GLN  |
| 1   | F     | 5235 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 14   | ASN  |
| 1   | A     | 101  | HIS  |
| 1   | A     | 179  | HIS  |
| 1   | A     | 188  | GLN  |
| 1   | B     | 1017 | GLN  |
| 1   | B     | 1083 | GLN  |
| 1   | B     | 1152 | HIS  |
| 1   | B     | 1179 | HIS  |
| 1   | B     | 1188 | GLN  |
| 1   | B     | 1226 | GLN  |
| 1   | B     | 1236 | GLN  |
| 1   | C     | 2047 | HIS  |
| 1   | C     | 2152 | HIS  |
| 1   | C     | 2179 | HIS  |
| 1   | C     | 2209 | GLN  |
| 1   | C     | 2225 | GLN  |
| 1   | C     | 2240 | HIS  |
| 1   | D     | 3099 | GLN  |
| 1   | D     | 3166 | GLN  |
| 1   | D     | 3194 | ASN  |
| 1   | D     | 3230 | ASN  |
| 1   | D     | 3236 | GLN  |
| 1   | E     | 4008 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 4101 | HIS  |
| 1   | E     | 4179 | HIS  |
| 1   | E     | 4226 | GLN  |
| 1   | F     | 5008 | HIS  |
| 1   | F     | 5122 | HIS  |
| 1   | F     | 5152 | HIS  |
| 1   | F     | 5240 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.