



# Full wwPDB X-ray Structure Validation Report i

Nov 14, 2023 – 02:05 PM JST

PDB ID : 5ZJE  
Title : LDHA-mla  
Authors : Han, C.W.; Jang, S.B.  
Deposited on : 2018-03-20  
Resolution : 2.93 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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

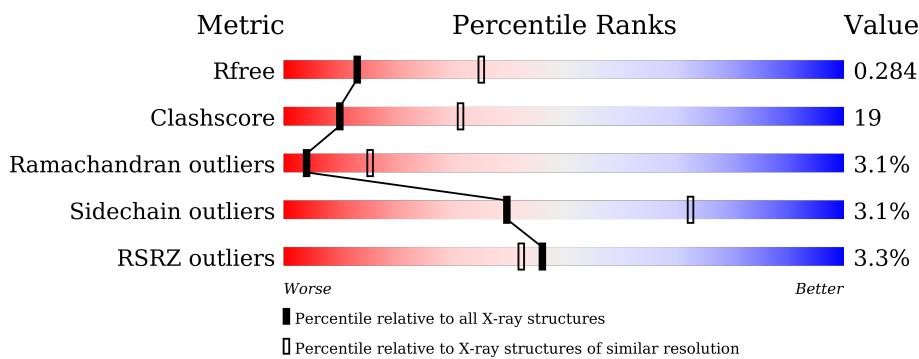
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|----------------------------------------------------|
| $R_{free}$            | 130704                   | 2307 (2.94-2.90)                                   |
| Clashscore            | 141614                   | 2531 (2.94-2.90)                                   |
| Ramachandran outliers | 138981                   | 2462 (2.94-2.90)                                   |
| Sidechain outliers    | 138945                   | 2464 (2.94-2.90)                                   |
| RSRZ outliers         | 127900                   | 2248 (2.94-2.90)                                   |

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



Continued on next page...

*Continued from previous page...*



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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | MLI  | A     | 601 | -         | X        | X       | -                |
| 2   | MLI  | D     | 601 | -         | X        | X       | -                |
| 2   | MLI  | E     | 601 | -         | X        | X       | -                |
| 2   | MLI  | G     | 601 | -         | X        | X       | -                |
| 2   | MLI  | J     | 601 | -         | X        | X       | -                |
| 2   | MLI  | K     | 601 | -         | X        | -       | -                |

## 2 Entry composition [\(i\)](#)

There are 3 unique types of molecules in this entry. The entry contains 31204 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 L-lactate dehydrogenase A chain.

| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 1   | A     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | B     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | C     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | D     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | E     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | F     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | G     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | H     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | I     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | J     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | K     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |
| 1   | L     | 331      | Total<br>2568 | C<br>1639 | N<br>439 | O<br>477 | S<br>13 | 0       | 0       | 0     |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -5      | HIS      | -      | expression tag | UNP P00338 |
| A     | -4      | HIS      | -      | expression tag | UNP P00338 |
| A     | -3      | HIS      | -      | expression tag | UNP P00338 |
| A     | -2      | HIS      | -      | expression tag | UNP P00338 |
| A     | -1      | HIS      | -      | expression tag | UNP P00338 |

*Continued on next page...*

*Continued from previous page...*

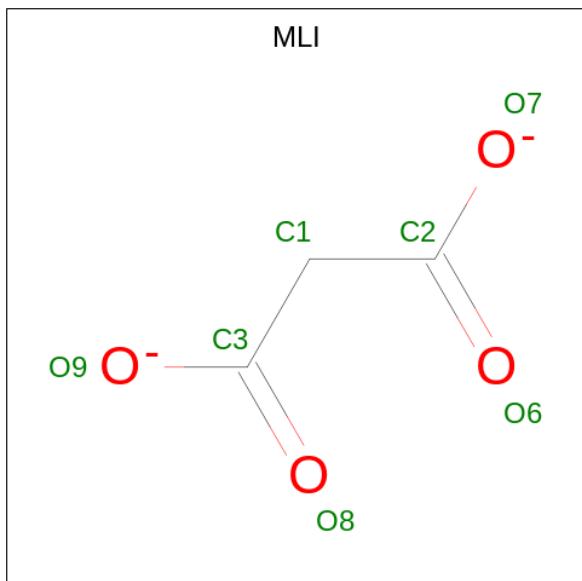
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 0       | HIS      | -      | expression tag | UNP P00338 |
| B     | -5      | HIS      | -      | expression tag | UNP P00338 |
| B     | -4      | HIS      | -      | expression tag | UNP P00338 |
| B     | -3      | HIS      | -      | expression tag | UNP P00338 |
| B     | -2      | HIS      | -      | expression tag | UNP P00338 |
| B     | -1      | HIS      | -      | expression tag | UNP P00338 |
| B     | 0       | HIS      | -      | expression tag | UNP P00338 |
| C     | -5      | HIS      | -      | expression tag | UNP P00338 |
| C     | -4      | HIS      | -      | expression tag | UNP P00338 |
| C     | -3      | HIS      | -      | expression tag | UNP P00338 |
| C     | -2      | HIS      | -      | expression tag | UNP P00338 |
| C     | -1      | HIS      | -      | expression tag | UNP P00338 |
| C     | 0       | HIS      | -      | expression tag | UNP P00338 |
| D     | -5      | HIS      | -      | expression tag | UNP P00338 |
| D     | -4      | HIS      | -      | expression tag | UNP P00338 |
| D     | -3      | HIS      | -      | expression tag | UNP P00338 |
| D     | -2      | HIS      | -      | expression tag | UNP P00338 |
| D     | -1      | HIS      | -      | expression tag | UNP P00338 |
| D     | 0       | HIS      | -      | expression tag | UNP P00338 |
| E     | -5      | HIS      | -      | expression tag | UNP P00338 |
| E     | -4      | HIS      | -      | expression tag | UNP P00338 |
| E     | -3      | HIS      | -      | expression tag | UNP P00338 |
| E     | -2      | HIS      | -      | expression tag | UNP P00338 |
| E     | -1      | HIS      | -      | expression tag | UNP P00338 |
| E     | 0       | HIS      | -      | expression tag | UNP P00338 |
| F     | -5      | HIS      | -      | expression tag | UNP P00338 |
| F     | -4      | HIS      | -      | expression tag | UNP P00338 |
| F     | -3      | HIS      | -      | expression tag | UNP P00338 |
| F     | -2      | HIS      | -      | expression tag | UNP P00338 |
| F     | -1      | HIS      | -      | expression tag | UNP P00338 |
| F     | 0       | HIS      | -      | expression tag | UNP P00338 |
| G     | -5      | HIS      | -      | expression tag | UNP P00338 |
| G     | -4      | HIS      | -      | expression tag | UNP P00338 |
| G     | -3      | HIS      | -      | expression tag | UNP P00338 |
| G     | -2      | HIS      | -      | expression tag | UNP P00338 |
| G     | -1      | HIS      | -      | expression tag | UNP P00338 |
| G     | 0       | HIS      | -      | expression tag | UNP P00338 |
| H     | -5      | HIS      | -      | expression tag | UNP P00338 |
| H     | -4      | HIS      | -      | expression tag | UNP P00338 |
| H     | -3      | HIS      | -      | expression tag | UNP P00338 |
| H     | -2      | HIS      | -      | expression tag | UNP P00338 |
| H     | -1      | HIS      | -      | expression tag | UNP P00338 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | 0       | HIS      | -      | expression tag | UNP P00338 |
| I     | -5      | HIS      | -      | expression tag | UNP P00338 |
| I     | -4      | HIS      | -      | expression tag | UNP P00338 |
| I     | -3      | HIS      | -      | expression tag | UNP P00338 |
| I     | -2      | HIS      | -      | expression tag | UNP P00338 |
| I     | -1      | HIS      | -      | expression tag | UNP P00338 |
| I     | 0       | HIS      | -      | expression tag | UNP P00338 |
| J     | -5      | HIS      | -      | expression tag | UNP P00338 |
| J     | -4      | HIS      | -      | expression tag | UNP P00338 |
| J     | -3      | HIS      | -      | expression tag | UNP P00338 |
| J     | -2      | HIS      | -      | expression tag | UNP P00338 |
| J     | -1      | HIS      | -      | expression tag | UNP P00338 |
| J     | 0       | HIS      | -      | expression tag | UNP P00338 |
| K     | -5      | HIS      | -      | expression tag | UNP P00338 |
| K     | -4      | HIS      | -      | expression tag | UNP P00338 |
| K     | -3      | HIS      | -      | expression tag | UNP P00338 |
| K     | -2      | HIS      | -      | expression tag | UNP P00338 |
| K     | -1      | HIS      | -      | expression tag | UNP P00338 |
| K     | 0       | HIS      | -      | expression tag | UNP P00338 |
| L     | -5      | HIS      | -      | expression tag | UNP P00338 |
| L     | -4      | HIS      | -      | expression tag | UNP P00338 |
| L     | -3      | HIS      | -      | expression tag | UNP P00338 |
| L     | -2      | HIS      | -      | expression tag | UNP P00338 |
| L     | -1      | HIS      | -      | expression tag | UNP P00338 |
| L     | 0       | HIS      | -      | expression tag | UNP P00338 |

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2   | A     | 1        | Total C O<br>7 3 4 | 0       | 0       |
| 2   | D     | 1        | Total C O<br>7 3 4 | 0       | 0       |
| 2   | E     | 1        | Total C O<br>7 3 4 | 0       | 0       |
| 2   | G     | 1        | Total C O<br>7 3 4 | 0       | 0       |
| 2   | J     | 1        | Total C O<br>7 3 4 | 0       | 0       |
| 2   | K     | 1        | Total C O<br>7 3 4 | 0       | 0       |

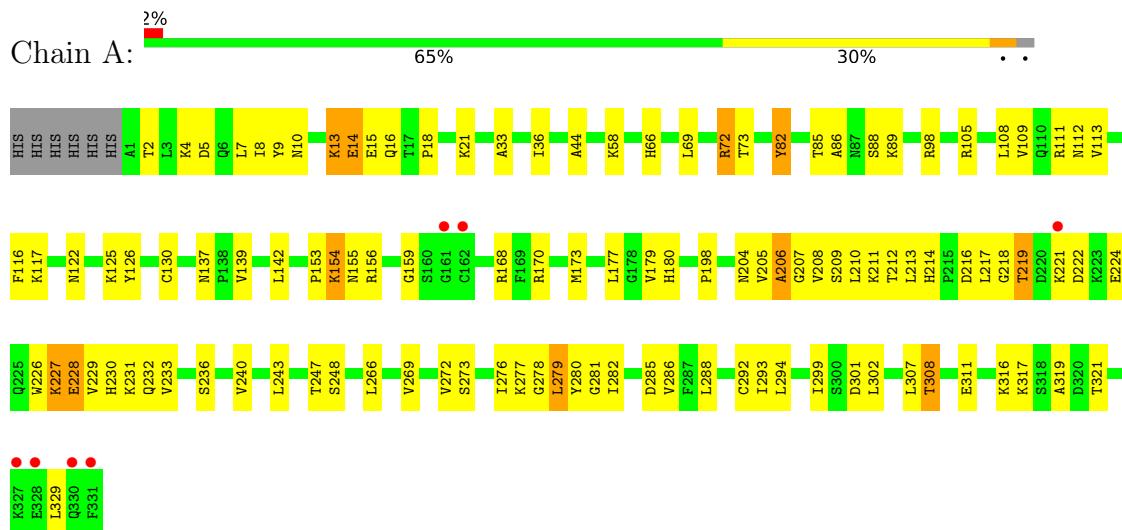
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | A     | 29       | Total O<br>29 29 | 0       | 0       |
| 3   | B     | 26       | Total O<br>26 26 | 0       | 0       |
| 3   | C     | 20       | Total O<br>20 20 | 0       | 0       |
| 3   | D     | 46       | Total O<br>46 46 | 0       | 0       |
| 3   | E     | 37       | Total O<br>37 37 | 0       | 0       |
| 3   | F     | 30       | Total O<br>30 30 | 0       | 0       |
| 3   | G     | 34       | Total O<br>34 34 | 0       | 0       |
| 3   | H     | 23       | Total O<br>23 23 | 0       | 0       |
| 3   | I     | 23       | Total O<br>23 23 | 0       | 0       |
| 3   | J     | 33       | Total O<br>33 33 | 0       | 0       |
| 3   | K     | 23       | Total O<br>23 23 | 0       | 0       |
| 3   | L     | 22       | Total O<br>22 22 | 0       | 0       |

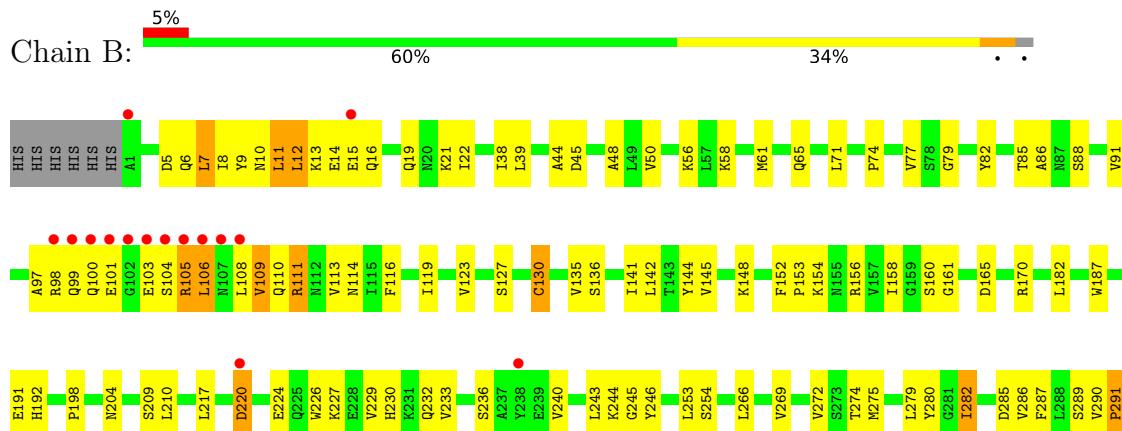
### 3 Residue-property plots

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

- Molecule 1: L-lactate dehydrogenase A chain

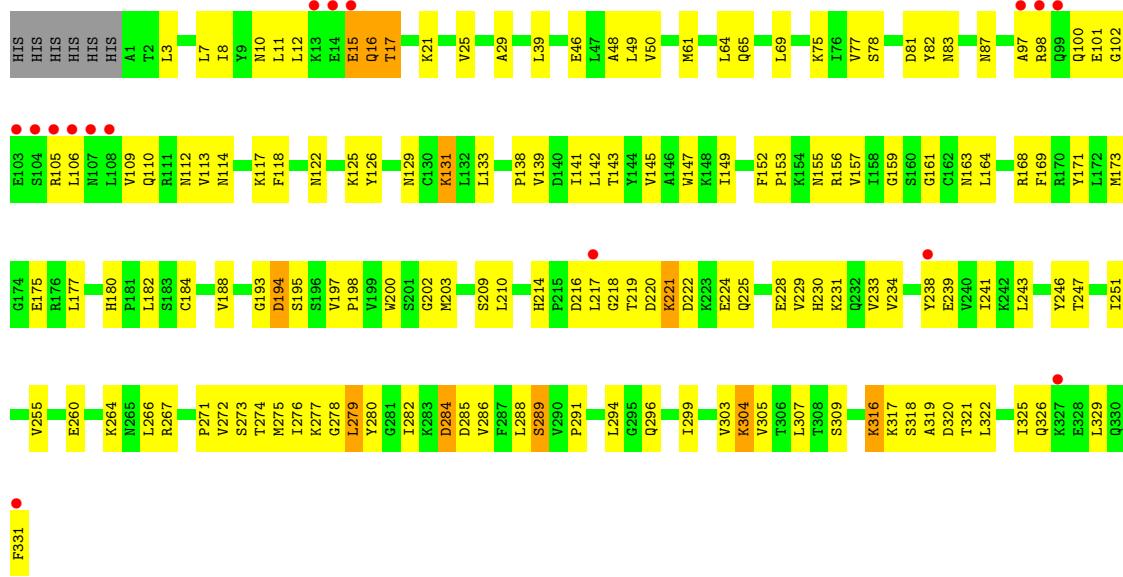


- Molecule 1: L-lactate dehydrogenase A chain

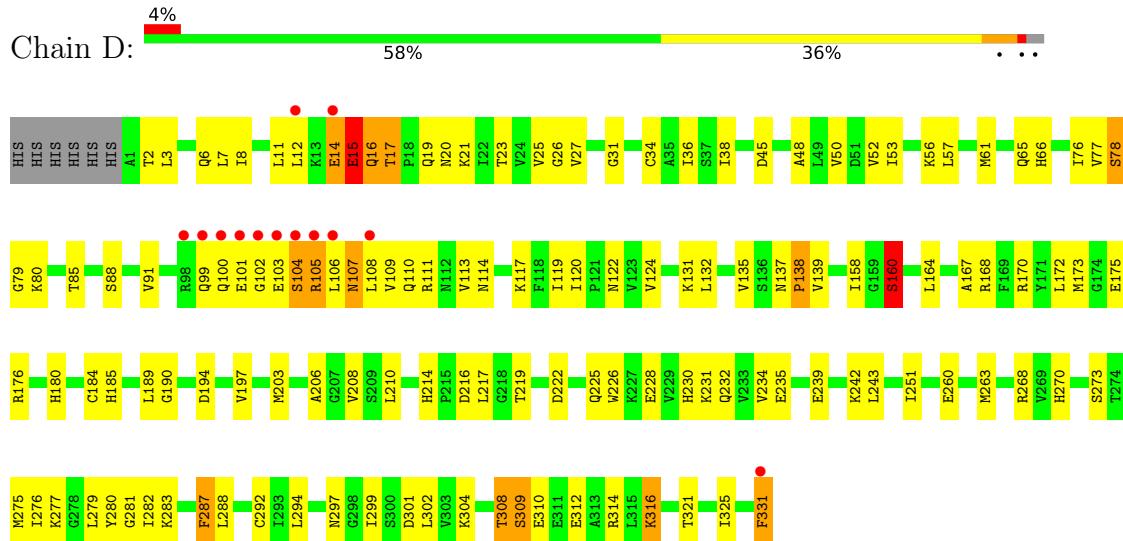


- Molecule 1: L-lactate dehydrogenase A chain

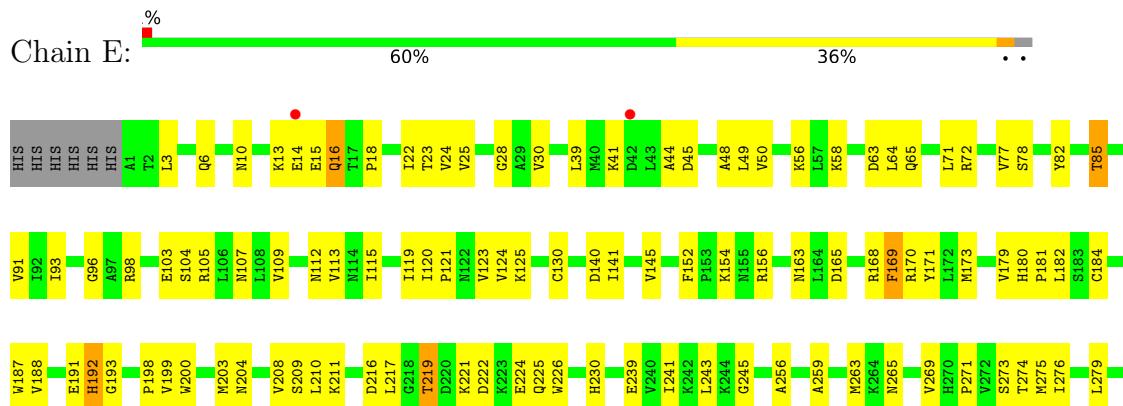




- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain

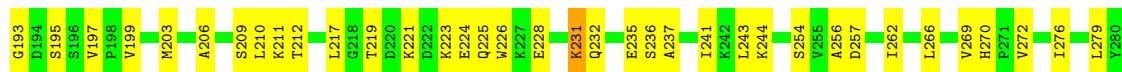




- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain

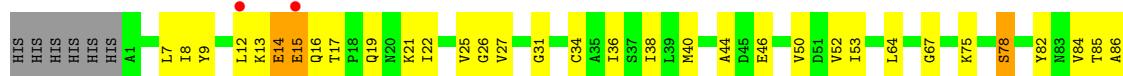




- Molecule 1: L-lactate dehydrogenase A chain

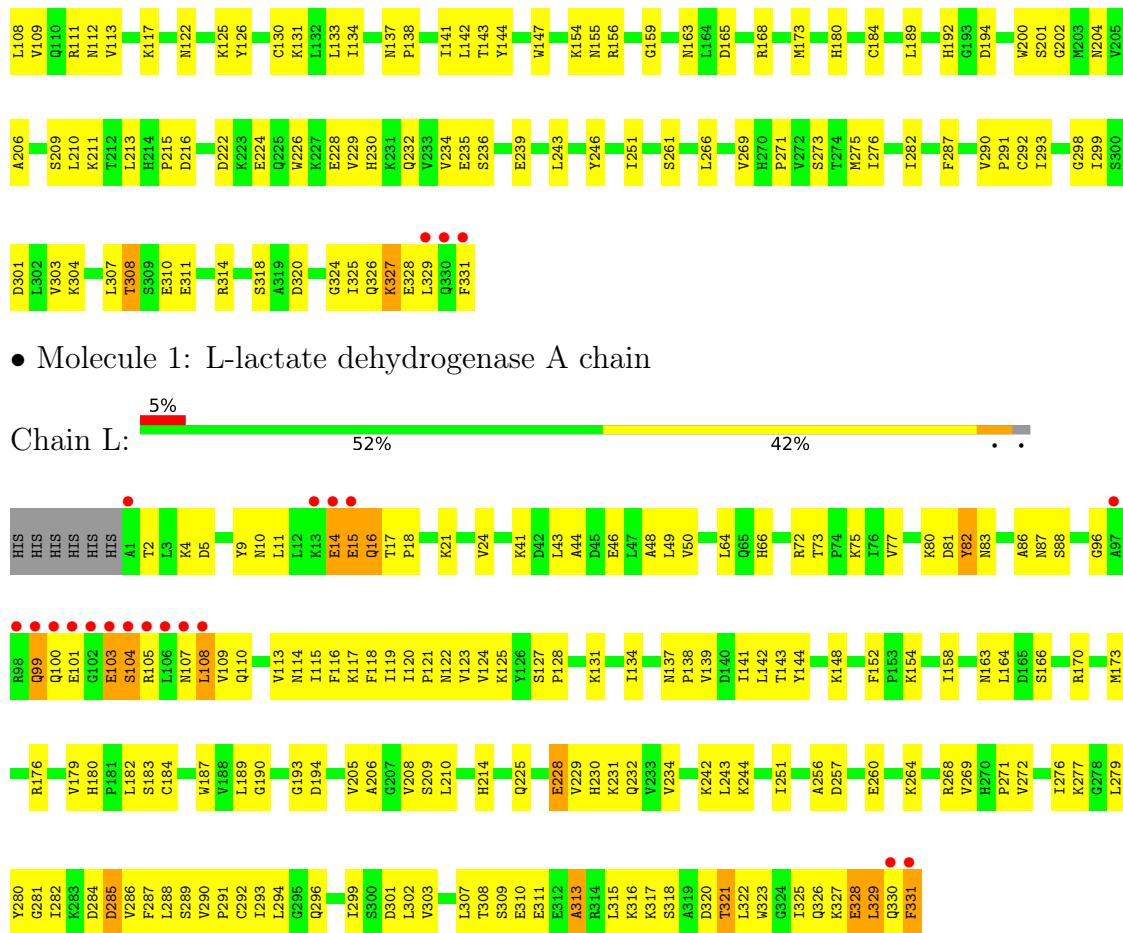


- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain





## 4 Data and refinement statistics i

| Property                                                                | Value                                                         | Source           |
|-------------------------------------------------------------------------|---------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 85.59 Å    219.33 Å    112.79 Å<br>90.00°    92.28°    90.00° | Depositor        |
| Resolution (Å)                                                          | 30.19 – 2.93<br>30.19 – 2.93                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.5 (30.19-2.93)<br>97.5 (30.19-2.93)                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.17                                                          | Depositor        |
| $R_{sym}$                                                               | (Not available)                                               | Depositor        |
| $\langle I/\sigma(I) \rangle^1$                                         | 2.80 (at 2.95 Å)                                              | Xtriage          |
| Refinement program                                                      | PHENIX (1.14_3260: ???)                                       | Depositor        |
| $R$ , $R_{free}$                                                        | 0.188 , 0.284<br>0.188 , 0.284                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4358 reflections (5.02%)                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 53.7                                                          | Xtriage          |
| Anisotropy                                                              | 0.481                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 53.4                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$   | Xtriage          |
| Estimated twinning fraction                                             | 0.065 for h,-k,-l                                             | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                          | EDS              |
| Total number of atoms                                                   | 31204                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 51.0                                                          | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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     | 0.47         | 0/2612         | 0.67        | 1/3532 (0.0%)   |
| 1   | B     | 0.47         | 1/2612 (0.0%)  | 0.66        | 3/3532 (0.1%)   |
| 1   | C     | 0.46         | 0/2612         | 0.68        | 2/3532 (0.1%)   |
| 1   | D     | 0.49         | 0/2612         | 0.67        | 0/3532          |
| 1   | E     | 0.50         | 0/2612         | 0.67        | 0/3532          |
| 1   | F     | 0.48         | 1/2612 (0.0%)  | 0.66        | 2/3532 (0.1%)   |
| 1   | G     | 0.53         | 1/2612 (0.0%)  | 0.69        | 1/3532 (0.0%)   |
| 1   | H     | 0.50         | 2/2612 (0.1%)  | 0.69        | 1/3532 (0.0%)   |
| 1   | I     | 0.49         | 0/2612         | 0.69        | 2/3532 (0.1%)   |
| 1   | J     | 0.46         | 0/2612         | 0.66        | 2/3532 (0.1%)   |
| 1   | K     | 0.48         | 0/2612         | 0.67        | 0/3532          |
| 1   | L     | 0.49         | 1/2612 (0.0%)  | 0.67        | 0/3532          |
| All | All   | 0.49         | 6/31344 (0.0%) | 0.67        | 14/42384 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| 1   | I     | 0                   | 2                   |
| 1   | J     | 0                   | 3                   |
| 1   | L     | 0                   | 3                   |
| All | All   | 0                   | 14                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 283 | LYS  | CD-CE | -6.47 | 1.35        | 1.51     |
| 1   | G     | 310 | GLU  | CG-CD | -6.26 | 1.42        | 1.51     |
| 1   | B     | 111 | ARG  | NE-CZ | 5.28  | 1.40        | 1.33     |
| 1   | L     | 103 | GLU  | CB-CG | 5.26  | 1.62        | 1.52     |
| 1   | H     | 221 | LYS  | CE-NZ | -5.07 | 1.36        | 1.49     |
| 1   | H     | 184 | CYS  | CB-SG | -5.00 | 1.73        | 1.81     |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 310 | GLU  | CA-CB-CG  | 8.37  | 131.82      | 113.40   |
| 1   | I     | 108 | LEU  | CA-CB-CG  | 7.32  | 132.14      | 115.30   |
| 1   | F     | 283 | LYS  | CB-CG-CD  | -6.99 | 93.42       | 111.60   |
| 1   | B     | 111 | ARG  | NE-CZ-NH1 | -6.65 | 116.97      | 120.30   |
| 1   | J     | 108 | LEU  | CA-CB-CG  | 6.06  | 129.23      | 115.30   |
| 1   | I     | 12  | LEU  | CA-CB-CG  | 5.99  | 129.06      | 115.30   |
| 1   | F     | 283 | LYS  | CD-CE-NZ  | -5.49 | 99.07       | 111.70   |
| 1   | C     | 279 | LEU  | CA-CB-CG  | 5.40  | 127.71      | 115.30   |
| 1   | B     | 11  | LEU  | CA-CB-CG  | 5.34  | 127.59      | 115.30   |
| 1   | B     | 111 | ARG  | CG-CD-NE  | 5.32  | 122.96      | 111.80   |
| 1   | H     | 216 | ASP  | CB-CG-OD2 | -5.11 | 113.70      | 118.30   |
| 1   | C     | 275 | MET  | CA-CB-CG  | -5.04 | 104.74      | 113.30   |
| 1   | A     | 279 | LEU  | CA-CB-CG  | 5.02  | 126.84      | 115.30   |
| 1   | J     | 106 | LEU  | CA-CB-CG  | 5.00  | 126.81      | 115.30   |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 14  | GLU  | Peptide |
| 1   | C     | 15  | GLU  | Peptide |
| 1   | D     | 15  | GLU  | Peptide |
| 1   | D     | 308 | THR  | Peptide |
| 1   | E     | 16  | GLN  | Peptide |
| 1   | G     | 16  | GLN  | Peptide |
| 1   | I     | 107 | ASN  | Peptide |
| 1   | I     | 150 | SER  | Peptide |
| 1   | J     | 100 | GLN  | Peptide |
| 1   | J     | 15  | GLU  | Peptide |
| 1   | J     | 99  | GLN  | Peptide |
| 1   | L     | 108 | LEU  | Peptide |
| 1   | L     | 14  | GLU  | Peptide |
| 1   | L     | 15  | GLU  | Peptide |

## 5.2 Too-close contacts [\(i\)](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2568  | 0        | 2656     | 93      | 0            |
| 1   | B     | 2568  | 0        | 2656     | 111     | 0            |
| 1   | C     | 2568  | 0        | 2656     | 118     | 0            |
| 1   | D     | 2568  | 0        | 2656     | 117     | 0            |
| 1   | E     | 2568  | 0        | 2656     | 96      | 0            |
| 1   | F     | 2568  | 0        | 2656     | 99      | 1            |
| 1   | G     | 2568  | 0        | 2656     | 111     | 0            |
| 1   | H     | 2568  | 0        | 2656     | 107     | 0            |
| 1   | I     | 2568  | 0        | 2656     | 127     | 1            |
| 1   | J     | 2568  | 0        | 2656     | 98      | 0            |
| 1   | K     | 2568  | 0        | 2656     | 100     | 0            |
| 1   | L     | 2568  | 0        | 2656     | 127     | 0            |
| 2   | A     | 7     | 0        | 2        | 2       | 0            |
| 2   | D     | 7     | 0        | 2        | 4       | 0            |
| 2   | E     | 7     | 0        | 2        | 5       | 0            |
| 2   | G     | 7     | 0        | 2        | 3       | 0            |
| 2   | J     | 7     | 0        | 2        | 2       | 0            |
| 2   | K     | 7     | 0        | 2        | 1       | 0            |
| 3   | A     | 29    | 0        | 0        | 4       | 0            |
| 3   | B     | 26    | 0        | 0        | 2       | 0            |
| 3   | C     | 20    | 0        | 0        | 3       | 0            |
| 3   | D     | 46    | 0        | 0        | 12      | 0            |
| 3   | E     | 37    | 0        | 0        | 1       | 0            |
| 3   | F     | 30    | 0        | 0        | 1       | 0            |
| 3   | G     | 34    | 0        | 0        | 4       | 0            |
| 3   | H     | 23    | 0        | 0        | 6       | 0            |
| 3   | I     | 23    | 0        | 0        | 7       | 0            |
| 3   | J     | 33    | 0        | 0        | 5       | 0            |
| 3   | K     | 23    | 0        | 0        | 9       | 0            |
| 3   | L     | 22    | 0        | 0        | 1       | 0            |
| All | All   | 31204 | 0        | 31884    | 1190    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1190) 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:G:32:MET:HE2   | 1:G:60:GLU:OE1   | 1.36                     | 1.24              |
| 1:B:220:ASP:OD2  | 1:B:227:LYS:NZ   | 1.84                     | 1.09              |
| 1:L:316:LYS:NZ   | 1:L:317:LYS:HD3  | 1.76                     | 1.01              |
| 1:K:324:GLY:HA2  | 1:K:327:LYS:NZ   | 1.75                     | 0.98              |
| 1:E:105:ARG:HH21 | 2:E:601:MLI:H11  | 1.28                     | 0.98              |
| 1:I:106:LEU:HD22 | 1:I:325:ILE:HD13 | 1.47                     | 0.97              |
| 1:L:327:LYS:HD2  | 1:L:328:GLU:HG2  | 1.47                     | 0.96              |
| 1:A:10:ASN:HD21  | 1:A:13:LYS:HD3   | 1.31                     | 0.94              |
| 1:B:330:GLN:NE2  | 3:B:401:HOH:O    | 2.02                     | 0.93              |
| 1:H:291:PRO:HB2  | 1:H:303:VAL:HB   | 1.48                     | 0.92              |
| 1:B:300:SER:CB   | 1:C:12:LEU:HD22  | 2.01                     | 0.90              |
| 1:J:99:GLN:HG2   | 1:J:100:GLN:H    | 1.35                     | 0.90              |
| 1:G:91:VAL:HG11  | 1:G:123:VAL:HG21 | 1.52                     | 0.89              |
| 1:L:99:GLN:HB2   | 1:L:103:GLU:HB3  | 1.53                     | 0.88              |
| 1:L:316:LYS:HZ3  | 1:L:317:LYS:HD3  | 1.34                     | 0.88              |
| 1:I:100:GLN:O    | 1:I:102:GLY:N    | 2.06                     | 0.88              |
| 1:A:276:ILE:HG12 | 1:A:288:LEU:HD12 | 1.55                     | 0.88              |
| 1:C:100:GLN:O    | 1:C:102:GLY:N    | 2.06                     | 0.87              |
| 1:F:9:TYR:HB2    | 1:G:304:LYS:HE2  | 1.55                     | 0.87              |
| 1:L:144:TYR:HE2  | 1:L:326:GLN:HB3  | 1.41                     | 0.86              |
| 1:D:2:THR:O      | 1:D:6:GLN:OE1    | 1.94                     | 0.85              |
| 1:H:216:ASP:O    | 1:H:219:THR:HG22 | 1.76                     | 0.85              |
| 1:D:251:ILE:HD11 | 2:D:601:MLI:H11  | 1.57                     | 0.85              |
| 1:L:9:TYR:HD1    | 1:L:10:ASN:H     | 1.20                     | 0.84              |
| 1:G:13:LYS:NZ    | 3:G:701:HOH:O    | 2.05                     | 0.84              |
| 1:F:260:GLU:OE2  | 1:G:72:ARG:NH1   | 2.10                     | 0.84              |
| 1:A:72:ARG:NH1   | 1:D:260:GLU:OE1  | 2.10                     | 0.84              |
| 1:B:100:GLN:HB3  | 1:B:103:GLU:HB2  | 1.59                     | 0.84              |
| 1:H:324:GLY:HA2  | 1:H:327:LYS:HE3  | 1.58                     | 0.83              |
| 1:K:111:ARG:HD2  | 3:K:707:HOH:O    | 1.78                     | 0.82              |
| 1:D:283:LYS:NZ   | 3:D:704:HOH:O    | 2.13                     | 0.82              |
| 1:I:75:LYS:NZ    | 3:I:404:HOH:O    | 2.13                     | 0.82              |
| 1:E:222:ASP:O    | 1:E:225:GLN:NE2  | 2.12                     | 0.81              |
| 1:I:189:LEU:HD21 | 1:I:291:PRO:HD3  | 1.62                     | 0.81              |
| 1:H:97:ALA:O     | 1:H:108:LEU:HD13 | 1.81                     | 0.80              |
| 1:A:204:ASN:HA   | 1:A:210:LEU:HD13 | 1.62                     | 0.79              |
| 1:B:154:LYS:HD3  | 1:B:275:MET:HE1  | 1.64                     | 0.79              |
| 1:J:131:LYS:NZ   | 1:J:296:GLN:O    | 2.15                     | 0.79              |
| 1:C:291:PRO:HB2  | 1:C:303:VAL:HB   | 1.64                     | 0.78              |
| 1:D:275:MET:HG2  | 1:D:287:PHE:CE1  | 2.19                     | 0.78              |
| 1:I:245:GLY:O    | 3:I:401:HOH:O    | 2.01                     | 0.78              |
| 1:D:107:ASN:ND2  | 3:D:706:HOH:O    | 2.16                     | 0.78              |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:108:LEU:O    | 1:B:110:GLN:N    | 2.16                     | 0.78              |
| 1:B:274:THR:HB   | 1:B:299:ILE:HD12 | 1.65                     | 0.78              |
| 1:K:141:ILE:HD12 | 1:K:326:GLN:HG3  | 1.66                     | 0.77              |
| 1:A:307:LEU:HD22 | 1:A:311:GLU:HB3  | 1.65                     | 0.77              |
| 1:I:107:ASN:O    | 3:I:402:HOH:O    | 2.01                     | 0.77              |
| 1:F:291:PRO:HB2  | 1:F:303:VAL:HB   | 1.66                     | 0.77              |
| 1:F:260:GLU:CD   | 1:G:72:ARG:HH11  | 1.87                     | 0.77              |
| 1:L:313:ALA:O    | 1:L:316:LYS:N    | 2.18                     | 0.77              |
| 1:B:110:GLN:O    | 1:B:114:ASN:ND2  | 2.18                     | 0.77              |
| 1:L:313:ALA:HA   | 1:L:316:LYS:HG2  | 1.67                     | 0.77              |
| 1:L:228:GLU:O    | 1:L:231:LYS:N    | 2.16                     | 0.76              |
| 1:C:118:PHE:O    | 1:C:122:ASN:ND2  | 2.18                     | 0.76              |
| 1:I:189:LEU:HD23 | 1:I:290:VAL:HA   | 1.68                     | 0.76              |
| 1:K:246:TYR:HB2  | 3:K:702:HOH:O    | 1.84                     | 0.76              |
| 1:I:210:LEU:HD21 | 1:J:7:LEU:HD22   | 1.67                     | 0.76              |
| 1:I:106:LEU:HD22 | 1:I:325:ILE:CD1  | 2.15                     | 0.75              |
| 1:G:39:LEU:HD22  | 1:G:71:LEU:HD13  | 1.66                     | 0.75              |
| 1:I:276:ILE:HD13 | 1:I:288:LEU:HD12 | 1.66                     | 0.75              |
| 1:L:109:VAL:O    | 1:L:113:VAL:HG23 | 1.87                     | 0.75              |
| 1:L:164:LEU:HD22 | 1:L:251:ILE:HG13 | 1.66                     | 0.74              |
| 1:K:324:GLY:HA2  | 1:K:327:LYS:HZ3  | 1.51                     | 0.74              |
| 1:D:281:GLY:O    | 1:D:316:LYS:NZ   | 2.14                     | 0.74              |
| 1:D:110:GLN:OE1  | 3:D:701:HOH:O    | 2.06                     | 0.73              |
| 1:J:224:GLU:OE2  | 3:J:701:HOH:O    | 2.05                     | 0.73              |
| 1:J:104:SER:O    | 1:J:106:LEU:N    | 2.21                     | 0.73              |
| 1:F:96:GLY:HA2   | 1:F:115:ILE:HD12 | 1.69                     | 0.73              |
| 1:I:291:PRO:HB2  | 1:I:303:VAL:HB   | 1.71                     | 0.73              |
| 1:J:108:LEU:O    | 3:J:702:HOH:O    | 2.06                     | 0.72              |
| 1:B:279:LEU:HB3  | 1:B:280:TYR:CD1  | 2.23                     | 0.72              |
| 1:D:110:GLN:NE2  | 3:D:707:HOH:O    | 2.20                     | 0.72              |
| 1:C:230:HIS:O    | 1:C:234:VAL:HG23 | 1.90                     | 0.72              |
| 1:E:170:ARG:HD3  | 1:E:184:CYS:O    | 1.90                     | 0.72              |
| 1:B:300:SER:HB3  | 1:C:12:LEU:HD22  | 1.69                     | 0.71              |
| 1:K:113:VAL:HG12 | 1:K:117:LYS:HE2  | 1.71                     | 0.71              |
| 1:A:226:TRP:O    | 1:A:229:VAL:HG22 | 1.90                     | 0.71              |
| 1:B:279:LEU:HB3  | 1:B:280:TYR:HD1  | 1.54                     | 0.71              |
| 1:C:143:THR:HG23 | 1:C:157:VAL:HG12 | 1.71                     | 0.71              |
| 1:E:243:LEU:HD22 | 1:F:55:ASP:HB2   | 1.72                     | 0.71              |
| 1:J:155:ASN:ND2  | 1:K:12:LEU:HD11  | 2.06                     | 0.71              |
| 1:K:324:GLY:HA2  | 1:K:327:LYS:HZ1  | 1.56                     | 0.71              |
| 1:I:107:ASN:HB2  | 1:I:108:LEU:HD13 | 1.72                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:32:MET:HE1   | 1:G:60:GLU:HB3   | 1.73                     | 0.71              |
| 1:B:158:ILE:HG23 | 1:B:299:ILE:HD11 | 1.72                     | 0.71              |
| 1:A:276:ILE:HD11 | 1:A:286:VAL:HG13 | 1.73                     | 0.70              |
| 1:D:105:ARG:O    | 1:D:106:LEU:HD12 | 1.91                     | 0.70              |
| 1:D:189:LEU:O    | 1:D:197:VAL:N    | 2.22                     | 0.70              |
| 1:I:61:MET:O     | 1:I:65:GLN:HG3   | 1.90                     | 0.70              |
| 1:K:189:LEU:HD22 | 1:K:290:VAL:HA   | 1.71                     | 0.70              |
| 1:E:105:ARG:NH2  | 2:E:601:MLI:H11  | 2.02                     | 0.70              |
| 1:G:293:ILE:HD12 | 1:G:301:ASP:HB2  | 1.71                     | 0.70              |
| 1:H:222:ASP:O    | 1:H:225:GLN:NE2  | 2.23                     | 0.70              |
| 1:D:222:ASP:O    | 1:D:225:GLN:NE2  | 2.25                     | 0.70              |
| 1:E:276:ILE:HD13 | 1:E:282:ILE:HD13 | 1.72                     | 0.70              |
| 1:B:302:LEU:HD12 | 1:C:11:LEU:HD11  | 1.72                     | 0.69              |
| 1:A:108:LEU:HD23 | 1:A:111:ARG:NH2  | 2.08                     | 0.69              |
| 1:B:279:LEU:HD23 | 1:B:280:TYR:HE1  | 1.57                     | 0.69              |
| 1:H:143:THR:HG23 | 1:H:157:VAL:HG12 | 1.73                     | 0.69              |
| 1:J:276:ILE:HD11 | 1:J:288:LEU:HD12 | 1.72                     | 0.69              |
| 1:C:276:ILE:HG21 | 1:C:288:LEU:HD12 | 1.72                     | 0.69              |
| 1:B:291:PRO:HB2  | 1:B:303:VAL:HB   | 1.72                     | 0.69              |
| 1:C:229:VAL:O    | 1:C:233:VAL:HG23 | 1.93                     | 0.69              |
| 1:B:5:ASP:O      | 1:C:304:LYS:NZ   | 2.26                     | 0.68              |
| 1:B:105:ARG:HH21 | 1:B:192:HIS:CE1  | 2.12                     | 0.68              |
| 1:H:290:VAL:HG12 | 1:H:291:PRO:HD2  | 1.75                     | 0.68              |
| 1:I:65:GLN:O     | 1:I:68:SER:OG    | 2.10                     | 0.68              |
| 1:I:124:VAL:HG22 | 1:I:152:PHE:CZ   | 2.28                     | 0.68              |
| 1:I:279:LEU:O    | 1:I:282:ILE:HG12 | 1.92                     | 0.68              |
| 1:L:110:GLN:O    | 1:L:114:ASN:ND2  | 2.26                     | 0.68              |
| 1:J:107:ASN:O    | 3:J:703:HOH:O    | 2.12                     | 0.68              |
| 1:K:98:ARG:NH2   | 3:K:702:HOH:O    | 2.27                     | 0.68              |
| 1:E:302:LEU:HD13 | 1:H:11:LEU:HD11  | 1.76                     | 0.68              |
| 1:G:237:ALA:O    | 1:G:241:ILE:HG13 | 1.94                     | 0.68              |
| 1:I:235:GLU:O    | 1:I:237:ALA:N    | 2.26                     | 0.68              |
| 1:F:216:ASP:O    | 1:F:219:THR:HG22 | 1.92                     | 0.68              |
| 1:I:216:ASP:O    | 1:I:219:THR:HG22 | 1.93                     | 0.68              |
| 1:L:123:VAL:O    | 1:L:127:SER:OG   | 2.07                     | 0.68              |
| 1:J:237:ALA:HB2  | 2:J:601:MLI:H11  | 1.76                     | 0.68              |
| 1:D:122:ASN:ND2  | 3:D:709:HOH:O    | 2.26                     | 0.67              |
| 1:C:3:LEU:HD13   | 1:D:214:HIS:HB2  | 1.75                     | 0.67              |
| 1:L:276:ILE:HG21 | 1:L:288:LEU:HB2  | 1.74                     | 0.67              |
| 1:L:230:HIS:O    | 1:L:234:VAL:HG23 | 1.95                     | 0.67              |
| 1:J:9:TYR:HB2    | 1:K:304:LYS:HE2  | 1.74                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:224:GLU:HG2  | 3:A:728:HOH:O    | 1.95                     | 0.67              |
| 1:F:293:ILE:HD12 | 1:F:301:ASP:HB2  | 1.74                     | 0.67              |
| 1:C:219:THR:HB   | 1:C:221:LYS:HD2  | 1.75                     | 0.67              |
| 1:C:274:THR:HB   | 1:C:299:ILE:HD13 | 1.76                     | 0.67              |
| 1:H:21:LYS:NZ    | 1:H:46:GLU:OE1   | 2.23                     | 0.67              |
| 1:J:285:ASP:HB2  | 1:J:323:TRP:HZ3  | 1.60                     | 0.67              |
| 1:F:12:LEU:HD11  | 1:G:155:ASN:ND2  | 2.09                     | 0.66              |
| 1:K:224:GLU:HB3  | 1:K:226:TRP:CD1  | 2.30                     | 0.66              |
| 1:L:46:GLU:HG3   | 1:L:75:LYS:HB3   | 1.77                     | 0.66              |
| 1:B:148:LYS:HG2  | 1:B:331:PHE:CZ   | 2.30                     | 0.66              |
| 1:I:141:ILE:O    | 1:I:145:VAL:HG23 | 1.94                     | 0.66              |
| 1:L:316:LYS:HZ3  | 1:L:317:LYS:CD   | 2.08                     | 0.66              |
| 1:C:29:ALA:H     | 1:C:98:ARG:HH22  | 1.43                     | 0.66              |
| 1:J:214:HIS:CD2  | 1:J:216:ASP:HB2  | 2.29                     | 0.66              |
| 1:C:318:SER:O    | 1:C:322:LEU:HD12 | 1.96                     | 0.66              |
| 1:G:199:VAL:O    | 3:G:702:HOH:O    | 2.14                     | 0.66              |
| 1:C:221:LYS:HD2  | 1:C:221:LYS:H    | 1.59                     | 0.66              |
| 1:D:117:LYS:HE2  | 1:D:331:PHE:HB2  | 1.78                     | 0.66              |
| 1:G:211:LYS:HD2  | 1:G:217:LEU:HB3  | 1.75                     | 0.66              |
| 1:G:6:GLN:HG2    | 1:H:213:LEU:HD22 | 1.78                     | 0.66              |
| 1:G:7:LEU:HG     | 1:G:8:ILE:HG13   | 1.78                     | 0.66              |
| 1:I:270:HIS:HD2  | 1:I:294:LEU:HD13 | 1.61                     | 0.66              |
| 1:D:103:GLU:OE2  | 3:D:705:HOH:O    | 2.14                     | 0.66              |
| 1:G:221:LYS:HE2  | 1:G:223:LYS:HE2  | 1.78                     | 0.66              |
| 1:A:2:THR:HB     | 1:A:5:ASP:OD2    | 1.96                     | 0.66              |
| 1:A:302:LEU:HD13 | 1:D:11:LEU:HD11  | 1.77                     | 0.66              |
| 1:D:308:THR:O    | 1:D:310:GLU:N    | 2.29                     | 0.66              |
| 1:E:276:ILE:HD11 | 1:E:282:ILE:HG21 | 1.78                     | 0.66              |
| 1:F:216:ASP:HB3  | 1:F:222:ASP:HB2  | 1.76                     | 0.66              |
| 1:H:110:GLN:OE1  | 3:H:401:HOH:O    | 2.12                     | 0.66              |
| 1:B:330:GLN:OE1  | 1:B:330:GLN:N    | 2.20                     | 0.65              |
| 1:H:261:SER:HA   | 1:H:266:LEU:HD12 | 1.78                     | 0.65              |
| 1:J:100:GLN:HG3  | 1:J:101:GLU:N    | 2.10                     | 0.65              |
| 1:H:231:LYS:NZ   | 3:H:404:HOH:O    | 2.24                     | 0.65              |
| 1:L:229:VAL:HA   | 1:L:232:GLN:HE21 | 1.60                     | 0.65              |
| 1:B:21:LYS:HB3   | 1:B:88:SER:HA    | 1.78                     | 0.65              |
| 1:A:105:ARG:HH21 | 2:A:601:MLI:H12  | 1.60                     | 0.65              |
| 1:C:284:ASP:HB2  | 1:C:286:VAL:HG23 | 1.77                     | 0.65              |
| 1:L:103:GLU:HG2  | 1:L:107:ASN:HB2  | 1.77                     | 0.65              |
| 1:F:222:ASP:O    | 1:F:225:GLN:NE2  | 2.29                     | 0.65              |
| 1:G:270:HIS:HB2  | 1:G:294:LEU:HD13 | 1.79                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:32:MET:CE    | 1:G:60:GLU:HB3   | 2.26                     | 0.65              |
| 1:L:316:LYS:HZ1  | 1:L:317:LYS:HD3  | 1.57                     | 0.65              |
| 1:G:32:MET:CE    | 1:G:60:GLU:OE1   | 2.29                     | 0.65              |
| 1:L:286:VAL:HG22 | 1:L:287:PHE:H    | 1.61                     | 0.65              |
| 1:B:154:LYS:HE3  | 1:C:11:LEU:HD23  | 1.79                     | 0.65              |
| 1:E:25:VAL:HG22  | 1:E:50:VAL:CG2   | 2.27                     | 0.65              |
| 1:H:237:ALA:O    | 1:H:241:ILE:HG13 | 1.96                     | 0.65              |
| 1:A:85:THR:O     | 1:A:88:SER:OG    | 2.16                     | 0.64              |
| 1:D:23:THR:HB    | 1:D:91:VAL:HG22  | 1.79                     | 0.64              |
| 1:G:25:VAL:CG2   | 1:G:93:ILE:HD13  | 2.27                     | 0.64              |
| 1:H:25:VAL:HG22  | 1:H:50:VAL:HG12  | 1.77                     | 0.64              |
| 1:K:25:VAL:HA    | 1:K:50:VAL:HG23  | 1.79                     | 0.64              |
| 1:G:10:ASN:ND2   | 1:G:12:LEU:O     | 2.30                     | 0.64              |
| 1:B:302:LEU:CD1  | 1:C:11:LEU:HD11  | 2.28                     | 0.64              |
| 1:C:277:LYS:HA   | 1:C:282:ILE:HG22 | 1.80                     | 0.64              |
| 1:C:280:TYR:OH   | 1:C:305:VAL:O    | 2.15                     | 0.64              |
| 1:E:168:ARG:NH1  | 2:E:601:MLI:O7   | 2.31                     | 0.64              |
| 1:F:189:LEU:HD22 | 1:F:290:VAL:HA   | 1.78                     | 0.64              |
| 1:F:260:GLU:CD   | 1:G:72:ARG:NH1   | 2.51                     | 0.64              |
| 1:A:177:LEU:O    | 1:A:179:VAL:HG23 | 1.98                     | 0.64              |
| 1:L:18:PRO:HG3   | 1:L:21:LYS:HD2   | 1.79                     | 0.64              |
| 1:B:109:VAL:O    | 1:B:113:VAL:HG23 | 1.96                     | 0.64              |
| 1:I:107:ASN:HB2  | 1:I:108:LEU:CD1  | 2.28                     | 0.64              |
| 1:K:204:ASN:HA   | 1:K:210:LEU:HD13 | 1.77                     | 0.64              |
| 1:E:199:VAL:O    | 3:E:701:HOH:O    | 2.15                     | 0.63              |
| 1:K:58:LYS:HD3   | 1:L:243:LEU:HD21 | 1.80                     | 0.63              |
| 1:L:277:LYS:HA   | 1:L:282:ILE:HG22 | 1.80                     | 0.63              |
| 1:I:21:LYS:NZ    | 1:I:84:VAL:O     | 2.28                     | 0.63              |
| 1:A:308:THR:HG1  | 1:A:311:GLU:H    | 1.46                     | 0.63              |
| 1:F:187:TRP:CZ2  | 1:H:206:ALA:HA   | 2.34                     | 0.62              |
| 1:L:100:GLN:HG3  | 1:L:101:GLU:HG2  | 1.80                     | 0.62              |
| 1:E:204:ASN:HA   | 1:E:210:LEU:HD13 | 1.80                     | 0.62              |
| 1:I:273:SER:HA   | 1:I:289:SER:HA   | 1.82                     | 0.62              |
| 1:A:155:ASN:HB2  | 1:A:299:ILE:O    | 1.99                     | 0.62              |
| 1:I:110:GLN:HG3  | 1:I:111:ARG:HG3  | 1.81                     | 0.62              |
| 1:A:7:LEU:HB3    | 1:A:8:ILE:HD12   | 1.81                     | 0.62              |
| 1:I:293:ILE:HD12 | 1:I:301:ASP:HB2  | 1.82                     | 0.62              |
| 1:I:330:GLN:O    | 1:I:330:GLN:HG2  | 1.99                     | 0.62              |
| 1:K:192:HIS:N    | 3:K:705:HOH:O    | 2.33                     | 0.62              |
| 1:G:279:LEU:HD11 | 1:G:302:LEU:HD23 | 1.81                     | 0.62              |
| 1:L:120:ILE:O    | 1:L:124:VAL:HG23 | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:141:ILE:O    | 1:L:144:TYR:HB3  | 2.00                     | 0.62              |
| 1:D:12:LEU:HB3   | 1:D:14:GLU:OE2   | 2.00                     | 0.62              |
| 1:D:309:SER:HA   | 1:D:312:GLU:HB3  | 1.81                     | 0.62              |
| 1:A:159:GLY:HA3  | 1:A:273:SER:HB3  | 1.81                     | 0.62              |
| 1:E:224:GLU:HG2  | 1:I:283:LYS:HD2  | 1.82                     | 0.62              |
| 1:E:276:ILE:C    | 1:E:276:ILE:HD12 | 2.20                     | 0.62              |
| 1:G:231:LYS:HE3  | 1:G:235:GLU:OE1  | 2.00                     | 0.62              |
| 1:C:222:ASP:OD1  | 1:C:224:GLU:N    | 2.33                     | 0.62              |
| 1:I:308:THR:OG1  | 3:I:403:HOH:O    | 2.03                     | 0.62              |
| 1:K:211:LYS:O    | 1:K:215:PRO:HA   | 2.00                     | 0.62              |
| 1:A:113:VAL:HG21 | 1:A:329:LEU:HD11 | 1.82                     | 0.61              |
| 1:D:105:ARG:O    | 1:D:138:PRO:HB3  | 2.00                     | 0.61              |
| 1:I:270:HIS:CD2  | 1:I:294:LEU:HD13 | 2.35                     | 0.61              |
| 1:I:189:LEU:CD2  | 1:I:291:PRO:HD3  | 2.30                     | 0.61              |
| 1:J:99:GLN:HG3   | 1:J:103:GLU:O    | 2.00                     | 0.61              |
| 1:D:107:ASN:O    | 3:D:707:HOH:O    | 2.16                     | 0.61              |
| 1:D:110:GLN:NE2  | 3:D:703:HOH:O    | 2.12                     | 0.61              |
| 1:I:233:VAL:O    | 1:I:236:SER:OG   | 2.18                     | 0.61              |
| 1:L:48:ALA:HA    | 1:L:77:VAL:O     | 1.99                     | 0.61              |
| 1:H:107:ASN:O    | 1:H:110:GLN:NE2  | 2.33                     | 0.61              |
| 1:A:317:LYS:O    | 1:A:321:THR:HG23 | 2.00                     | 0.61              |
| 1:B:301:ASP:OD1  | 1:C:10:ASN:ND2   | 2.34                     | 0.61              |
| 1:F:153:PRO:O    | 1:F:155:ASN:N    | 2.34                     | 0.61              |
| 1:I:304:LYS:HZ1  | 1:L:9:TYR:N      | 1.99                     | 0.61              |
| 1:J:185:HIS:O    | 1:J:203:MET:HA   | 2.01                     | 0.61              |
| 1:B:22:ILE:HD12  | 1:B:44:ALA:HB2   | 1.83                     | 0.60              |
| 1:K:134:ILE:HG13 | 1:K:143:THR:HA   | 1.82                     | 0.60              |
| 1:I:22:ILE:HG12  | 1:I:90:LEU:HB3   | 1.83                     | 0.60              |
| 1:G:21:LYS:HB3   | 1:G:88:SER:HA    | 1.81                     | 0.60              |
| 1:K:138:PRO:HG2  | 1:K:141:ILE:HB   | 1.83                     | 0.60              |
| 1:K:159:GLY:HA3  | 1:K:273:SER:OG   | 2.02                     | 0.60              |
| 1:A:240:VAL:HB   | 1:A:247:THR:HG22 | 1.82                     | 0.60              |
| 1:A:281:GLY:O    | 1:A:316:LYS:HE2  | 2.02                     | 0.60              |
| 1:K:194:ASP:HA   | 1:K:234:VAL:HG13 | 1.82                     | 0.60              |
| 1:F:265:ASN:ND2  | 1:F:265:ASN:O    | 2.34                     | 0.60              |
| 1:J:237:ALA:CB   | 2:J:601:MLI:H11  | 2.32                     | 0.60              |
| 1:E:82:TYR:O     | 1:E:85:THR:HB    | 2.02                     | 0.60              |
| 1:F:130:CYS:O    | 1:F:156:ARG:HD2  | 2.02                     | 0.60              |
| 1:F:220:ASP:C    | 1:F:222:ASP:H    | 2.04                     | 0.60              |
| 1:K:269:VAL:HA   | 1:K:292:CYS:O    | 2.02                     | 0.60              |
| 1:A:154:LYS:NZ   | 1:D:11:LEU:HG    | 2.17                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:306:THR:O    | 1:F:307:LEU:HD23 | 2.02                     | 0.60              |
| 1:I:14:GLU:N     | 1:I:14:GLU:OE2   | 2.32                     | 0.60              |
| 1:I:168:ARG:NH1  | 1:I:237:ALA:HB2  | 2.17                     | 0.60              |
| 1:K:324:GLY:CA   | 1:K:327:LYS:NZ   | 2.59                     | 0.60              |
| 1:H:269:VAL:HA   | 1:H:292:CYS:O    | 2.01                     | 0.60              |
| 1:H:274:THR:HA   | 1:H:287:PHE:CD2  | 2.37                     | 0.60              |
| 1:I:239:GLU:O    | 1:I:243:LEU:HD13 | 2.01                     | 0.60              |
| 1:C:139:VAL:HG21 | 1:C:161:GLY:H    | 1.66                     | 0.59              |
| 1:J:270:HIS:HB2  | 1:J:294:LEU:HD13 | 1.82                     | 0.59              |
| 1:B:300:SER:HB2  | 1:C:12:LEU:HD22  | 1.83                     | 0.59              |
| 1:E:3:LEU:HD21   | 1:F:210:LEU:HD23 | 1.84                     | 0.59              |
| 1:D:230:HIS:O    | 1:D:234:VAL:HG13 | 2.02                     | 0.59              |
| 1:E:291:PRO:HG2  | 1:E:305:VAL:HG21 | 1.85                     | 0.59              |
| 1:F:147:TRP:CZ3  | 1:F:148:LYS:HE3  | 2.38                     | 0.59              |
| 1:G:83:ASN:OD1   | 1:G:84:VAL:N     | 2.34                     | 0.59              |
| 1:K:1:ALA:HB2    | 3:K:723:HOH:O    | 2.00                     | 0.59              |
| 1:K:112:ASN:HB3  | 1:K:142:LEU:HD11 | 1.85                     | 0.59              |
| 1:L:96:GLY:HA2   | 1:L:115:ILE:HD12 | 1.85                     | 0.59              |
| 1:B:100:GLN:HG3  | 1:B:101:GLU:N    | 2.18                     | 0.59              |
| 1:B:145:VAL:HG22 | 1:B:329:LEU:HD21 | 1.83                     | 0.59              |
| 1:H:16:GLN:HG3   | 1:H:17:THR:H     | 1.67                     | 0.59              |
| 1:D:292:CYS:HB3  | 1:D:299:ILE:HG23 | 1.84                     | 0.59              |
| 1:A:278:GLY:O    | 1:A:279:LEU:HG   | 2.03                     | 0.59              |
| 1:E:10:ASN:HA    | 1:H:301:ASP:OD1  | 2.03                     | 0.59              |
| 1:C:110:GLN:NE2  | 3:C:401:HOH:O    | 2.15                     | 0.59              |
| 1:C:169:PHE:HD1  | 1:C:233:VAL:HG21 | 1.68                     | 0.59              |
| 1:C:277:LYS:NZ   | 1:C:285:ASP:OD1  | 2.36                     | 0.58              |
| 1:D:15:GLU:HG3   | 1:D:16:GLN:N     | 2.17                     | 0.58              |
| 1:I:99:GLN:HA    | 1:I:103:GLU:HG3  | 1.85                     | 0.58              |
| 1:J:34:CYS:O     | 1:J:38:ILE:HG13  | 2.02                     | 0.58              |
| 1:K:109:VAL:HG22 | 1:K:138:PRO:HG3  | 1.85                     | 0.58              |
| 1:L:291:PRO:HB2  | 1:L:303:VAL:HB   | 1.85                     | 0.58              |
| 1:A:213:LEU:O    | 1:B:6:GLN:NE2    | 2.37                     | 0.58              |
| 1:B:226:TRP:O    | 1:B:229:VAL:HG22 | 2.03                     | 0.58              |
| 1:D:107:ASN:O    | 1:D:110:GLN:NE2  | 2.36                     | 0.58              |
| 1:D:239:GLU:O    | 1:D:243:LEU:HD12 | 2.04                     | 0.58              |
| 1:E:103:GLU:HG3  | 1:E:107:ASN:HD22 | 1.68                     | 0.58              |
| 1:F:99:GLN:NE2   | 1:F:103:GLU:O    | 2.36                     | 0.58              |
| 1:I:260:GLU:HG3  | 1:I:264:LYS:HE2  | 1.84                     | 0.58              |
| 1:J:206:ALA:HA   | 1:L:187:TRP:CZ2  | 2.38                     | 0.58              |
| 1:D:110:GLN:OE1  | 3:D:708:HOH:O    | 2.17                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:216:ASP:HB3  | 1:H:222:ASP:HB2  | 1.84                     | 0.58              |
| 1:K:261:SER:HA   | 1:K:266:LEU:HD12 | 1.85                     | 0.58              |
| 1:B:282:ILE:HD13 | 1:B:282:ILE:H    | 1.67                     | 0.58              |
| 1:L:139:VAL:O    | 1:L:143:THR:OG1  | 2.14                     | 0.58              |
| 1:D:52:VAL:HG23  | 1:D:53:ILE:HG12  | 1.86                     | 0.58              |
| 1:A:205:VAL:O    | 1:A:208:VAL:N    | 2.35                     | 0.58              |
| 1:C:21:LYS:NZ    | 1:C:46:GLU:OE2   | 2.23                     | 0.58              |
| 1:C:219:THR:HB   | 1:C:221:LYS:CD   | 2.33                     | 0.58              |
| 1:F:11:LEU:HD11  | 1:G:302:LEU:HD13 | 1.86                     | 0.58              |
| 1:G:272:VAL:O    | 1:G:289:SER:HA   | 2.04                     | 0.58              |
| 1:I:220:ASP:OD2  | 1:I:221:LYS:N    | 2.37                     | 0.58              |
| 1:K:276:ILE:C    | 1:K:276:ILE:HD12 | 2.24                     | 0.58              |
| 1:B:39:LEU:HD22  | 1:B:71:LEU:HD13  | 1.86                     | 0.58              |
| 1:G:209:SER:HB3  | 1:G:212:THR:HG23 | 1.85                     | 0.58              |
| 1:B:266:LEU:O    | 1:D:180:HIS:HB2  | 2.03                     | 0.58              |
| 1:D:135:VAL:HA   | 1:D:160:SER:HB3  | 1.86                     | 0.57              |
| 1:C:7:LEU:HD23   | 1:C:8:ILE:HG13   | 1.86                     | 0.57              |
| 1:F:109:VAL:HG21 | 1:F:325:ILE:HG21 | 1.86                     | 0.57              |
| 1:L:110:GLN:OE1  | 1:L:114:ASN:ND2  | 2.37                     | 0.57              |
| 1:I:99:GLN:OE1   | 1:I:241:ILE:HD13 | 2.04                     | 0.57              |
| 1:I:72:ARG:NH2   | 1:J:182:LEU:HD21 | 2.19                     | 0.57              |
| 1:K:7:LEU:HD21   | 1:L:205:VAL:HB   | 1.86                     | 0.57              |
| 1:B:98:ARG:HB2   | 1:B:99:GLN:HG2   | 1.85                     | 0.57              |
| 1:B:282:ILE:HD11 | 1:B:316:LYS:HA   | 1.85                     | 0.57              |
| 1:C:16:GLN:CG    | 1:C:17:THR:H     | 2.16                     | 0.57              |
| 1:L:103:GLU:O    | 1:L:104:SER:O    | 2.22                     | 0.57              |
| 1:H:274:THR:HA   | 1:H:287:PHE:HD2  | 1.69                     | 0.57              |
| 1:I:11:LEU:O     | 1:I:12:LEU:HD23  | 2.04                     | 0.57              |
| 1:I:99:GLN:NE2   | 3:I:401:HOH:O    | 1.71                     | 0.57              |
| 1:B:104:SER:O    | 1:B:106:LEU:N    | 2.32                     | 0.57              |
| 1:H:143:THR:HG23 | 1:H:157:VAL:CG1  | 2.34                     | 0.57              |
| 1:H:248:SER:O    | 1:H:251:ILE:HG22 | 2.05                     | 0.57              |
| 1:G:61:MET:O     | 1:G:65:GLN:HG3   | 2.04                     | 0.57              |
| 1:H:203:MET:HE2  | 1:H:217:LEU:HD21 | 1.85                     | 0.57              |
| 1:H:276:ILE:HG21 | 1:H:290:VAL:HG21 | 1.87                     | 0.57              |
| 1:B:61:MET:O     | 1:B:65:GLN:HG3   | 2.05                     | 0.57              |
| 1:G:137:ASN:ND2  | 2:G:601:MLI:O9   | 2.38                     | 0.57              |
| 1:H:25:VAL:HG22  | 1:H:50:VAL:CG1   | 2.35                     | 0.57              |
| 1:I:266:LEU:HD12 | 1:I:268:ARG:HH11 | 1.68                     | 0.57              |
| 1:J:108:LEU:HA   | 3:J:716:HOH:O    | 2.05                     | 0.57              |
| 1:K:292:CYS:HB3  | 1:K:299:ILE:HG23 | 1.87                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:50:VAL:HG11  | 1:B:82:TYR:CZ    | 2.40                     | 0.56              |
| 1:D:276:ILE:HD11 | 1:D:280:TYR:CD1  | 2.40                     | 0.56              |
| 1:F:141:ILE:O    | 1:F:145:VAL:HG23 | 2.05                     | 0.56              |
| 1:I:151:GLY:O    | 1:I:152:PHE:CD1  | 2.58                     | 0.56              |
| 1:L:308:THR:HG22 | 1:L:310:GLU:H    | 1.69                     | 0.56              |
| 1:E:22:ILE:HD12  | 1:E:44:ALA:HB2   | 1.86                     | 0.56              |
| 1:L:24:VAL:HB    | 1:L:49:LEU:HD23  | 1.87                     | 0.56              |
| 1:C:193:GLY:O    | 1:C:195:SER:N    | 2.38                     | 0.56              |
| 1:E:30:VAL:H     | 1:E:98:ARG:NH2   | 2.03                     | 0.56              |
| 1:E:284:ASP:O    | 1:E:286:VAL:N    | 2.33                     | 0.56              |
| 1:F:268:ARG:HD3  | 1:H:182:LEU:HD23 | 1.87                     | 0.56              |
| 1:B:144:TYR:CE2  | 1:B:326:GLN:HB3  | 2.40                     | 0.56              |
| 1:C:260:GLU:HG3  | 1:C:264:LYS:HE2  | 1.86                     | 0.56              |
| 1:I:155:ASN:HB2  | 1:I:299:ILE:O    | 2.06                     | 0.56              |
| 1:J:141:ILE:O    | 1:J:145:VAL:HG23 | 2.06                     | 0.56              |
| 1:B:148:LYS:HG2  | 1:B:331:PHE:CE2  | 2.40                     | 0.56              |
| 1:L:279:LEU:HB3  | 1:L:280:TYR:CD2  | 2.40                     | 0.56              |
| 1:E:28:GLY:HA3   | 1:E:98:ARG:HH22  | 1.71                     | 0.56              |
| 1:F:109:VAL:HG23 | 1:F:141:ILE:HG21 | 1.88                     | 0.56              |
| 1:C:125:LYS:HD3  | 1:C:126:TYR:CE2  | 2.41                     | 0.56              |
| 1:D:228:GLU:O    | 1:D:232:GLN:HG3  | 2.06                     | 0.56              |
| 1:H:103:GLU:OE1  | 3:H:402:HOH:O    | 2.18                     | 0.56              |
| 1:I:155:ASN:ND2  | 1:I:156:ARG:HG3  | 2.19                     | 0.56              |
| 1:L:293:ILE:HD12 | 1:L:301:ASP:HB2  | 1.87                     | 0.56              |
| 1:I:14:GLU:CD    | 1:I:14:GLU:H     | 2.09                     | 0.56              |
| 1:C:214:HIS:HB3  | 1:D:3:LEU:HD13   | 1.88                     | 0.56              |
| 1:E:3:LEU:HD13   | 1:F:214:HIS:HB2  | 1.88                     | 0.56              |
| 1:I:139:VAL:O    | 1:I:143:THR:OG1  | 2.17                     | 0.56              |
| 1:K:320:ASP:O    | 1:K:324:GLY:N    | 2.39                     | 0.56              |
| 1:A:180:HIS:HB2  | 1:C:266:LEU:O    | 2.06                     | 0.56              |
| 1:F:249:TRP:O    | 1:F:253:LEU:HD12 | 2.06                     | 0.56              |
| 1:L:21:LYS:HG3   | 1:L:46:GLU:HB3   | 1.88                     | 0.56              |
| 1:G:284:ASP:O    | 1:G:286:VAL:N    | 2.33                     | 0.55              |
| 1:B:220:ASP:CG   | 1:B:227:LYS:NZ   | 2.59                     | 0.55              |
| 1:C:228:GLU:O    | 1:C:231:LYS:HG2  | 2.06                     | 0.55              |
| 1:E:18:PRO:HB2   | 1:E:45:ASP:OD1   | 2.06                     | 0.55              |
| 1:G:105:ARG:NE   | 2:G:601:MLI:O8   | 2.38                     | 0.55              |
| 1:D:190:GLY:O    | 1:D:288:LEU:HB2  | 2.05                     | 0.55              |
| 1:E:130:CYS:O    | 1:E:156:ARG:HD2  | 2.05                     | 0.55              |
| 1:F:61:MET:O     | 1:F:65:GLN:HG3   | 2.06                     | 0.55              |
| 1:G:25:VAL:HG21  | 1:G:93:ILE:HD13  | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:197:VAL:HG21 | 1:G:315:LEU:HA   | 1.88                     | 0.55              |
| 1:J:308:THR:O    | 1:J:311:GLU:N    | 2.39                     | 0.55              |
| 1:L:131:LYS:HD3  | 1:L:296:GLN:O    | 2.06                     | 0.55              |
| 1:A:82:TYR:O     | 1:A:85:THR:HB    | 2.06                     | 0.55              |
| 1:E:140:ASP:OD1  | 1:E:273:SER:OG   | 2.23                     | 0.55              |
| 1:L:121:PRO:O    | 1:L:125:LYS:HG2  | 2.07                     | 0.55              |
| 1:F:14:GLU:CD    | 1:F:14:GLU:H     | 2.10                     | 0.55              |
| 1:F:82:TYR:OH    | 1:F:119:ILE:HG23 | 2.06                     | 0.55              |
| 1:I:203:MET:HE1  | 1:I:226:TRP:CZ3  | 2.42                     | 0.55              |
| 1:G:69:LEU:HD21  | 1:H:170:ARG:NH2  | 2.21                     | 0.55              |
| 1:I:109:VAL:O    | 1:I:113:VAL:HG23 | 2.05                     | 0.55              |
| 1:C:141:ILE:HG23 | 1:C:326:GLN:HG2  | 1.88                     | 0.55              |
| 1:C:125:LYS:NZ   | 1:C:126:TYR:OH   | 2.37                     | 0.55              |
| 1:I:23:THR:HB    | 1:I:91:VAL:HG22  | 1.88                     | 0.55              |
| 1:K:173:MET:HG2  | 1:K:184:CYS:HB3  | 1.87                     | 0.55              |
| 1:L:44:ALA:O     | 1:L:73:THR:HG23  | 2.06                     | 0.55              |
| 1:C:163:ASN:HA   | 1:C:271:PRO:HG2  | 1.88                     | 0.55              |
| 1:G:93:ILE:HD12  | 1:G:119:ILE:HG21 | 1.88                     | 0.55              |
| 1:I:85:THR:HG21  | 1:I:123:VAL:HG23 | 1.89                     | 0.55              |
| 1:I:329:LEU:HB3  | 1:I:331:PHE:CE1  | 2.42                     | 0.55              |
| 1:C:129:ASN:HA   | 1:C:156:ARG:HH12 | 1.72                     | 0.55              |
| 1:E:169:PHE:HD2  | 1:E:188:VAL:CG2  | 2.19                     | 0.55              |
| 1:F:82:TYR:O     | 1:F:85:THR:HB    | 2.07                     | 0.55              |
| 1:G:219:THR:HG22 | 1:G:221:LYS:N    | 2.22                     | 0.55              |
| 1:E:141:ILE:HD11 | 1:E:322:LEU:HD22 | 1.88                     | 0.54              |
| 1:I:147:TRP:NE1  | 1:I:152:PHE:O    | 2.40                     | 0.54              |
| 1:D:276:ILE:HD11 | 1:D:280:TYR:HD1  | 1.71                     | 0.54              |
| 1:G:15:GLU:O     | 1:G:16:GLN:OE1   | 2.26                     | 0.54              |
| 1:B:292:CYS:HB3  | 1:B:299:ILE:HG23 | 1.90                     | 0.54              |
| 1:E:241:ILE:HG23 | 1:E:245:GLY:O    | 2.08                     | 0.54              |
| 1:I:21:LYS:NZ    | 1:I:46:GLU:OE2   | 2.36                     | 0.54              |
| 1:K:98:ARG:HB2   | 3:K:722:HOH:O    | 2.07                     | 0.54              |
| 1:K:324:GLY:HA2  | 1:K:327:LYS:CE   | 2.36                     | 0.54              |
| 1:A:72:ARG:NE    | 1:D:260:GLU:OE2  | 2.41                     | 0.54              |
| 1:B:290:VAL:HG11 | 1:B:302:LEU:HD23 | 1.89                     | 0.54              |
| 1:F:19:GLN:O     | 1:F:89:LYS:HE2   | 2.07                     | 0.54              |
| 1:G:105:ARG:HH12 | 1:G:193:GLY:HA2  | 1.72                     | 0.54              |
| 1:L:18:PRO:CG    | 1:L:21:LYS:HD2   | 2.38                     | 0.54              |
| 1:A:205:VAL:O    | 1:A:207:GLY:N    | 2.40                     | 0.54              |
| 1:C:276:ILE:HG12 | 1:C:276:ILE:O    | 2.08                     | 0.54              |
| 1:C:16:GLN:HG2   | 1:C:17:THR:H     | 1.72                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:244:LYS:HE2  | 1:H:60:GLU:CD    | 2.28                     | 0.54              |
| 1:I:110:GLN:HG3  | 1:I:111:ARG:N    | 2.23                     | 0.54              |
| 1:I:292:CYS:SG   | 1:I:299:ILE:HD13 | 2.47                     | 0.54              |
| 1:J:280:TYR:HB2  | 1:J:282:ILE:HD12 | 1.90                     | 0.54              |
| 1:K:137:ASN:HD21 | 2:K:601:MLI:C3   | 2.21                     | 0.54              |
| 1:F:269:VAL:HA   | 1:F:292:CYS:O    | 2.08                     | 0.54              |
| 1:H:130:CYS:O    | 1:H:156:ARG:NH1  | 2.34                     | 0.54              |
| 1:C:278:GLY:N    | 1:C:282:ILE:O    | 2.32                     | 0.54              |
| 1:G:138:PRO:HG2  | 1:G:141:ILE:HB   | 1.89                     | 0.54              |
| 1:G:25:VAL:HB    | 1:G:93:ILE:HD13  | 1.90                     | 0.54              |
| 1:J:25:VAL:HG13  | 1:J:50:VAL:HG13  | 1.89                     | 0.54              |
| 1:C:216:ASP:O    | 1:C:219:THR:OG1  | 2.25                     | 0.53              |
| 1:D:277:LYS:HD2  | 1:D:283:LYS:O    | 2.09                     | 0.53              |
| 1:E:180:HIS:HB2  | 1:G:266:LEU:O    | 2.09                     | 0.53              |
| 1:F:266:LEU:O    | 1:H:180:HIS:HB2  | 2.08                     | 0.53              |
| 1:K:293:ILE:HD13 | 1:K:301:ASP:HB2  | 1.89                     | 0.53              |
| 1:A:72:ARG:HH11  | 1:D:260:GLU:CD   | 2.08                     | 0.53              |
| 1:D:27:VAL:HG23  | 1:D:56:LYS:HE3   | 1.90                     | 0.53              |
| 1:F:105:ARG:C    | 1:F:107:ASN:H    | 2.11                     | 0.53              |
| 1:C:203:MET:HE2  | 1:C:210:LEU:HD12 | 1.91                     | 0.53              |
| 1:J:108:LEU:HG   | 1:J:111:ARG:HD3  | 1.91                     | 0.53              |
| 1:L:205:VAL:O    | 1:L:208:VAL:HG12 | 2.08                     | 0.53              |
| 1:H:244:LYS:O    | 1:H:244:LYS:HG2  | 2.09                     | 0.53              |
| 1:D:197:VAL:HG22 | 1:D:314:ARG:HD3  | 1.89                     | 0.53              |
| 1:D:321:THR:O    | 1:D:325:ILE:HD12 | 2.08                     | 0.53              |
| 1:B:10:ASN:O     | 1:B:11:LEU:HD12  | 2.08                     | 0.53              |
| 1:C:251:ILE:HD12 | 1:C:251:ILE:N    | 2.24                     | 0.53              |
| 1:D:279:LEU:HD11 | 1:D:302:LEU:HD23 | 1.90                     | 0.53              |
| 1:K:239:GLU:O    | 1:K:243:LEU:HD12 | 2.09                     | 0.53              |
| 1:A:58:LYS:HG2   | 1:B:243:LEU:HD13 | 1.90                     | 0.53              |
| 1:B:22:ILE:HG21  | 1:B:38:ILE:HD13  | 1.89                     | 0.53              |
| 1:J:291:PRO:HB2  | 1:J:303:VAL:HB   | 1.91                     | 0.53              |
| 1:A:272:VAL:HG11 | 1:A:294:LEU:HD11 | 1.91                     | 0.53              |
| 1:B:14:GLU:OE1   | 1:B:16:GLN:N     | 2.41                     | 0.53              |
| 1:D:14:GLU:O     | 1:D:15:GLU:HB3   | 2.08                     | 0.53              |
| 1:D:216:ASP:HB3  | 1:D:222:ASP:HB2  | 1.91                     | 0.53              |
| 1:E:293:ILE:HD12 | 1:E:301:ASP:HB2  | 1.91                     | 0.53              |
| 1:J:204:ASN:HA   | 1:J:210:LEU:HD13 | 1.91                     | 0.53              |
| 1:L:269:VAL:HA   | 1:L:292:CYS:O    | 2.09                     | 0.53              |
| 1:A:308:THR:OG1  | 1:A:311:GLU:N    | 2.41                     | 0.53              |
| 1:I:145:VAL:HG12 | 1:I:149:ILE:CD1  | 2.40                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:99:GLN:HG2   | 1:J:100:GLN:N    | 2.16                     | 0.53              |
| 1:L:103:GLU:HG2  | 1:L:107:ASN:CB   | 2.39                     | 0.53              |
| 1:A:44:ALA:O     | 1:A:73:THR:HG23  | 2.09                     | 0.52              |
| 1:A:276:ILE:CG1  | 1:A:288:LEU:HD12 | 2.33                     | 0.52              |
| 1:B:56:LYS:NZ    | 3:B:404:HOH:O    | 2.38                     | 0.52              |
| 1:C:141:ILE:O    | 1:C:145:VAL:HG23 | 2.09                     | 0.52              |
| 1:E:120:ILE:O    | 1:E:124:VAL:HG23 | 2.09                     | 0.52              |
| 1:F:206:ALA:HA   | 1:H:187:TRP:CZ2  | 2.43                     | 0.52              |
| 1:G:25:VAL:HG13  | 1:G:50:VAL:HG23  | 1.90                     | 0.52              |
| 1:D:282:ILE:HG13 | 1:D:316:LYS:HE3  | 1.91                     | 0.52              |
| 1:H:129:ASN:HA   | 1:H:156:ARG:NH1  | 2.24                     | 0.52              |
| 1:H:179:VAL:HG23 | 1:H:184:CYS:SG   | 2.48                     | 0.52              |
| 1:K:310:GLU:OE1  | 1:K:314:ARG:HD2  | 2.10                     | 0.52              |
| 1:D:21:LYS:HB3   | 1:D:88:SER:HA    | 1.90                     | 0.52              |
| 1:H:164:LEU:HD22 | 1:H:251:ILE:HD12 | 1.90                     | 0.52              |
| 1:L:2:THR:HB     | 1:L:5:ASP:HB2    | 1.90                     | 0.52              |
| 1:L:190:GLY:HA2  | 1:L:288:LEU:HD23 | 1.91                     | 0.52              |
| 1:D:168:ARG:HH22 | 2:D:601:MLI:C2   | 2.22                     | 0.52              |
| 1:I:269:VAL:HA   | 1:I:292:CYS:O    | 2.10                     | 0.52              |
| 1:B:330:GLN:O    | 1:B:330:GLN:HG2  | 2.08                     | 0.52              |
| 1:F:44:ALA:O     | 1:F:73:THR:HG23  | 2.09                     | 0.52              |
| 1:F:284:ASP:O    | 1:F:286:VAL:N    | 2.41                     | 0.52              |
| 1:I:238:TYR:HA   | 1:I:241:ILE:HB   | 1.92                     | 0.52              |
| 1:I:286:VAL:HG11 | 1:I:319:ALA:HA   | 1.92                     | 0.52              |
| 1:J:304:LYS:HE2  | 1:K:9:TYR:HB2    | 1.92                     | 0.52              |
| 1:K:21:LYS:HB3   | 1:K:88:SER:HA    | 1.91                     | 0.52              |
| 1:H:123:VAL:HG11 | 1:H:132:LEU:HD21 | 1.92                     | 0.52              |
| 1:I:238:TYR:O    | 1:I:242:LYS:N    | 2.38                     | 0.52              |
| 1:K:21:LYS:HG3   | 1:K:46:GLU:HB3   | 1.90                     | 0.52              |
| 1:A:116:PHE:CE2  | 1:A:142:LEU:HB3  | 2.44                     | 0.52              |
| 1:F:141:ILE:HG13 | 1:F:322:LEU:CD2  | 2.40                     | 0.52              |
| 1:G:25:VAL:HG21  | 1:G:93:ILE:CD1   | 2.39                     | 0.52              |
| 1:J:304:LYS:HE3  | 1:K:5:ASP:O      | 2.10                     | 0.52              |
| 1:L:41:LYS:HB3   | 1:L:43:LEU:HG    | 1.92                     | 0.52              |
| 1:G:291:PRO:HB2  | 1:G:303:VAL:HB   | 1.90                     | 0.52              |
| 1:A:18:PRO:HB2   | 1:A:21:LYS:HB2   | 1.92                     | 0.52              |
| 1:B:153:PRO:HD2  | 1:B:156:ARG:HH21 | 1.75                     | 0.52              |
| 1:B:236:SER:O    | 1:B:240:VAL:HG23 | 2.09                     | 0.52              |
| 1:E:269:VAL:HA   | 1:E:292:CYS:O    | 2.10                     | 0.52              |
| 1:B:136:SER:O    | 1:B:142:LEU:HD12 | 2.10                     | 0.52              |
| 1:D:105:ARG:NH2  | 2:D:601:MLI:O8   | 2.44                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:15:GLU:O     | 1:G:16:GLN:HB2   | 2.09                     | 0.52              |
| 1:I:286:VAL:HG21 | 1:I:319:ALA:O    | 2.10                     | 0.52              |
| 1:J:206:ALA:HB3  | 1:L:303:VAL:HG11 | 1.90                     | 0.51              |
| 1:K:106:LEU:O    | 1:K:109:VAL:HG23 | 2.10                     | 0.51              |
| 1:K:108:LEU:HD23 | 1:K:111:ARG:NH2  | 2.25                     | 0.51              |
| 1:A:113:VAL:HG12 | 1:A:117:LYS:HE2  | 1.93                     | 0.51              |
| 1:B:154:LYS:HD3  | 1:B:275:MET:CE   | 2.37                     | 0.51              |
| 1:K:144:TYR:HB2  | 1:K:287:PHE:CD1  | 2.45                     | 0.51              |
| 1:B:7:LEU:HD23   | 1:B:8:ILE:HG13   | 1.92                     | 0.51              |
| 1:K:10:ASN:ND2   | 1:K:13:LYS:HE2   | 2.25                     | 0.51              |
| 1:K:168:ARG:HD2  | 3:K:716:HOH:O    | 2.10                     | 0.51              |
| 1:G:41:LYS:HB2   | 1:G:41:LYS:HZ3   | 1.75                     | 0.51              |
| 1:J:230:HIS:O    | 1:J:233:VAL:HG12 | 2.10                     | 0.51              |
| 1:L:110:GLN:HA   | 1:L:113:VAL:HB   | 1.91                     | 0.51              |
| 1:L:260:GLU:HG2  | 1:L:264:LYS:HE2  | 1.92                     | 0.51              |
| 1:C:159:GLY:HA3  | 1:C:273:SER:HB2  | 1.91                     | 0.51              |
| 1:E:265:ASN:HB2  | 1:E:296:GLN:HB3  | 1.91                     | 0.51              |
| 1:G:137:ASN:HD21 | 2:G:601:MLI:C3   | 2.24                     | 0.51              |
| 1:H:96:GLY:O     | 3:H:403:HOH:O    | 2.19                     | 0.51              |
| 1:D:34:CYS:O     | 1:D:38:ILE:HG13  | 2.10                     | 0.51              |
| 1:E:105:ARG:HH21 | 2:E:601:MLI:C1   | 2.13                     | 0.51              |
| 1:J:251:ILE:HA   | 1:J:254:SER:HB3  | 1.93                     | 0.51              |
| 1:K:13:LYS:O     | 1:K:14:GLU:O     | 2.28                     | 0.51              |
| 1:A:228:GLU:O    | 1:A:232:GLN:HG3  | 2.11                     | 0.51              |
| 1:F:57:LEU:HD21  | 1:F:79:GLY:N     | 2.25                     | 0.51              |
| 1:F:61:MET:HB2   | 1:F:78:SER:HB3   | 1.93                     | 0.51              |
| 1:H:82:TYR:O     | 1:H:85:THR:HB    | 2.11                     | 0.51              |
| 1:I:236:SER:O    | 1:I:240:VAL:HG23 | 2.10                     | 0.51              |
| 1:L:144:TYR:CE2  | 1:L:326:GLN:HB3  | 2.31                     | 0.51              |
| 1:L:251:ILE:HD12 | 1:L:251:ILE:H    | 1.74                     | 0.51              |
| 1:A:153:PRO:HB2  | 1:A:155:ASN:OD1  | 2.11                     | 0.51              |
| 1:I:163:ASN:HA   | 1:I:271:PRO:HD2  | 1.92                     | 0.51              |
| 1:C:278:GLY:C    | 1:C:279:LEU:HD12 | 2.31                     | 0.51              |
| 1:E:63:ASP:O     | 1:F:250:ALA:HB2  | 2.11                     | 0.51              |
| 1:E:208:VAL:HG21 | 1:G:305:VAL:HA   | 1.93                     | 0.51              |
| 1:B:220:ASP:HA   | 1:B:227:LYS:HZ3  | 1.75                     | 0.50              |
| 1:I:180:HIS:HB2  | 1:K:266:LEU:O    | 2.11                     | 0.50              |
| 1:J:50:VAL:HG21  | 1:J:82:TYR:CE1   | 2.47                     | 0.50              |
| 1:L:105:ARG:O    | 1:L:138:PRO:HB3  | 2.11                     | 0.50              |
| 1:C:200:TRP:HB3  | 1:C:217:LEU:HD23 | 1.92                     | 0.50              |
| 1:C:273:SER:HA   | 1:C:288:LEU:O    | 2.10                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:104:SER:O    | 1:E:107:ASN:HB2  | 2.11                     | 0.50              |
| 1:F:144:TYR:HB2  | 1:F:287:PHE:CD1  | 2.46                     | 0.50              |
| 1:G:244:LYS:HE2  | 1:H:60:GLU:OE1   | 2.11                     | 0.50              |
| 1:H:14:GLU:O     | 1:H:15:GLU:HG3   | 2.11                     | 0.50              |
| 1:H:180:HIS:CE1  | 1:H:182:LEU:HD13 | 2.46                     | 0.50              |
| 1:K:63:ASP:OD2   | 1:L:244:LYS:NZ   | 2.43                     | 0.50              |
| 1:B:45:ASP:O     | 1:B:74:PRO:HD2   | 2.11                     | 0.50              |
| 1:C:319:ALA:HA   | 1:C:322:LEU:HD13 | 1.94                     | 0.50              |
| 1:D:20:ASN:HB3   | 1:D:263:MET:HE3  | 1.92                     | 0.50              |
| 1:H:292:CYS:SG   | 1:H:302:LEU:HD23 | 2.51                     | 0.50              |
| 1:I:145:VAL:HG12 | 1:I:149:ILE:HD12 | 1.93                     | 0.50              |
| 1:K:25:VAL:CG2   | 1:K:93:ILE:HD13  | 2.41                     | 0.50              |
| 1:A:277:LYS:HD2  | 1:A:285:ASP:OD1  | 2.11                     | 0.50              |
| 1:D:14:GLU:HG2   | 1:D:15:GLU:N     | 2.27                     | 0.50              |
| 1:D:108:LEU:HA   | 3:D:701:HOH:O    | 2.10                     | 0.50              |
| 1:L:118:PHE:CE1  | 1:L:122:ASN:ND2  | 2.80                     | 0.50              |
| 1:L:173:MET:SD   | 1:L:184:CYS:HB3  | 2.51                     | 0.50              |
| 1:L:279:LEU:HB3  | 1:L:280:TYR:HD2  | 1.76                     | 0.50              |
| 1:C:49:LEU:HB2   | 1:C:78:SER:HB2   | 1.94                     | 0.50              |
| 1:E:327:LYS:NZ   | 1:E:327:LYS:HB3  | 2.27                     | 0.50              |
| 1:F:300:SER:O    | 1:G:11:LEU:HB2   | 2.12                     | 0.50              |
| 1:H:226:TRP:CE3  | 1:H:229:VAL:HG21 | 2.47                     | 0.50              |
| 1:I:153:PRO:HG2  | 1:I:156:ARG:HD3  | 1.93                     | 0.50              |
| 1:J:189:LEU:HD11 | 1:J:291:PRO:HD3  | 1.94                     | 0.50              |
| 1:J:316:LYS:HD3  | 1:J:320:ASP:CG   | 2.31                     | 0.50              |
| 1:D:61:MET:HB2   | 1:D:78:SER:HB3   | 1.92                     | 0.50              |
| 1:C:168:ARG:HG2  | 1:D:66:HIS:HB3   | 1.94                     | 0.50              |
| 1:D:19:GLN:N     | 1:D:45:ASP:OD2   | 2.44                     | 0.50              |
| 1:E:3:LEU:HD23   | 1:F:226:TRP:CZ2  | 2.46                     | 0.50              |
| 1:A:214:HIS:CE1  | 1:A:216:ASP:HB2  | 2.47                     | 0.50              |
| 1:C:48:ALA:HA    | 1:C:77:VAL:O     | 2.11                     | 0.50              |
| 1:H:170:ARG:NH2  | 3:H:406:HOH:O    | 2.43                     | 0.50              |
| 1:I:185:HIS:O    | 1:I:203:MET:HA   | 2.11                     | 0.50              |
| 1:I:303:VAL:HG11 | 1:K:206:ALA:HB3  | 1.93                     | 0.50              |
| 1:E:179:VAL:HB   | 1:E:184:CYS:SG   | 2.52                     | 0.50              |
| 1:F:176:ARG:HD2  | 1:F:226:TRP:CH2  | 2.47                     | 0.50              |
| 1:H:50:VAL:HG23  | 1:H:79:GLY:O     | 2.12                     | 0.50              |
| 1:I:322:LEU:O    | 1:I:326:GLN:HB2  | 2.11                     | 0.50              |
| 1:L:180:HIS:ND1  | 1:L:182:LEU:HB2  | 2.27                     | 0.50              |
| 1:L:290:VAL:HG22 | 1:L:291:PRO:HD2  | 1.93                     | 0.50              |
| 1:A:266:LEU:O    | 1:C:180:HIS:HB2  | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:135:VAL:HA   | 1:B:160:SER:OG   | 2.12                     | 0.49              |
| 1:B:154:LYS:HE3  | 1:C:11:LEU:CD2   | 2.40                     | 0.49              |
| 1:C:251:ILE:HD12 | 1:C:251:ILE:H    | 1.75                     | 0.49              |
| 1:D:176:ARG:HG3  | 1:D:226:TRP:CH2  | 2.47                     | 0.49              |
| 1:E:115:ILE:HG22 | 1:E:119:ILE:CD1  | 2.42                     | 0.49              |
| 1:G:257:ASP:OD2  | 1:G:270:HIS:HE1  | 1.95                     | 0.49              |
| 1:K:276:ILE:C    | 1:K:276:ILE:CD1  | 2.80                     | 0.49              |
| 1:B:111:ARG:H    | 1:B:111:ARG:HD3  | 1.77                     | 0.49              |
| 1:E:198:PRO:HD3  | 1:E:230:HIS:CE1  | 2.46                     | 0.49              |
| 1:J:99:GLN:CG    | 1:J:100:GLN:H    | 2.17                     | 0.49              |
| 1:J:120:ILE:O    | 1:J:124:VAL:HG13 | 2.12                     | 0.49              |
| 1:C:171:TYR:O    | 1:C:175:GLU:OE1  | 2.29                     | 0.49              |
| 1:E:271:PRO:HA   | 1:E:290:VAL:O    | 2.12                     | 0.49              |
| 1:K:293:ILE:N    | 1:K:293:ILE:HD12 | 2.27                     | 0.49              |
| 1:A:21:LYS:NZ    | 1:A:86:ALA:O     | 2.36                     | 0.49              |
| 1:B:269:VAL:HA   | 1:B:292:CYS:O    | 2.12                     | 0.49              |
| 1:C:17:THR:HG22  | 1:C:87:ASN:ND2   | 2.27                     | 0.49              |
| 1:H:288:LEU:HD13 | 1:H:315:LEU:HD11 | 1.94                     | 0.49              |
| 1:D:14:GLU:CD    | 1:D:14:GLU:H     | 2.15                     | 0.49              |
| 1:G:225:GLN:O    | 1:G:228:GLU:HB2  | 2.12                     | 0.49              |
| 1:L:96:GLY:HA2   | 1:L:115:ILE:CD1  | 2.42                     | 0.49              |
| 1:F:153:PRO:C    | 1:F:155:ASN:H    | 2.16                     | 0.49              |
| 1:F:284:ASP:O    | 1:F:286:VAL:HG23 | 2.13                     | 0.49              |
| 1:L:311:GLU:O    | 1:L:315:LEU:HB2  | 2.13                     | 0.49              |
| 1:A:5:ASP:O      | 1:D:304:LYS:NZ   | 2.39                     | 0.49              |
| 1:A:280:TYR:CE1  | 1:A:307:LEU:HD12 | 2.48                     | 0.49              |
| 1:D:203:MET:HB3  | 1:D:210:LEU:HD12 | 1.93                     | 0.49              |
| 1:H:32:MET:SD    | 1:H:60:GLU:HB3   | 2.52                     | 0.49              |
| 1:F:109:VAL:O    | 1:F:113:VAL:HG23 | 2.13                     | 0.49              |
| 1:F:220:ASP:C    | 1:F:222:ASP:N    | 2.66                     | 0.49              |
| 1:G:243:LEU:HB3  | 1:H:55:ASP:O     | 2.13                     | 0.49              |
| 1:H:216:ASP:OD1  | 1:H:221:LYS:HB2  | 2.13                     | 0.49              |
| 1:L:225:GLN:O    | 1:L:228:GLU:N    | 2.33                     | 0.49              |
| 1:L:320:ASP:O    | 1:L:322:LEU:N    | 2.46                     | 0.49              |
| 1:A:33:ALA:O     | 1:A:36:ILE:HG22  | 2.13                     | 0.49              |
| 1:G:26:GLY:O     | 1:G:31:GLY:HA3   | 2.13                     | 0.49              |
| 1:H:124:VAL:C    | 1:H:126:TYR:H    | 2.16                     | 0.49              |
| 1:K:25:VAL:HG21  | 1:K:93:ILE:HD13  | 1.95                     | 0.49              |
| 1:L:10:ASN:C     | 1:L:11:LEU:HD12  | 2.33                     | 0.49              |
| 1:L:276:ILE:HD11 | 1:L:282:ILE:HG12 | 1.95                     | 0.49              |
| 1:A:125:LYS:NZ   | 3:A:701:HOH:O    | 2.17                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:141:ILE:O    | 1:B:144:TYR:HB3  | 2.13                     | 0.48              |
| 1:C:46:GLU:HA    | 1:C:75:LYS:O     | 2.12                     | 0.48              |
| 1:C:180:HIS:CE1  | 1:C:182:LEU:HD12 | 2.48                     | 0.48              |
| 1:D:16:GLN:N     | 3:D:710:HOH:O    | 2.46                     | 0.48              |
| 1:D:57:LEU:HG    | 1:D:78:SER:HB2   | 1.95                     | 0.48              |
| 1:D:103:GLU:OE1  | 1:D:108:LEU:HD11 | 2.13                     | 0.48              |
| 1:I:280:TYR:HB3  | 1:I:312:GLU:HG3  | 1.95                     | 0.48              |
| 1:A:154:LYS:HZ3  | 1:D:11:LEU:HG    | 1.78                     | 0.48              |
| 1:H:95:ALA:O     | 1:H:136:SER:OG   | 2.24                     | 0.48              |
| 1:J:26:GLY:O     | 1:J:31:GLY:HA3   | 2.13                     | 0.48              |
| 1:B:127:SER:HB3  | 1:B:130:CYS:HB3  | 1.96                     | 0.48              |
| 1:C:105:ARG:NH1  | 3:C:406:HOH:O    | 2.46                     | 0.48              |
| 1:D:107:ASN:ND2  | 3:D:702:HOH:O    | 2.10                     | 0.48              |
| 1:I:281:GLY:C    | 1:I:282:ILE:HD13 | 2.34                     | 0.48              |
| 1:J:292:CYS:HB3  | 1:J:299:ILE:HG23 | 1.95                     | 0.48              |
| 1:D:231:LYS:HD3  | 1:D:235:GLU:OE1  | 2.12                     | 0.48              |
| 1:J:118:PHE:O    | 1:J:121:PRO:HD2  | 2.13                     | 0.48              |
| 1:J:135:VAL:CG1  | 1:J:251:ILE:HD11 | 2.43                     | 0.48              |
| 1:K:291:PRO:HB2  | 1:K:303:VAL:HB   | 1.96                     | 0.48              |
| 1:K:276:ILE:HD11 | 1:K:282:ILE:HG21 | 1.95                     | 0.48              |
| 1:L:134:ILE:HG22 | 1:L:139:VAL:HG23 | 1.94                     | 0.48              |
| 1:B:154:LYS:CD   | 1:B:275:MET:CE   | 2.91                     | 0.48              |
| 1:B:282:ILE:HD13 | 1:B:282:ILE:N    | 2.28                     | 0.48              |
| 1:F:274:THR:OG1  | 1:F:275:MET:N    | 2.46                     | 0.48              |
| 1:I:106:LEU:O    | 3:I:405:HOH:O    | 2.20                     | 0.48              |
| 1:I:205:VAL:HB   | 1:J:7:LEU:HD11   | 1.96                     | 0.48              |
| 1:I:329:LEU:HD23 | 1:I:331:PHE:CE1  | 2.48                     | 0.48              |
| 1:K:324:GLY:CA   | 1:K:327:LYS:HZ1  | 2.23                     | 0.48              |
| 1:B:97:ALA:O     | 1:B:108:LEU:HD13 | 2.14                     | 0.48              |
| 1:B:274:THR:HB   | 1:B:299:ILE:CD1  | 2.37                     | 0.48              |
| 1:E:187:TRP:CZ2  | 1:G:206:ALA:HA   | 2.49                     | 0.48              |
| 1:G:117:LYS:HE2  | 1:G:331:PHE:HA   | 1.95                     | 0.48              |
| 1:G:143:THR:HG22 | 1:G:287:PHE:CE2  | 2.47                     | 0.48              |
| 1:I:214:HIS:CD2  | 1:I:216:ASP:HB2  | 2.49                     | 0.48              |
| 1:D:104:SER:C    | 1:D:106:LEU:H    | 2.17                     | 0.48              |
| 1:E:115:ILE:HG22 | 1:E:119:ILE:HD12 | 1.95                     | 0.48              |
| 1:J:112:ASN:HB3  | 1:J:142:LEU:HD21 | 1.95                     | 0.48              |
| 1:K:19:GLN:O     | 1:K:89:LYS:HE2   | 2.14                     | 0.48              |
| 1:B:282:ILE:CD1  | 1:B:316:LYS:HA   | 2.44                     | 0.48              |
| 1:C:241:ILE:HG13 | 1:C:247:THR:HG23 | 1.95                     | 0.48              |
| 1:D:164:LEU:HD12 | 1:D:167:ALA:HB3  | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:214:HIS:O    | 1:H:217:LEU:N    | 2.46                     | 0.48              |
| 1:J:187:TRP:CZ3  | 1:J:271:PRO:HD3  | 2.49                     | 0.48              |
| 1:A:130:CYS:O    | 1:A:156:ARG:HD2  | 2.14                     | 0.48              |
| 1:A:218:GLY:O    | 1:A:219:THR:O    | 2.30                     | 0.48              |
| 1:C:109:VAL:O    | 1:C:113:VAL:HG23 | 2.14                     | 0.48              |
| 1:D:185:HIS:O    | 1:D:203:MET:HA   | 2.13                     | 0.48              |
| 1:J:78:SER:O     | 1:J:84:VAL:HG21  | 2.14                     | 0.48              |
| 1:K:3:LEU:HD21   | 1:L:210:LEU:HD23 | 1.95                     | 0.48              |
| 1:A:66:HIS:CE1   | 1:B:236:SER:HB3  | 2.49                     | 0.47              |
| 1:B:204:ASN:HA   | 1:B:210:LEU:HD13 | 1.96                     | 0.47              |
| 1:C:97:ALA:N     | 3:C:403:HOH:O    | 2.25                     | 0.47              |
| 1:C:284:ASP:HB2  | 1:C:286:VAL:CG2  | 2.44                     | 0.47              |
| 1:A:269:VAL:HA   | 1:A:292:CYS:O    | 2.14                     | 0.47              |
| 1:C:112:ASN:HB3  | 1:C:142:LEU:HD21 | 1.96                     | 0.47              |
| 1:E:322:LEU:HD23 | 1:E:322:LEU:HA   | 1.73                     | 0.47              |
| 1:F:109:VAL:CG2  | 1:F:141:ILE:HG21 | 2.44                     | 0.47              |
| 1:A:230:HIS:HA   | 1:A:233:VAL:HG12 | 1.95                     | 0.47              |
| 1:A:308:THR:HG23 | 1:A:311:GLU:OE2  | 2.13                     | 0.47              |
| 1:H:46:GLU:OE2   | 1:H:75:LYS:HD3   | 2.14                     | 0.47              |
| 1:K:125:LYS:HD3  | 1:K:126:TYR:CE2  | 2.50                     | 0.47              |
| 1:L:138:PRO:O    | 1:L:142:LEU:HG   | 2.14                     | 0.47              |
| 1:C:147:TRP:CD1  | 1:C:152:PHE:O    | 2.67                     | 0.47              |
| 1:D:61:MET:O     | 1:D:65:GLN:HG3   | 2.15                     | 0.47              |
| 1:D:216:ASP:O    | 1:D:219:THR:HB   | 2.14                     | 0.47              |
| 1:E:154:LYS:HE3  | 1:E:275:MET:HE2  | 1.96                     | 0.47              |
| 1:G:25:VAL:CB    | 1:G:93:ILE:HD13  | 2.43                     | 0.47              |
| 1:H:323:TRP:O    | 1:H:327:LYS:HG2  | 2.14                     | 0.47              |
| 1:I:11:LEU:HD11  | 1:L:302:LEU:HD13 | 1.95                     | 0.47              |
| 1:L:287:PHE:O    | 1:L:288:LEU:HD12 | 2.14                     | 0.47              |
| 1:B:279:LEU:HD23 | 1:B:280:TYR:CE1  | 2.43                     | 0.47              |
| 1:C:21:LYS:HD2   | 1:C:46:GLU:CD    | 2.34                     | 0.47              |
| 1:C:106:LEU:HD21 | 1:C:141:ILE:HD11 | 1.95                     | 0.47              |
| 1:H:188:VAL:CG1  | 1:H:196:SER:HB3  | 2.43                     | 0.47              |
| 1:L:158:ILE:HG23 | 1:L:299:ILE:HD11 | 1.96                     | 0.47              |
| 1:L:318:SER:HA   | 1:L:321:THR:HB   | 1.96                     | 0.47              |
| 1:C:147:TRP:NE1  | 1:C:152:PHE:O    | 2.48                     | 0.47              |
| 1:C:194:ASP:H    | 1:C:234:VAL:CG1  | 2.27                     | 0.47              |
| 1:E:39:LEU:HD11  | 1:E:64:LEU:HD13  | 1.97                     | 0.47              |
| 1:G:224:GLU:O    | 1:G:225:GLN:HB2  | 2.15                     | 0.47              |
| 1:H:21:LYS:HB3   | 1:H:88:SER:HA    | 1.96                     | 0.47              |
| 1:H:108:LEU:O    | 1:H:112:ASN:HB2  | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:281:GLY:O    | 1:A:316:LYS:CE   | 2.63                     | 0.47              |
| 1:B:100:GLN:HG3  | 1:B:101:GLU:H    | 1.78                     | 0.47              |
| 1:C:61:MET:O     | 1:C:65:GLN:HG3   | 2.15                     | 0.47              |
| 1:D:109:VAL:O    | 1:D:113:VAL:HG23 | 2.14                     | 0.47              |
| 1:E:65:GLN:HB3   | 1:F:171:TYR:CZ   | 2.49                     | 0.47              |
| 1:F:91:VAL:HB    | 1:F:132:LEU:HD23 | 1.97                     | 0.47              |
| 1:H:29:ALA:N     | 1:H:98:ARG:HH12  | 2.12                     | 0.47              |
| 1:I:198:PRO:HG3  | 1:I:230:HIS:CG   | 2.49                     | 0.47              |
| 1:L:108:LEU:HD12 | 1:L:137:ASN:O    | 2.14                     | 0.47              |
| 1:L:166:SER:O    | 1:L:170:ARG:HG3  | 2.14                     | 0.47              |
| 1:L:179:VAL:CG1  | 1:L:183:SER:HB2  | 2.45                     | 0.47              |
| 1:B:217:LEU:HD12 | 1:B:226:TRP:CD1  | 2.50                     | 0.47              |
| 1:C:11:LEU:N     | 1:C:11:LEU:HD12  | 2.30                     | 0.47              |
| 1:E:191:GLU:O    | 1:E:193:GLY:N    | 2.48                     | 0.47              |
| 1:G:47:LEU:HB3   | 1:G:76:ILE:HG12  | 1.97                     | 0.47              |
| 1:G:224:GLU:HB3  | 1:G:226:TRP:CD1  | 2.49                     | 0.47              |
| 1:H:103:GLU:OE2  | 1:H:108:LEU:HD21 | 2.15                     | 0.47              |
| 1:H:105:ARG:HD3  | 1:H:137:ASN:HB3  | 1.95                     | 0.47              |
| 1:I:327:LYS:C    | 1:I:329:LEU:H    | 2.18                     | 0.47              |
| 1:K:109:VAL:O    | 1:K:113:VAL:HG23 | 2.15                     | 0.47              |
| 1:K:230:HIS:O    | 1:K:234:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:112:ASN:ND2  | 1:A:137:ASN:O    | 2.48                     | 0.47              |
| 1:B:187:TRP:CZ2  | 1:D:206:ALA:HA   | 2.50                     | 0.47              |
| 1:B:329:LEU:HD12 | 1:B:329:LEU:HA   | 1.69                     | 0.47              |
| 1:F:109:VAL:HG21 | 1:F:325:ILE:CG2  | 2.45                     | 0.47              |
| 1:G:105:ARG:HD3  | 1:G:137:ASN:ND2  | 2.30                     | 0.47              |
| 1:I:3:LEU:HD12   | 1:I:3:LEU:HA     | 1.63                     | 0.47              |
| 1:I:110:GLN:O    | 1:I:330:GLN:NE2  | 2.48                     | 0.47              |
| 1:K:55:ASP:O     | 1:L:243:LEU:HG   | 2.15                     | 0.47              |
| 1:L:100:GLN:HG3  | 1:L:101:GLU:CG   | 2.43                     | 0.47              |
| 1:A:4:LYS:O      | 1:A:4:LYS:HG2    | 2.14                     | 0.47              |
| 1:A:219:THR:O    | 1:A:222:ASP:HB2  | 2.15                     | 0.47              |
| 1:D:104:SER:O    | 1:D:106:LEU:N    | 2.48                     | 0.47              |
| 1:K:194:ASP:HA   | 1:K:234:VAL:CG1  | 2.43                     | 0.47              |
| 1:A:269:VAL:HG22 | 1:A:293:ILE:HG13 | 1.96                     | 0.46              |
| 1:A:292:CYS:HB3  | 1:A:299:ILE:HG23 | 1.96                     | 0.46              |
| 1:I:198:PRO:HG2  | 1:I:200:TRP:CZ2  | 2.50                     | 0.46              |
| 1:C:317:LYS:O    | 1:C:321:THR:HG23 | 2.16                     | 0.46              |
| 1:E:163:ASN:OD1  | 1:E:271:PRO:HD2  | 2.16                     | 0.46              |
| 1:F:140:ASP:OD2  | 1:F:191:GLU:HA   | 2.16                     | 0.46              |
| 1:B:182:LEU:HD13 | 1:D:268:ARG:HD3  | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:48:ALA:HA    | 1:E:77:VAL:O     | 2.15                     | 0.46              |
| 1:E:221:LYS:O    | 1:E:221:LYS:HG3  | 2.15                     | 0.46              |
| 1:G:99:GLN:HG3   | 1:G:241:ILE:CD1  | 2.45                     | 0.46              |
| 1:I:116:PHE:CE1  | 1:I:142:LEU:HD22 | 2.50                     | 0.46              |
| 1:L:14:GLU:O     | 1:L:16:GLN:N     | 2.49                     | 0.46              |
| 1:E:191:GLU:HG3  | 1:E:322:LEU:HD11 | 1.96                     | 0.46              |
| 1:H:32:MET:HE1   | 1:H:64:LEU:HD11  | 1.98                     | 0.46              |
| 1:H:61:MET:O     | 1:H:65:GLN:HG3   | 2.15                     | 0.46              |
| 1:H:129:ASN:HA   | 1:H:156:ARG:HH12 | 1.79                     | 0.46              |
| 1:I:173:MET:SD   | 1:I:184:CYS:HB3  | 2.56                     | 0.46              |
| 1:J:100:GLN:HG3  | 1:J:101:GLU:H    | 1.78                     | 0.46              |
| 1:L:110:GLN:HE21 | 1:L:329:LEU:HA   | 1.78                     | 0.46              |
| 1:L:193:GLY:O    | 1:L:234:VAL:HG13 | 2.15                     | 0.46              |
| 1:B:191:GLU:OE2  | 1:B:322:LEU:HD11 | 2.15                     | 0.46              |
| 1:D:276:ILE:HG21 | 1:D:288:LEU:HG   | 1.97                     | 0.46              |
| 1:E:208:VAL:CG2  | 1:G:305:VAL:HA   | 2.46                     | 0.46              |
| 1:E:279:LEU:HD11 | 1:E:302:LEU:HD23 | 1.97                     | 0.46              |
| 1:F:12:LEU:HB3   | 1:F:14:GLU:OE2   | 2.15                     | 0.46              |
| 1:F:46:GLU:CD    | 1:F:75:LYS:HD2   | 2.36                     | 0.46              |
| 1:G:262:ILE:HG13 | 1:G:294:LEU:HD23 | 1.97                     | 0.46              |
| 1:I:303:VAL:O    | 1:I:305:VAL:N    | 2.46                     | 0.46              |
| 1:J:52:VAL:HG23  | 1:J:53:ILE:HD12  | 1.97                     | 0.46              |
| 1:K:25:VAL:HA    | 1:K:50:VAL:CG2   | 2.45                     | 0.46              |
| 1:K:324:GLY:CA   | 1:K:327:LYS:HZ3  | 2.24                     | 0.46              |
| 1:B:91:VAL:HG11  | 1:B:123:VAL:HG11 | 1.97                     | 0.46              |
| 1:E:91:VAL:HG11  | 1:E:123:VAL:HG11 | 1.96                     | 0.46              |
| 1:E:145:VAL:HG13 | 1:E:331:PHE:CE1  | 2.50                     | 0.46              |
| 1:E:200:TRP:CE3  | 1:E:203:MET:HE3  | 2.50                     | 0.46              |
| 1:E:291:PRO:HG2  | 1:E:305:VAL:CG2  | 2.45                     | 0.46              |
| 1:G:99:GLN:HG3   | 1:G:241:ILE:HD13 | 1.95                     | 0.46              |
| 1:G:133:LEU:HD23 | 1:G:133:LEU:HA   | 1.55                     | 0.46              |
| 1:I:280:TYR:CD2  | 1:I:307:LEU:HD12 | 2.50                     | 0.46              |
| 1:J:21:LYS:HG3   | 1:J:46:GLU:HB3   | 1.98                     | 0.46              |
| 1:L:272:VAL:O    | 1:L:289:SER:HA   | 2.15                     | 0.46              |
| 1:A:168:ARG:HB2  | 1:A:233:VAL:HG23 | 1.96                     | 0.46              |
| 1:C:316:LYS:HA   | 1:C:319:ALA:HB3  | 1.98                     | 0.46              |
| 1:E:50:VAL:HG21  | 1:E:82:TYR:CE2   | 2.50                     | 0.46              |
| 1:G:99:GLN:OE1   | 1:G:105:ARG:HG2  | 2.16                     | 0.46              |
| 1:L:308:THR:HG22 | 1:L:309:SER:N    | 2.30                     | 0.46              |
| 1:C:200:TRP:CE2  | 1:C:218:GLY:HA3  | 2.51                     | 0.46              |
| 1:J:214:HIS:HD2  | 1:J:216:ASP:HB2  | 1.76                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:251:ILE:O    | 1:C:255:VAL:HG23 | 2.15                     | 0.46              |
| 1:J:180:HIS:CE1  | 1:J:182:LEU:HD13 | 2.51                     | 0.46              |
| 1:K:130:CYS:O    | 1:K:156:ARG:NH1  | 2.43                     | 0.46              |
| 1:L:18:PRO:HB2   | 1:L:21:LYS:HB2   | 1.96                     | 0.46              |
| 1:A:286:VAL:HG22 | 1:A:288:LEU:HG   | 1.97                     | 0.46              |
| 1:C:164:LEU:HD22 | 1:C:251:ILE:HG13 | 1.97                     | 0.46              |
| 1:C:203:MET:HE2  | 1:C:203:MET:HB3  | 1.75                     | 0.46              |
| 1:E:96:GLY:HA3   | 1:E:112:ASN:OD1  | 2.16                     | 0.46              |
| 1:F:261:SER:OG   | 1:F:268:ARG:HB2  | 2.16                     | 0.46              |
| 1:J:111:ARG:O    | 1:J:115:ILE:HG13 | 2.16                     | 0.46              |
| 1:L:257:ASP:OD1  | 1:L:268:ARG:NH1  | 2.49                     | 0.46              |
| 1:C:173:MET:SD   | 1:C:184:CYS:HB3  | 2.56                     | 0.45              |
| 1:D:172:LEU:O    | 1:D:175:GLU:HB2  | 2.16                     | 0.45              |
| 1:E:310:GLU:O    | 1:E:314:ARG:HG3  | 2.16                     | 0.45              |
| 1:G:16:GLN:HB3   | 1:G:17:THR:H     | 1.60                     | 0.45              |
| 1:H:46:GLU:HG3   | 1:H:75:LYS:HB3   | 1.98                     | 0.45              |
| 1:J:119:ILE:HG13 | 1:J:120:ILE:N    | 2.32                     | 0.45              |
| 1:J:219:THR:OG1  | 1:J:222:ASP:HB2  | 2.16                     | 0.45              |
| 1:A:137:ASN:HD22 | 1:A:139:VAL:H    | 1.62                     | 0.45              |
| 1:C:105:ARG:O    | 1:C:138:PRO:HB3  | 2.16                     | 0.45              |
| 1:E:173:MET:HE1  | 1:E:203:MET:HG3  | 1.99                     | 0.45              |
| 1:F:293:ILE:HD13 | 1:H:179:VAL:HG12 | 1.97                     | 0.45              |
| 1:I:257:ASP:OD1  | 1:I:268:ARG:NH2  | 2.46                     | 0.45              |
| 1:J:309:SER:OG   | 1:J:310:GLU:N    | 2.49                     | 0.45              |
| 1:A:198:PRO:HG3  | 1:A:230:HIS:CG   | 2.51                     | 0.45              |
| 1:F:11:LEU:CD1   | 1:G:302:LEU:HD13 | 2.46                     | 0.45              |
| 1:F:220:ASP:O    | 1:F:222:ASP:N    | 2.49                     | 0.45              |
| 1:G:99:GLN:H     | 1:G:99:GLN:HG2   | 1.48                     | 0.45              |
| 1:G:180:HIS:ND1  | 1:G:182:LEU:HB2  | 2.30                     | 0.45              |
| 1:H:171:TYR:HA   | 1:H:181:PRO:HG3  | 1.97                     | 0.45              |
| 1:I:200:TRP:HB3  | 1:I:217:LEU:HD23 | 1.97                     | 0.45              |
| 1:J:145:VAL:O    | 1:J:149:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:58:LYS:HE2   | 1:B:243:LEU:HD11 | 1.99                     | 0.45              |
| 1:E:109:VAL:O    | 1:E:113:VAL:HG23 | 2.16                     | 0.45              |
| 1:F:21:LYS:NZ    | 1:F:84:VAL:O     | 2.38                     | 0.45              |
| 1:H:229:VAL:O    | 1:H:233:VAL:HG23 | 2.16                     | 0.45              |
| 1:L:317:LYS:HA   | 1:L:317:LYS:HD2  | 1.46                     | 0.45              |
| 1:B:50:VAL:HG22  | 1:B:79:GLY:O     | 2.16                     | 0.45              |
| 1:H:244:LYS:HD3  | 1:H:246:TYR:CZ   | 2.52                     | 0.45              |
| 1:I:110:GLN:HG2  | 3:I:402:HOH:O    | 2.15                     | 0.45              |
| 1:A:98:ARG:NE    | 3:A:703:HOH:O    | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:198:PRO:HG3  | 1:C:230:HIS:CG   | 2.51                     | 0.45              |
| 1:E:256:ALA:HA   | 1:E:259:ALA:HB3  | 1.98                     | 0.45              |
| 1:G:72:ARG:HH21  | 1:H:182:LEU:HD21 | 1.81                     | 0.45              |
| 1:J:173:MET:SD   | 1:J:184:CYS:HB3  | 2.57                     | 0.45              |
| 1:D:276:ILE:HG13 | 1:D:276:ILE:O    | 2.16                     | 0.45              |
| 1:F:97:ALA:O     | 1:F:108:LEU:HD23 | 2.16                     | 0.45              |
| 1:H:108:LEU:N    | 1:H:108:LEU:HD23 | 2.32                     | 0.45              |
| 1:J:64:LEU:O     | 1:J:67:GLY:N     | 2.32                     | 0.45              |
| 1:K:10:ASN:HD21  | 1:K:13:LYS:HE2   | 1.80                     | 0.45              |
| 1:B:280:TYR:HE2  | 1:B:307:LEU:HG   | 1.82                     | 0.45              |
| 1:E:16:GLN:N     | 1:E:16:GLN:OE1   | 2.49                     | 0.45              |
| 1:F:159:GLY:HA3  | 1:F:273:SER:HB3  | 1.98                     | 0.45              |
| 1:F:227:LYS:HG2  | 3:F:402:HOH:O    | 2.16                     | 0.45              |
| 1:G:195:SER:O    | 1:G:318:SER:OG   | 2.34                     | 0.45              |
| 1:L:320:ASP:O    | 1:L:323:TRP:N    | 2.49                     | 0.45              |
| 1:A:13:LYS:HG3   | 1:A:14:GLU:H     | 1.82                     | 0.45              |
| 1:B:274:THR:HG21 | 1:B:299:ILE:HG21 | 1.98                     | 0.45              |
| 1:F:274:THR:O    | 1:F:287:PHE:HA   | 2.16                     | 0.45              |
| 1:G:276:ILE:HD13 | 1:G:288:LEU:HD11 | 1.98                     | 0.45              |
| 1:I:280:TYR:O    | 1:I:316:LYS:HD3  | 2.16                     | 0.45              |
| 1:L:189:LEU:HD22 | 1:L:291:PRO:HD3  | 1.98                     | 0.45              |
| 1:D:132:LEU:HD23 | 1:D:132:LEU:HA   | 1.59                     | 0.45              |
| 1:H:131:LYS:HB2  | 1:H:131:LYS:HE2  | 1.73                     | 0.45              |
| 1:J:135:VAL:HG12 | 1:J:135:VAL:O    | 2.17                     | 0.45              |
| 1:K:83:ASN:HA    | 1:K:126:TYR:CD1  | 2.52                     | 0.45              |
| 1:D:120:ILE:O    | 1:D:124:VAL:HG13 | 2.16                     | 0.44              |
| 1:G:117:LYS:CE   | 1:G:331:PHE:HA   | 2.48                     | 0.44              |
| 1:J:14:GLU:OE1   | 1:J:14:GLU:N     | 2.39                     | 0.44              |
| 1:K:236:SER:HB3  | 1:L:66:HIS:CE1   | 2.52                     | 0.44              |
| 1:K:308:THR:HG1  | 1:K:311:GLU:H    | 1.59                     | 0.44              |
| 1:B:304:LYS:HB2  | 1:B:304:LYS:HE2  | 1.68                     | 0.44              |
| 1:E:216:ASP:O    | 1:E:219:THR:OG1  | 2.22                     | 0.44              |
| 1:I:25:VAL:HG11  | 1:I:93:ILE:HD13  | 1.99                     | 0.44              |
| 1:I:281:GLY:O    | 1:I:282:ILE:HD13 | 2.17                     | 0.44              |
| 1:J:153:PRO:HA   | 3:J:717:HOH:O    | 2.17                     | 0.44              |
| 1:J:308:THR:O    | 1:J:310:GLU:N    | 2.50                     | 0.44              |
| 1:K:307:LEU:HD22 | 1:K:311:GLU:HB3  | 1.99                     | 0.44              |
| 1:L:194:ASP:HB2  | 3:L:416:HOH:O    | 2.16                     | 0.44              |
| 1:A:301:ASP:HB3  | 1:D:8:ILE:CG2    | 2.48                     | 0.44              |
| 1:E:25:VAL:HB    | 1:E:93:ILE:HA    | 2.00                     | 0.44              |
| 1:E:180:HIS:CE1  | 1:E:182:LEU:HD12 | 2.53                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:200:TRP:HB3  | 1:E:217:LEU:HD23 | 1.99                     | 0.44              |
| 1:F:303:VAL:HG11 | 1:H:206:ALA:HB3  | 1.97                     | 0.44              |
| 1:H:57:LEU:HD21  | 1:H:79:GLY:H     | 1.83                     | 0.44              |
| 1:I:58:LYS:HG2   | 1:J:243:LEU:HD23 | 2.00                     | 0.44              |
| 1:I:284:ASP:HB2  | 1:I:286:VAL:HG23 | 1.97                     | 0.44              |
| 1:K:86:ALA:HA    | 1:K:126:TYR:O    | 2.18                     | 0.44              |
| 1:L:81:ASP:O     | 1:L:83:ASN:N     | 2.50                     | 0.44              |
| 1:I:170:ARG:HD3  | 1:I:184:CYS:O    | 2.18                     | 0.44              |
| 1:L:279:LEU:O    | 1:L:281:GLY:N    | 2.50                     | 0.44              |
| 1:C:21:LYS:HD2   | 1:C:46:GLU:CG    | 2.48                     | 0.44              |
| 1:C:210:LEU:HD23 | 1:C:210:LEU:HA   | 1.73                     | 0.44              |
| 1:I:147:TRP:CD1  | 1:I:152:PHE:O    | 2.70                     | 0.44              |
| 1:I:189:LEU:CD1  | 1:I:199:VAL:HG21 | 2.47                     | 0.44              |
| 1:K:3:LEU:HD13   | 1:L:214:HIS:HB2  | 2.00                     | 0.44              |
| 1:L:137:ASN:HA   | 1:L:139:VAL:N    | 2.33                     | 0.44              |
| 1:A:69:LEU:HD21  | 1:B:170:ARG:NH2  | 2.33                     | 0.44              |
| 1:B:198:PRO:HD3  | 1:B:230:HIS:CD2  | 2.52                     | 0.44              |
| 1:D:36:ILE:HD12  | 1:D:36:ILE:HA    | 1.78                     | 0.44              |
| 1:D:61:MET:HG3   | 1:D:76:ILE:HG22  | 1.99                     | 0.44              |
| 1:E:325:ILE:O    | 1:E:328:GLU:HB2  | 2.18                     | 0.44              |
| 1:H:141:ILE:O    | 1:H:145:VAL:HG23 | 2.18                     | 0.44              |
| 1:I:326:GLN:O    | 1:I:329:LEU:HB2  | 2.17                     | 0.44              |
| 1:J:17:THR:HG22  | 1:J:19:GLN:OE1   | 2.16                     | 0.44              |
| 1:J:274:THR:HB   | 1:J:299:ILE:HD13 | 2.00                     | 0.44              |
| 1:H:306:THR:O    | 1:H:307:LEU:HD23 | 2.18                     | 0.44              |
| 1:B:105:ARG:HE   | 1:B:192:HIS:CE1  | 2.36                     | 0.44              |
| 1:E:211:LYS:HD2  | 1:E:217:LEU:HB3  | 1.99                     | 0.44              |
| 1:F:105:ARG:C    | 1:F:107:ASN:N    | 2.71                     | 0.44              |
| 1:F:179:VAL:HG22 | 1:H:293:ILE:HD13 | 2.00                     | 0.44              |
| 1:F:305:VAL:HG12 | 1:H:208:VAL:CG2  | 2.48                     | 0.44              |
| 1:J:86:ALA:HA    | 1:J:126:TYR:HB3  | 1.99                     | 0.44              |
| 1:K:18:PRO:HB3   | 1:K:46:GLU:OE1   | 2.17                     | 0.44              |
| 1:L:21:LYS:HB3   | 1:L:88:SER:HA    | 2.00                     | 0.44              |
| 1:L:328:GLU:HB2  | 1:L:329:LEU:H    | 1.42                     | 0.44              |
| 1:E:56:LYS:HE2   | 1:E:56:LYS:HB2   | 1.72                     | 0.44              |
| 1:G:203:MET:O    | 1:G:210:LEU:HG   | 2.18                     | 0.44              |
| 1:H:235:GLU:O    | 1:H:239:GLU:HG2  | 2.18                     | 0.44              |
| 1:H:261:SER:OG   | 1:H:268:ARG:HB2  | 2.17                     | 0.44              |
| 1:J:36:ILE:O     | 1:J:40:MET:HG3   | 2.17                     | 0.44              |
| 1:D:105:ARG:C    | 1:D:106:LEU:HD12 | 2.38                     | 0.43              |
| 1:K:209:SER:O    | 1:K:213:LEU:HD23 | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:119:ILE:O    | 1:L:122:ASN:HB2  | 2.18                     | 0.43              |
| 1:A:125:LYS:HG2  | 1:A:126:TYR:CD2  | 2.53                     | 0.43              |
| 1:D:228:GLU:HG2  | 1:D:231:LYS:HD2  | 2.00                     | 0.43              |
| 1:D:270:HIS:HB2  | 1:D:294:LEU:HD13 | 1.99                     | 0.43              |
| 1:E:58:LYS:HG2   | 1:F:243:LEU:HD13 | 2.00                     | 0.43              |
| 1:G:323:TRP:HA   | 1:G:326:GLN:HB2  | 1.99                     | 0.43              |
| 1:H:273:SER:HA   | 1:H:289:SER:HA   | 2.00                     | 0.43              |
| 1:I:11:LEU:HD11  | 1:L:302:LEU:CD1  | 2.49                     | 0.43              |
| 1:K:30:VAL:HG22  | 1:K:251:ILE:HG21 | 2.00                     | 0.43              |
| 1:C:25:VAL:HG22  | 1:C:50:VAL:CG2   | 2.48                     | 0.43              |
| 1:C:169:PHE:CD1  | 1:C:233:VAL:HG21 | 2.50                     | 0.43              |
| 1:E:124:VAL:HG13 | 1:E:152:PHE:CE1  | 2.53                     | 0.43              |
| 1:E:239:GLU:OE2  | 1:E:243:LEU:HG   | 2.17                     | 0.43              |
| 1:F:24:VAL:HG22  | 1:F:92:ILE:HB    | 1.99                     | 0.43              |
| 1:F:227:LYS:HB2  | 1:F:227:LYS:HE3  | 1.57                     | 0.43              |
| 1:G:105:ARG:NH1  | 1:G:193:GLY:HA2  | 2.34                     | 0.43              |
| 1:I:264:LYS:HE3  | 1:L:72:ARG:HG2   | 2.00                     | 0.43              |
| 1:J:127:SER:HB3  | 1:J:130:CYS:HB3  | 2.00                     | 0.43              |
| 1:A:218:GLY:C    | 1:A:227:LYS:HD3  | 2.39                     | 0.43              |
| 1:B:297:ASN:HB2  | 1:C:12:LEU:HD21  | 2.00                     | 0.43              |
| 1:D:25:VAL:HG22  | 1:D:50:VAL:CG2   | 2.48                     | 0.43              |
| 1:F:56:LYS:HE2   | 1:F:60:GLU:OE2   | 2.19                     | 0.43              |
| 1:H:284:ASP:O    | 1:H:286:VAL:N    | 2.52                     | 0.43              |
| 1:J:261:SER:HA   | 1:J:266:LEU:HG   | 2.00                     | 0.43              |
| 1:K:111:ARG:NH1  | 3:K:707:HOH:O    | 2.48                     | 0.43              |
| 1:L:294:LEU:HD12 | 1:L:294:LEU:HA   | 1.81                     | 0.43              |
| 1:B:9:TYR:HB2    | 1:C:304:LYS:HD2  | 2.00                     | 0.43              |
| 1:C:147:TRP:HA   | 1:C:157:VAL:HG21 | 2.00                     | 0.43              |
| 1:D:275:MET:HG2  | 1:D:287:PHE:CZ   | 2.52                     | 0.43              |
| 1:H:111:ARG:HG3  | 3:H:410:HOH:O    | 2.18                     | 0.43              |
| 1:I:57:LEU:HD21  | 1:I:79:GLY:N     | 2.33                     | 0.43              |
| 1:L:163:ASN:HA   | 1:L:271:PRO:HG2  | 2.00                     | 0.43              |
| 1:A:82:TYR:CG    | 1:A:122:ASN:HB3  | 2.53                     | 0.43              |
| 1:E:22:ILE:HD11  | 1:E:263:MET:HG3  | 1.99                     | 0.43              |
| 1:G:72:ARG:NH2   | 1:H:182:LEU:HD21 | 2.33                     | 0.43              |
| 1:J:116:PHE:CZ   | 1:J:142:LEU:HD22 | 2.53                     | 0.43              |
| 1:F:173:MET:SD   | 1:F:184:CYS:HB3  | 2.59                     | 0.43              |
| 1:G:139:VAL:HG21 | 1:G:160:SER:HB3  | 2.00                     | 0.43              |
| 1:J:7:LEU:HG     | 1:J:8:ILE:CG1    | 2.48                     | 0.43              |
| 1:K:25:VAL:HG21  | 1:K:93:ILE:CD1   | 2.48                     | 0.43              |
| 1:C:171:TYR:CE1  | 1:C:175:GLU:HG2  | 2.53                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:100:GLN:HG2  | 1:D:101:GLU:H    | 1.82                     | 0.43              |
| 1:E:243:LEU:HB3  | 1:F:55:ASP:O     | 2.19                     | 0.43              |
| 1:G:54:GLU:OE2   | 1:G:80:LYS:HD2   | 2.18                     | 0.43              |
| 1:G:57:LEU:HD21  | 1:G:79:GLY:H     | 1.84                     | 0.43              |
| 1:G:329:LEU:O    | 1:G:330:GLN:HG2  | 2.18                     | 0.43              |
| 1:H:14:GLU:HG3   | 1:H:15:GLU:HB3   | 2.01                     | 0.43              |
| 1:I:210:LEU:HD23 | 1:I:210:LEU:HA   | 1.79                     | 0.43              |
| 1:J:187:TRP:CZ2  | 1:L:206:ALA:HA   | 2.54                     | 0.43              |
| 1:K:228:GLU:O    | 1:K:232:GLN:HG3  | 2.18                     | 0.43              |
| 1:K:276:ILE:CD1  | 1:K:276:ILE:O    | 2.67                     | 0.43              |
| 1:K:331:PHE:HD1  | 1:K:331:PHE:OXT  | 2.01                     | 0.43              |
| 1:L:110:GLN:HG2  | 1:L:329:LEU:HD22 | 2.00                     | 0.43              |
| 1:D:111:ARG:O    | 1:D:114:ASN:HB2  | 2.18                     | 0.43              |
| 1:F:7:LEU:HD23   | 1:F:8:ILE:HG13   | 2.01                     | 0.43              |
| 1:I:172:LEU:O    | 1:I:175:GLU:HB3  | 2.18                     | 0.43              |
| 1:J:228:GLU:O    | 1:J:232:GLN:HG3  | 2.19                     | 0.43              |
| 1:J:277:LYS:HB3  | 1:J:277:LYS:HE3  | 1.63                     | 0.43              |
| 1:K:147:TRP:CH2  | 1:K:275:MET:HE1  | 2.53                     | 0.43              |
| 1:K:276:ILE:CD1  | 1:K:282:ILE:HG21 | 2.48                     | 0.43              |
| 1:A:231:LYS:HD3  | 1:A:231:LYS:HA   | 1.74                     | 0.43              |
| 1:D:173:MET:SD   | 1:D:184:CYS:HB3  | 2.59                     | 0.43              |
| 1:F:331:PHE:O    | 1:F:331:PHE:CG   | 2.71                     | 0.43              |
| 1:G:21:LYS:HD3   | 1:G:86:ALA:O     | 2.19                     | 0.43              |
| 1:H:165:ASP:OD2  | 1:H:192:HIS:ND1  | 2.52                     | 0.43              |
| 1:I:236:SER:C    | 1:I:238:TYR:H    | 2.22                     | 0.43              |
| 1:I:275:MET:HE1  | 1:I:277:LYS:HD2  | 2.01                     | 0.43              |
| 1:A:316:LYS:O    | 1:A:319:ALA:HB3  | 2.19                     | 0.42              |
| 1:B:305:VAL:HA   | 1:D:208:VAL:HG21 | 2.00                     | 0.42              |
| 1:D:16:GLN:O     | 1:D:17:THR:C     | 2.57                     | 0.42              |
| 1:E:23:THR:HB    | 1:E:91:VAL:HG22  | 2.00                     | 0.42              |
| 1:E:71:LEU:HD21  | 1:F:253:LEU:HD21 | 2.01                     | 0.42              |
| 1:F:51:ASP:N     | 1:F:57:LEU:HD13  | 2.34                     | 0.42              |
| 1:F:103:GLU:OE1  | 1:F:108:LEU:HD11 | 2.19                     | 0.42              |
| 1:G:3:LEU:N      | 1:H:224:GLU:OE1  | 2.50                     | 0.42              |
| 1:G:16:GLN:O     | 3:G:703:HOH:O    | 2.21                     | 0.42              |
| 1:H:2:THR:OG1    | 1:H:5:ASP:OD2    | 2.37                     | 0.42              |
| 1:H:180:HIS:ND1  | 1:H:181:PRO:HD2  | 2.34                     | 0.42              |
| 1:J:12:LEU:HB3   | 1:J:13:LYS:H     | 1.63                     | 0.42              |
| 1:J:231:LYS:HA   | 1:J:234:VAL:HG22 | 2.01                     | 0.42              |
| 1:L:276:ILE:HD13 | 1:L:288:LEU:HB2  | 2.01                     | 0.42              |
| 1:A:206:ALA:HB3  | 1:C:303:VAL:HG11 | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:114:ASN:HA   | 1:C:117:LYS:HG2  | 2.01                     | 0.42              |
| 1:C:131:LYS:HE3  | 1:C:296:GLN:O    | 2.19                     | 0.42              |
| 1:C:325:ILE:O    | 1:C:329:LEU:HD13 | 2.19                     | 0.42              |
| 1:G:281:GLY:HA3  | 1:G:316:LYS:NZ   | 2.35                     | 0.42              |
| 1:H:158:ILE:HG12 | 1:H:294:LEU:HD11 | 2.01                     | 0.42              |
| 1:H:188:VAL:HG12 | 1:H:196:SER:HB3  | 2.01                     | 0.42              |
| 1:I:266:LEU:HD12 | 1:I:268:ARG:NH1  | 2.34                     | 0.42              |
| 1:J:148:LYS:CB   | 1:J:331:PHE:HE2  | 2.33                     | 0.42              |
| 1:J:323:TRP:NE1  | 1:J:327:LYS:HB3  | 2.33                     | 0.42              |
| 1:B:227:LYS:HE2  | 1:B:227:LYS:HB3  | 1.90                     | 0.42              |
| 1:B:244:LYS:O    | 1:B:246:TYR:N    | 2.50                     | 0.42              |
| 1:C:177:LEU:HD11 | 1:C:210:LEU:HD11 | 2.02                     | 0.42              |
| 1:D:168:ARG:NH2  | 2:D:601:MLI:O7   | 2.42                     | 0.42              |
| 1:E:276:ILE:CD1  | 1:E:282:ILE:HG21 | 2.47                     | 0.42              |
| 1:K:122:ASN:OD1  | 1:K:122:ASN:N    | 2.51                     | 0.42              |
| 1:L:251:ILE:HD12 | 1:L:251:ILE:N    | 2.34                     | 0.42              |
| 1:D:158:ILE:HG12 | 1:D:299:ILE:HD11 | 2.01                     | 0.42              |
| 1:G:133:LEU:HD23 | 1:G:158:ILE:HB   | 2.01                     | 0.42              |
| 1:G:232:GLN:O    | 1:G:236:SER:HB3  | 2.19                     | 0.42              |
| 1:I:231:LYS:HE2  | 1:I:235:GLU:OE1  | 2.18                     | 0.42              |
| 1:J:219:THR:HB   | 1:J:221:LYS:H    | 1.85                     | 0.42              |
| 1:A:105:ARG:HD3  | 1:A:137:ASN:CG   | 2.39                     | 0.42              |
| 1:A:170:ARG:NH1  | 3:A:705:HOH:O    | 2.52                     | 0.42              |
| 1:B:48:ALA:HA    | 1:B:77:VAL:O     | 2.19                     | 0.42              |
| 1:B:320:ASP:O    | 1:B:322:LEU:N    | 2.52                     | 0.42              |
| 1:C:267:ARG:HE   | 1:C:267:ARG:HB3  | 1.74                     | 0.42              |
| 1:D:228:GLU:HG2  | 1:D:231:LYS:HB3  | 2.01                     | 0.42              |
| 1:F:142:LEU:HD23 | 1:F:142:LEU:HA   | 1.82                     | 0.42              |
| 1:F:272:VAL:O    | 1:F:289:SER:HA   | 2.19                     | 0.42              |
| 1:A:10:ASN:ND2   | 1:A:13:LYS:HD3   | 2.14                     | 0.42              |
| 1:A:13:LYS:HA    | 1:A:13:LYS:HD2   | 1.30                     | 0.42              |
| 1:B:108:LEU:O    | 1:B:111:ARG:N    | 2.44                     | 0.42              |
| 1:D:7:LEU:O      | 1:D:7:LEU:HG     | 2.20                     | 0.42              |
| 1:D:50:VAL:HA    | 1:D:79:GLY:O     | 2.20                     | 0.42              |
| 1:D:108:LEU:O    | 1:D:110:GLN:N    | 2.52                     | 0.42              |
| 1:G:41:LYS:NZ    | 1:G:256:ALA:HB1  | 2.35                     | 0.42              |
| 1:I:25:VAL:O     | 1:I:94:THR:OG1   | 2.30                     | 0.42              |
| 1:I:276:ILE:HG12 | 1:I:276:ILE:O    | 2.20                     | 0.42              |
| 1:I:283:LYS:HB2  | 1:I:283:LYS:HE3  | 1.89                     | 0.42              |
| 1:J:19:GLN:NE2   | 1:J:19:GLN:HA    | 2.35                     | 0.42              |
| 1:J:301:ASP:HB3  | 1:K:8:ILE:CG2    | 2.50                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:131:LYS:HB2  | 1:K:131:LYS:HE2  | 1.74                     | 0.42              |
| 1:B:82:TYR:O     | 1:B:85:THR:HB    | 2.19                     | 0.42              |
| 1:C:278:GLY:O    | 1:C:279:LEU:HD12 | 2.19                     | 0.42              |
| 1:G:70:PHE:CE2   | 1:H:254:SER:HA   | 2.55                     | 0.42              |
| 1:L:176:ARG:HH21 | 1:L:229:VAL:HG23 | 1.84                     | 0.42              |
| 1:A:105:ARG:HH21 | 2:A:601:MLI:C1   | 2.31                     | 0.42              |
| 1:G:69:LEU:HD12  | 1:H:182:LEU:HD12 | 2.01                     | 0.42              |
| 1:G:158:ILE:HG23 | 1:G:299:ILE:HD11 | 2.01                     | 0.42              |
| 1:J:105:ARG:NH1  | 1:J:238:TYR:OH   | 2.53                     | 0.42              |
| 1:B:11:LEU:O     | 1:B:12:LEU:HG    | 2.19                     | 0.42              |
| 1:B:229:VAL:HG12 | 1:B:232:GLN:NE2  | 2.35                     | 0.42              |
| 1:C:153:PRO:HB2  | 1:C:155:ASN:OD1  | 2.20                     | 0.42              |
| 1:I:13:LYS:N     | 1:I:14:GLU:OE2   | 2.44                     | 0.42              |
| 1:I:25:VAL:CG1   | 1:I:93:ILE:HD13  | 2.50                     | 0.42              |
| 1:I:304:LYS:HZ2  | 1:I:304:LYS:HG3  | 1.53                     | 0.42              |
| 1:A:211:LYS:HD2  | 1:A:217:LEU:HB3  | 2.01                     | 0.42              |
| 1:B:82:TYR:OH    | 1:B:119:ILE:HG23 | 2.20                     | 0.42              |
| 1:B:293:ILE:HB   | 1:B:301:ASP:HB2  | 2.02                     | 0.42              |
| 1:E:119:ILE:O    | 1:E:123:VAL:HG23 | 2.19                     | 0.42              |
| 1:J:316:LYS:HD3  | 1:J:320:ASP:OD2  | 2.19                     | 0.42              |
| 1:K:226:TRP:O    | 1:K:229:VAL:HB   | 2.19                     | 0.42              |
| 1:K:235:GLU:OE1  | 1:K:239:GLU:HG2  | 2.19                     | 0.42              |
| 1:L:50:VAL:HG11  | 1:L:82:TYR:CE1   | 2.55                     | 0.42              |
| 1:E:3:LEU:O      | 1:E:6:GLN:HB2    | 2.20                     | 0.41              |
| 1:E:192:HIS:NE2  | 2:E:601:MLI:O9   | 2.53                     | 0.41              |
| 1:G:244:LYS:HE2  | 1:H:60:GLU:OE2   | 2.20                     | 0.41              |
| 1:I:168:ARG:CZ   | 1:I:237:ALA:HB2  | 2.50                     | 0.41              |
| 1:J:96:GLY:HA3   | 1:J:112:ASN:HD21 | 1.85                     | 0.41              |
| 1:K:98:ARG:NH1   | 3:K:702:HOH:O    | 2.53                     | 0.41              |
| 1:K:216:ASP:O    | 1:K:222:ASP:HB2  | 2.20                     | 0.41              |
| 1:L:117:LYS:O    | 1:L:121:PRO:HG2  | 2.20                     | 0.41              |
| 1:B:244:LYS:HE3  | 1:B:246:TYR:O    | 2.20                     | 0.41              |
| 1:D:14:GLU:HG2   | 1:D:15:GLU:H     | 1.85                     | 0.41              |
| 1:I:36:ILE:HD12  | 1:I:36:ILE:HA    | 1.78                     | 0.41              |
| 1:J:21:LYS:HE3   | 1:J:46:GLU:HG2   | 2.02                     | 0.41              |
| 1:L:330:GLN:O    | 1:L:331:PHE:O    | 2.38                     | 0.41              |
| 1:A:243:LEU:HD11 | 1:B:58:LYS:HE3   | 2.03                     | 0.41              |
| 1:B:272:VAL:O    | 1:B:289:SER:HA   | 2.20                     | 0.41              |
| 1:C:69:LEU:HD21  | 1:D:170:ARG:NH2  | 2.34                     | 0.41              |
| 1:G:96:GLY:HA3   | 1:G:112:ASN:OD1  | 2.20                     | 0.41              |
| 1:I:25:VAL:CG1   | 1:I:93:ILE:HA    | 2.50                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:259:ALA:O    | 1:I:263:MET:HG2  | 2.21                     | 0.41              |
| 1:K:82:TYR:O     | 1:K:85:THR:HB    | 2.20                     | 0.41              |
| 1:L:110:GLN:NE2  | 1:L:329:LEU:HA   | 2.35                     | 0.41              |
| 1:L:243:LEU:HD12 | 1:L:243:LEU:HA   | 1.77                     | 0.41              |
| 1:B:300:SER:HB3  | 1:C:12:LEU:CD2   | 2.47                     | 0.41              |
| 1:C:17:THR:HG22  | 1:C:87:ASN:HD21  | 1.85                     | 0.41              |
| 1:C:145:VAL:O    | 1:C:149:ILE:HG13 | 2.19                     | 0.41              |
| 1:C:188:VAL:HA   | 1:C:197:VAL:O    | 2.21                     | 0.41              |
| 1:C:214:HIS:CB   | 1:D:3:LEU:HD13   | 2.51                     | 0.41              |
| 1:D:26:GLY:O     | 1:D:31:GLY:HA3   | 2.19                     | 0.41              |
| 1:E:169:PHE:HD2  | 1:E:188:VAL:HG22 | 1.82                     | 0.41              |
| 1:F:107:ASN:C    | 1:F:109:VAL:H    | 2.22                     | 0.41              |
| 1:F:214:HIS:O    | 1:F:216:ASP:N    | 2.53                     | 0.41              |
| 1:B:230:HIS:O    | 1:B:230:HIS:CG   | 2.73                     | 0.41              |
| 1:D:109:VAL:HG21 | 1:D:325:ILE:HG21 | 2.02                     | 0.41              |
| 1:D:219:THR:HG22 | 1:D:222:ASP:HB2  | 2.02                     | 0.41              |
| 1:F:165:ASP:OD1  | 1:F:192:HIS:CE1  | 2.73                     | 0.41              |
| 1:G:192:HIS:O    | 1:G:192:HIS:CG   | 2.73                     | 0.41              |
| 1:H:109:VAL:O    | 1:H:113:VAL:HG23 | 2.20                     | 0.41              |
| 1:H:197:VAL:HG13 | 1:H:314:ARG:HH11 | 1.85                     | 0.41              |
| 1:I:158:ILE:HG23 | 1:I:272:VAL:HG21 | 2.02                     | 0.41              |
| 1:K:133:LEU:HD12 | 1:K:133:LEU:HA   | 1.80                     | 0.41              |
| 1:K:200:TRP:C    | 1:K:202:GLY:H    | 2.23                     | 0.41              |
| 1:B:105:ARG:HH11 | 1:B:105:ARG:HG2  | 1.86                     | 0.41              |
| 1:B:230:HIS:O    | 1:B:233:VAL:HG22 | 2.21                     | 0.41              |
| 1:F:12:LEU:O     | 1:F:13:LYS:HB2   | 2.20                     | 0.41              |
| 1:F:121:PRO:HA   | 1:F:124:VAL:HG22 | 2.02                     | 0.41              |
| 1:H:107:ASN:O    | 1:H:109:VAL:N    | 2.45                     | 0.41              |
| 1:H:197:VAL:HG13 | 1:H:314:ARG:NH1  | 2.36                     | 0.41              |
| 1:I:9:TYR:CG     | 1:I:10:ASN:N     | 2.89                     | 0.41              |
| 1:J:216:ASP:O    | 1:J:219:THR:HG23 | 2.20                     | 0.41              |
| 1:K:147:TRP:CZ3  | 1:K:275:MET:HE1  | 2.55                     | 0.41              |
| 1:L:41:LYS:HD2   | 1:L:256:ALA:HB1  | 2.02                     | 0.41              |
| 1:L:80:LYS:HE3   | 1:L:80:LYS:HB3   | 1.82                     | 0.41              |
| 1:A:209:SER:OG   | 1:A:212:THR:HG23 | 2.21                     | 0.41              |
| 1:B:85:THR:HG22  | 1:B:127:SER:OG   | 2.20                     | 0.41              |
| 1:D:48:ALA:HA    | 1:D:77:VAL:O     | 2.20                     | 0.41              |
| 1:E:276:ILE:C    | 1:E:276:ILE:CD1  | 2.88                     | 0.41              |
| 1:H:189:LEU:HD12 | 1:H:199:VAL:HG21 | 2.03                     | 0.41              |
| 1:K:224:GLU:HB3  | 1:K:226:TRP:HD1  | 1.78                     | 0.41              |
| 1:L:99:GLN:HA    | 1:L:103:GLU:OE2  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:8:ILE:CG2    | 1:D:301:ASP:HB3  | 2.50                     | 0.41              |
| 1:A:173:MET:HE2  | 1:A:173:MET:HB2  | 1.78                     | 0.41              |
| 1:C:164:LEU:CD2  | 1:C:251:ILE:HG13 | 2.51                     | 0.41              |
| 1:C:294:LEU:HA   | 1:C:294:LEU:HD23 | 1.80                     | 0.41              |
| 1:E:41:LYS:HB3   | 1:E:41:LYS:HE3   | 1.92                     | 0.41              |
| 1:E:226:TRP:CZ2  | 1:F:3:LEU:HD23   | 2.56                     | 0.41              |
| 1:F:39:LEU:HD11  | 1:F:64:LEU:HD13  | 2.02                     | 0.41              |
| 1:F:57:LEU:HD21  | 1:F:79:GLY:H     | 1.85                     | 0.41              |
| 1:G:7:LEU:HD12   | 1:G:7:LEU:O      | 2.19                     | 0.41              |
| 1:J:162:CYS:HB3  | 1:J:165:ASP:HB2  | 2.03                     | 0.41              |
| 1:L:280:TYR:HE1  | 1:L:307:LEU:HG   | 1.86                     | 0.41              |
| 1:A:154:LYS:HZ1  | 1:D:11:LEU:HG    | 1.85                     | 0.41              |
| 1:A:282:ILE:HG21 | 1:A:286:VAL:CG1  | 2.51                     | 0.41              |
| 1:C:272:VAL:O    | 1:C:289:SER:HA   | 2.19                     | 0.41              |
| 1:D:85:THR:HG22  | 1:D:85:THR:O     | 2.21                     | 0.41              |
| 1:E:125:LYS:HB3  | 1:E:125:LYS:HE2  | 1.90                     | 0.41              |
| 1:E:274:THR:HG21 | 1:E:302:LEU:HD11 | 2.02                     | 0.41              |
| 1:G:13:LYS:O     | 1:G:15:GLU:HG3   | 2.21                     | 0.41              |
| 1:G:330:GLN:NE2  | 3:G:707:HOH:O    | 2.54                     | 0.41              |
| 1:H:91:VAL:HB    | 1:H:132:LEU:HD23 | 2.02                     | 0.41              |
| 1:H:113:VAL:HG13 | 1:H:145:VAL:HG11 | 2.03                     | 0.41              |
| 1:H:173:MET:HE1  | 1:H:203:MET:HG2  | 2.02                     | 0.41              |
| 1:H:277:LYS:HG3  | 1:H:284:ASP:N    | 2.36                     | 0.41              |
| 1:I:111:ARG:O    | 1:I:115:ILE:HG12 | 2.21                     | 0.41              |
| 1:I:267:ARG:HA   | 1:I:294:LEU:O    | 2.21                     | 0.41              |
| 1:J:22:ILE:HD12  | 1:J:44:ALA:HB2   | 2.03                     | 0.41              |
| 1:J:286:VAL:HG21 | 1:J:319:ALA:HB1  | 2.02                     | 0.41              |
| 1:K:155:ASN:O    | 1:K:298:GLY:HA3  | 2.21                     | 0.41              |
| 1:B:253:LEU:HA   | 1:B:253:LEU:HD23 | 1.87                     | 0.41              |
| 1:C:307:LEU:HD23 | 1:C:307:LEU:HA   | 1.77                     | 0.41              |
| 1:E:24:VAL:HB    | 1:E:49:LEU:HD23  | 2.02                     | 0.41              |
| 1:I:224:GLU:HB3  | 1:I:226:TRP:CD1  | 2.56                     | 0.41              |
| 1:J:82:TYR:O     | 1:J:85:THR:HB    | 2.20                     | 0.41              |
| 1:J:180:HIS:ND1  | 1:J:181:PRO:HD2  | 2.36                     | 0.41              |
| 1:J:308:THR:N    | 1:J:311:GLU:OE2  | 2.44                     | 0.41              |
| 1:B:286:VAL:CG1  | 1:B:287:PHE:N    | 2.84                     | 0.40              |
| 1:B:300:SER:CA   | 1:C:12:LEU:HD22  | 2.49                     | 0.40              |
| 1:E:120:ILE:HB   | 1:E:121:PRO:HD3  | 2.04                     | 0.40              |
| 1:G:98:ARG:NH2   | 1:G:136:SER:HA   | 2.35                     | 0.40              |
| 1:I:266:LEU:O    | 1:K:180:HIS:HB2  | 2.20                     | 0.40              |
| 1:L:120:ILE:HD13 | 1:L:120:ILE:HA   | 1.95                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:VAL:O    | 1:A:113:VAL:HG23 | 2.22                     | 0.40              |
| 1:B:111:ARG:HD3  | 1:B:111:ARG:N    | 2.36                     | 0.40              |
| 1:C:133:LEU:HD12 | 1:C:133:LEU:HA   | 1.91                     | 0.40              |
| 1:C:239:GLU:O    | 1:C:243:LEU:HD13 | 2.21                     | 0.40              |
| 1:F:189:LEU:HD23 | 1:F:189:LEU:HA   | 1.88                     | 0.40              |
| 1:F:301:ASP:HB3  | 1:G:8:ILE:CG2    | 2.51                     | 0.40              |
| 1:G:41:LYS:HZ3   | 1:G:41:LYS:CB    | 2.33                     | 0.40              |
| 1:G:47:LEU:HA    | 1:G:47:LEU:HD12  | 1.78                     | 0.40              |
| 1:G:187:TRP:CH2  | 1:G:269:VAL:HG12 | 2.56                     | 0.40              |
| 1:J:316:LYS:NZ   | 1:J:320:ASP:OD1  | 2.48                     | 0.40              |
| 1:C:39:LEU:CD1   | 1:C:64:LEU:HD22  | 2.52                     | 0.40              |
| 1:C:81:ASP:O     | 1:C:83:ASN:N     | 2.54                     | 0.40              |
| 1:D:15:GLU:CG    | 1:D:16:GLN:N     | 2.83                     | 0.40              |
| 1:F:256:ALA:HA   | 1:F:259:ALA:HB3  | 2.02                     | 0.40              |
| 1:H:276:ILE:HG22 | 1:H:302:LEU:HD13 | 2.03                     | 0.40              |
| 1:I:142:LEU:HD23 | 1:I:142:LEU:HA   | 1.93                     | 0.40              |
| 1:J:165:ASP:O    | 1:J:233:VAL:HG21 | 2.22                     | 0.40              |
| 1:K:163:ASN:HA   | 1:K:271:PRO:HG2  | 2.04                     | 0.40              |
| 1:L:4:LYS:HG2    | 1:L:4:LYS:O      | 2.22                     | 0.40              |
| 1:L:50:VAL:HG11  | 1:L:82:TYR:CZ    | 2.56                     | 0.40              |
| 1:L:144:TYR:HE1  | 1:L:148:LYS:HZ3  | 1.67                     | 0.40              |
| 1:L:279:LEU:C    | 1:L:281:GLY:H    | 2.25                     | 0.40              |
| 1:A:2:THR:HG23   | 1:B:224:GLU:OE2  | 2.20                     | 0.40              |
| 1:D:99:GLN:HE21  | 1:D:105:ARG:HA   | 1.85                     | 0.40              |
| 1:D:137:ASN:HA   | 1:D:139:VAL:N    | 2.36                     | 0.40              |
| 1:D:275:MET:HG2  | 1:D:287:PHE:CD1  | 2.55                     | 0.40              |
| 1:E:171:TYR:HA   | 1:E:181:PRO:HG3  | 2.02                     | 0.40              |
| 1:F:22:ILE:O     | 1:F:47:LEU:HA    | 2.21                     | 0.40              |
| 1:F:48:ALA:HA    | 1:F:77:VAL:O     | 2.21                     | 0.40              |
| 1:I:49:LEU:O     | 1:I:78:SER:HA    | 2.21                     | 0.40              |
| 1:J:50:VAL:HG21  | 1:J:82:TYR:CZ    | 2.56                     | 0.40              |
| 1:J:216:ASP:O    | 1:J:217:LEU:C    | 2.59                     | 0.40              |
| 1:L:109:VAL:HG21 | 1:L:325:ILE:HG21 | 2.03                     | 0.40              |
| 1:L:117:LYS:H    | 1:L:117:LYS:HG3  | 1.65                     | 0.40              |
| 1:A:72:ARG:HE    | 1:D:260:GLU:CD   | 2.25                     | 0.40              |
| 1:A:204:ASN:HB3  | 1:A:209:SER:HA   | 2.03                     | 0.40              |
| 1:G:71:LEU:HD23  | 1:G:71:LEU:HA    | 1.79                     | 0.40              |
| 1:G:97:ALA:O     | 1:G:108:LEU:HD22 | 2.21                     | 0.40              |
| 1:G:110:GLN:OE1  | 1:G:110:GLN:HA   | 2.21                     | 0.40              |
| 1:L:64:LEU:HA    | 1:L:64:LEU:HD23  | 1.81                     | 0.40              |
| 1:L:176:ARG:HD3  | 1:L:229:VAL:HG21 | 2.03                     | 0.40              |

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

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:F:117:LYS:NZ | 1:I:15:GLU:OE2[1_655] | 2.08                     | 0.12              |

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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     | 329/337 (98%)   | 304 (92%)  | 18 (6%)  | 7 (2%)   | 7 24        |
| 1   | B     | 329/337 (98%)   | 279 (85%)  | 38 (12%) | 12 (4%)  | 3 13        |
| 1   | C     | 329/337 (98%)   | 278 (84%)  | 40 (12%) | 11 (3%)  | 4 14        |
| 1   | D     | 329/337 (98%)   | 290 (88%)  | 27 (8%)  | 12 (4%)  | 3 13        |
| 1   | E     | 329/337 (98%)   | 302 (92%)  | 20 (6%)  | 7 (2%)   | 7 24        |
| 1   | F     | 329/337 (98%)   | 291 (88%)  | 29 (9%)  | 9 (3%)   | 5 18        |
| 1   | G     | 329/337 (98%)   | 303 (92%)  | 19 (6%)  | 7 (2%)   | 7 24        |
| 1   | H     | 329/337 (98%)   | 294 (89%)  | 26 (8%)  | 9 (3%)   | 5 18        |
| 1   | I     | 329/337 (98%)   | 274 (83%)  | 41 (12%) | 14 (4%)  | 2 9         |
| 1   | J     | 329/337 (98%)   | 287 (87%)  | 31 (9%)  | 11 (3%)  | 4 14        |
| 1   | K     | 329/337 (98%)   | 286 (87%)  | 34 (10%) | 9 (3%)   | 5 18        |
| 1   | L     | 329/337 (98%)   | 280 (85%)  | 33 (10%) | 16 (5%)  | 2 7         |
| All | All   | 3948/4044 (98%) | 3468 (88%) | 356 (9%) | 124 (3%) | 4 15        |

All (124) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | GLU  |
| 1   | A     | 219 | THR  |
| 1   | A     | 308 | THR  |
| 1   | B     | 15  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 105 | ARG  |
| 1   | B     | 109 | VAL  |
| 1   | B     | 152 | PHE  |
| 1   | B     | 282 | ILE  |
| 1   | B     | 321 | THR  |
| 1   | C     | 101 | GLU  |
| 1   | C     | 194 | ASP  |
| 1   | C     | 309 | SER  |
| 1   | D     | 14  | GLU  |
| 1   | D     | 16  | GLN  |
| 1   | D     | 105 | ARG  |
| 1   | D     | 217 | LEU  |
| 1   | E     | 14  | GLU  |
| 1   | E     | 192 | HIS  |
| 1   | E     | 285 | ASP  |
| 1   | F     | 154 | LYS  |
| 1   | F     | 285 | ASP  |
| 1   | G     | 16  | GLN  |
| 1   | G     | 160 | SER  |
| 1   | G     | 285 | ASP  |
| 1   | H     | 108 | LEU  |
| 1   | I     | 13  | LYS  |
| 1   | I     | 101 | GLU  |
| 1   | I     | 104 | SER  |
| 1   | I     | 105 | ARG  |
| 1   | I     | 151 | GLY  |
| 1   | I     | 236 | SER  |
| 1   | I     | 304 | LYS  |
| 1   | J     | 105 | ARG  |
| 1   | J     | 309 | SER  |
| 1   | K     | 14  | GLU  |
| 1   | K     | 201 | SER  |
| 1   | K     | 329 | LEU  |
| 1   | L     | 15  | GLU  |
| 1   | L     | 16  | GLN  |
| 1   | L     | 104 | SER  |
| 1   | L     | 152 | PHE  |
| 1   | L     | 321 | THR  |
| 1   | L     | 329 | LEU  |
| 1   | A     | 206 | ALA  |
| 1   | A     | 221 | LYS  |
| 1   | B     | 245 | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 15  | GLU  |
| 1   | C     | 16  | GLN  |
| 1   | C     | 82  | TYR  |
| 1   | C     | 246 | TYR  |
| 1   | D     | 15  | GLU  |
| 1   | D     | 107 | ASN  |
| 1   | D     | 309 | SER  |
| 1   | E     | 13  | LYS  |
| 1   | E     | 15  | GLU  |
| 1   | E     | 85  | THR  |
| 1   | E     | 219 | THR  |
| 1   | F     | 13  | LYS  |
| 1   | F     | 106 | LEU  |
| 1   | F     | 221 | LYS  |
| 1   | G     | 72  | ARG  |
| 1   | H     | 119 | ILE  |
| 1   | H     | 285 | ASP  |
| 1   | I     | 14  | GLU  |
| 1   | I     | 225 | GLN  |
| 1   | I     | 275 | MET  |
| 1   | J     | 14  | GLU  |
| 1   | J     | 15  | GLU  |
| 1   | J     | 98  | ARG  |
| 1   | J     | 103 | GLU  |
| 1   | J     | 109 | VAL  |
| 1   | J     | 217 | LEU  |
| 1   | K     | 308 | THR  |
| 1   | L     | 154 | LYS  |
| 1   | B     | 86  | ALA  |
| 1   | B     | 130 | CYS  |
| 1   | C     | 17  | THR  |
| 1   | D     | 102 | GLY  |
| 1   | D     | 160 | SER  |
| 1   | H     | 16  | GLN  |
| 1   | H     | 160 | SER  |
| 1   | H     | 196 | SER  |
| 1   | I     | 160 | SER  |
| 1   | I     | 237 | ALA  |
| 1   | J     | 16  | GLN  |
| 1   | J     | 129 | ASN  |
| 1   | K     | 68  | SER  |
| 1   | K     | 328 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 228 | GLU  |
| 1   | L     | 285 | ASP  |
| 1   | L     | 328 | GLU  |
| 1   | C     | 202 | GLY  |
| 1   | C     | 304 | LYS  |
| 1   | F     | 15  | GLU  |
| 1   | G     | 15  | GLU  |
| 1   | G     | 82  | TYR  |
| 1   | H     | 106 | LEU  |
| 1   | H     | 249 | TRP  |
| 1   | I     | 17  | THR  |
| 1   | K     | 15  | GLU  |
| 1   | L     | 86  | ALA  |
| 1   | L     | 87  | ASN  |
| 1   | L     | 313 | ALA  |
| 1   | B     | 220 | ASP  |
| 1   | C     | 225 | GLN  |
| 1   | D     | 17  | THR  |
| 1   | D     | 119 | ILE  |
| 1   | F     | 14  | GLU  |
| 1   | H     | 104 | SER  |
| 1   | I     | 27  | VAL  |
| 1   | L     | 17  | THR  |
| 1   | L     | 82  | TYR  |
| 1   | A     | 82  | TYR  |
| 1   | A     | 248 | SER  |
| 1   | F     | 17  | THR  |
| 1   | B     | 161 | GLY  |
| 1   | K     | 325 | ILE  |
| 1   | L     | 128 | PRO  |
| 1   | F     | 27  | VAL  |
| 1   | B     | 291 | PRO  |
| 1   | G     | 27  | VAL  |
| 1   | K     | 27  | VAL  |
| 1   | J     | 27  | VAL  |
| 1   | D     | 138 | PRO  |

### 5.3.2 Protein sidechains [\(i\)](#)

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     | 287/293 (98%)   | 278 (97%)  | 9 (3%)   | 40 72       |
| 1   | B     | 287/293 (98%)   | 276 (96%)  | 11 (4%)  | 33 65       |
| 1   | C     | 287/293 (98%)   | 277 (96%)  | 10 (4%)  | 36 68       |
| 1   | D     | 287/293 (98%)   | 274 (96%)  | 13 (4%)  | 27 59       |
| 1   | E     | 287/293 (98%)   | 279 (97%)  | 8 (3%)   | 43 75       |
| 1   | F     | 287/293 (98%)   | 277 (96%)  | 10 (4%)  | 36 68       |
| 1   | G     | 287/293 (98%)   | 279 (97%)  | 8 (3%)   | 43 75       |
| 1   | H     | 287/293 (98%)   | 280 (98%)  | 7 (2%)   | 49 78       |
| 1   | I     | 287/293 (98%)   | 276 (96%)  | 11 (4%)  | 33 65       |
| 1   | J     | 287/293 (98%)   | 281 (98%)  | 6 (2%)   | 53 80       |
| 1   | K     | 287/293 (98%)   | 281 (98%)  | 6 (2%)   | 53 80       |
| 1   | L     | 287/293 (98%)   | 280 (98%)  | 7 (2%)   | 49 78       |
| All | All   | 3444/3516 (98%) | 3338 (97%) | 106 (3%) | 40 72       |

All (106) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | TYR  |
| 1   | A     | 13  | LYS  |
| 1   | A     | 16  | GLN  |
| 1   | A     | 72  | ARG  |
| 1   | A     | 89  | LYS  |
| 1   | A     | 154 | LYS  |
| 1   | A     | 227 | LYS  |
| 1   | A     | 228 | GLU  |
| 1   | A     | 236 | SER  |
| 1   | B     | 7   | LEU  |
| 1   | B     | 12  | LEU  |
| 1   | B     | 13  | LYS  |
| 1   | B     | 19  | GLN  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 116 | PHE  |
| 1   | B     | 165 | ASP  |
| 1   | B     | 209 | SER  |
| 1   | B     | 254 | SER  |
| 1   | B     | 285 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 331 | PHE  |
| 1   | C     | 131 | LYS  |
| 1   | C     | 209 | SER  |
| 1   | C     | 220 | ASP  |
| 1   | C     | 221 | LYS  |
| 1   | C     | 238 | TYR  |
| 1   | C     | 284 | ASP  |
| 1   | C     | 289 | SER  |
| 1   | C     | 316 | LYS  |
| 1   | C     | 320 | ASP  |
| 1   | C     | 331 | PHE  |
| 1   | D     | 15  | GLU  |
| 1   | D     | 78  | SER  |
| 1   | D     | 80  | LYS  |
| 1   | D     | 104 | SER  |
| 1   | D     | 131 | LYS  |
| 1   | D     | 160 | SER  |
| 1   | D     | 194 | ASP  |
| 1   | D     | 242 | LYS  |
| 1   | D     | 273 | SER  |
| 1   | D     | 287 | PHE  |
| 1   | D     | 297 | ASN  |
| 1   | D     | 316 | LYS  |
| 1   | D     | 331 | PHE  |
| 1   | E     | 72  | ARG  |
| 1   | E     | 78  | SER  |
| 1   | E     | 165 | ASP  |
| 1   | E     | 169 | PHE  |
| 1   | E     | 209 | SER  |
| 1   | E     | 285 | ASP  |
| 1   | E     | 316 | LYS  |
| 1   | E     | 330 | GLN  |
| 1   | F     | 57  | LEU  |
| 1   | F     | 99  | GLN  |
| 1   | F     | 160 | SER  |
| 1   | F     | 165 | ASP  |
| 1   | F     | 221 | LYS  |
| 1   | F     | 261 | SER  |
| 1   | F     | 265 | ASN  |
| 1   | F     | 279 | LEU  |
| 1   | F     | 314 | ARG  |
| 1   | F     | 331 | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 5   | ASP  |
| 1   | G     | 19  | GLN  |
| 1   | G     | 42  | ASP  |
| 1   | G     | 55  | ASP  |
| 1   | G     | 89  | LYS  |
| 1   | G     | 160 | SER  |
| 1   | G     | 231 | LYS  |
| 1   | G     | 254 | SER  |
| 1   | H     | 9   | TYR  |
| 1   | H     | 131 | LYS  |
| 1   | H     | 140 | ASP  |
| 1   | H     | 220 | ASP  |
| 1   | H     | 221 | LYS  |
| 1   | H     | 222 | ASP  |
| 1   | H     | 316 | LYS  |
| 1   | I     | 131 | LYS  |
| 1   | I     | 152 | PHE  |
| 1   | I     | 165 | ASP  |
| 1   | I     | 194 | ASP  |
| 1   | I     | 209 | SER  |
| 1   | I     | 223 | LYS  |
| 1   | I     | 242 | LYS  |
| 1   | I     | 283 | LYS  |
| 1   | I     | 285 | ASP  |
| 1   | I     | 300 | SER  |
| 1   | I     | 301 | ASP  |
| 1   | J     | 75  | LYS  |
| 1   | J     | 78  | SER  |
| 1   | J     | 105 | ARG  |
| 1   | J     | 227 | LYS  |
| 1   | J     | 318 | SER  |
| 1   | J     | 331 | PHE  |
| 1   | K     | 5   | ASP  |
| 1   | K     | 14  | GLU  |
| 1   | K     | 154 | LYS  |
| 1   | K     | 165 | ASP  |
| 1   | K     | 318 | SER  |
| 1   | K     | 327 | LYS  |
| 1   | L     | 99  | GLN  |
| 1   | L     | 116 | PHE  |
| 1   | L     | 209 | SER  |
| 1   | L     | 242 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 284 | ASP  |
| 1   | L     | 285 | ASP  |
| 1   | L     | 331 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | ASN  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 185 | HIS  |
| 1   | C     | 114 | ASN  |
| 1   | D     | 107 | ASN  |
| 1   | D     | 225 | GLN  |
| 1   | E     | 107 | ASN  |
| 1   | E     | 214 | HIS  |
| 1   | E     | 296 | GLN  |
| 1   | F     | 107 | ASN  |
| 1   | J     | 112 | ASN  |
| 1   | J     | 214 | HIS  |
| 1   | K     | 10  | ASN  |
| 1   | K     | 137 | ASN  |
| 1   | L     | 137 | ASN  |
| 1   | L     | 232 | GLN  |

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | MLI  | K     | 601 | -    | 6,6,6        | 3.89 | 4 (66%)     | 7,7,7       | 3.37 | 5 (71%)     |
| 2   | MLI  | D     | 601 | -    | 6,6,6        | 3.96 | 6 (100%)    | 7,7,7       | 3.19 | 5 (71%)     |
| 2   | MLI  | G     | 601 | -    | 6,6,6        | 4.04 | 5 (83%)     | 7,7,7       | 3.48 | 5 (71%)     |
| 2   | MLI  | E     | 601 | -    | 6,6,6        | 3.86 | 4 (66%)     | 7,7,7       | 3.42 | 5 (71%)     |
| 2   | MLI  | J     | 601 | -    | 6,6,6        | 3.67 | 4 (66%)     | 7,7,7       | 3.51 | 5 (71%)     |
| 2   | MLI  | A     | 601 | -    | 6,6,6        | 3.83 | 4 (66%)     | 7,7,7       | 3.50 | 5 (71%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 2   | MLI  | K     | 601 | -    | -       | 1/4/4/4  | -     |
| 2   | MLI  | D     | 601 | -    | -       | 2/4/4/4  | -     |
| 2   | MLI  | G     | 601 | -    | -       | 2/4/4/4  | -     |
| 2   | MLI  | E     | 601 | -    | -       | 2/4/4/4  | -     |
| 2   | MLI  | J     | 601 | -    | -       | 1/4/4/4  | -     |
| 2   | MLI  | A     | 601 | -    | -       | 2/4/4/4  | -     |

All (27) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | K     | 601 | MLI  | O8-C3 | 6.07 | 1.42        | 1.22     |
| 2   | G     | 601 | MLI  | O6-C2 | 6.06 | 1.42        | 1.22     |
| 2   | E     | 601 | MLI  | O8-C3 | 6.00 | 1.42        | 1.22     |
| 2   | G     | 601 | MLI  | O8-C3 | 5.84 | 1.41        | 1.22     |
| 2   | D     | 601 | MLI  | O6-C2 | 5.81 | 1.41        | 1.22     |
| 2   | A     | 601 | MLI  | O6-C2 | 5.77 | 1.41        | 1.22     |
| 2   | D     | 601 | MLI  | O8-C3 | 5.71 | 1.41        | 1.22     |
| 2   | E     | 601 | MLI  | O6-C2 | 5.66 | 1.40        | 1.22     |
| 2   | J     | 601 | MLI  | O6-C2 | 5.60 | 1.40        | 1.22     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | K     | 601 | MLI  | O6-C2 | 5.57 | 1.40        | 1.22     |
| 2   | A     | 601 | MLI  | O8-C3 | 5.48 | 1.40        | 1.22     |
| 2   | J     | 601 | MLI  | O8-C3 | 5.44 | 1.40        | 1.22     |
| 2   | A     | 601 | MLI  | O7-C2 | 3.31 | 1.41        | 1.30     |
| 2   | A     | 601 | MLI  | O9-C3 | 3.19 | 1.41        | 1.30     |
| 2   | K     | 601 | MLI  | O9-C3 | 3.19 | 1.41        | 1.30     |
| 2   | D     | 601 | MLI  | O9-C3 | 3.18 | 1.41        | 1.30     |
| 2   | G     | 601 | MLI  | O9-C3 | 3.15 | 1.41        | 1.30     |
| 2   | G     | 601 | MLI  | O7-C2 | 3.15 | 1.41        | 1.30     |
| 2   | E     | 601 | MLI  | O9-C3 | 3.14 | 1.41        | 1.30     |
| 2   | K     | 601 | MLI  | O7-C2 | 3.10 | 1.41        | 1.30     |
| 2   | J     | 601 | MLI  | O9-C3 | 3.05 | 1.41        | 1.30     |
| 2   | D     | 601 | MLI  | O7-C2 | 3.02 | 1.40        | 1.30     |
| 2   | E     | 601 | MLI  | O7-C2 | 2.96 | 1.40        | 1.30     |
| 2   | J     | 601 | MLI  | O7-C2 | 2.93 | 1.40        | 1.30     |
| 2   | D     | 601 | MLI  | C1-C3 | 2.09 | 1.54        | 1.51     |
| 2   | G     | 601 | MLI  | C1-C3 | 2.09 | 1.54        | 1.51     |
| 2   | D     | 601 | MLI  | C1-C2 | 2.03 | 1.54        | 1.51     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | K     | 601 | MLI  | O6-C2-C1 | -5.68 | 105.48      | 122.08   |
| 2   | E     | 601 | MLI  | O6-C2-C1 | -5.59 | 105.75      | 122.08   |
| 2   | A     | 601 | MLI  | O8-C3-C1 | -5.18 | 106.93      | 122.08   |
| 2   | J     | 601 | MLI  | O8-C3-C1 | -5.16 | 107.00      | 122.08   |
| 2   | A     | 601 | MLI  | O6-C2-C1 | -5.09 | 107.20      | 122.08   |
| 2   | G     | 601 | MLI  | O9-C3-O8 | -4.97 | 110.92      | 123.30   |
| 2   | G     | 601 | MLI  | O6-C2-C1 | -4.93 | 107.68      | 122.08   |
| 2   | J     | 601 | MLI  | O6-C2-C1 | -4.60 | 108.64      | 122.08   |
| 2   | D     | 601 | MLI  | O7-C2-O6 | -4.49 | 112.11      | 123.30   |
| 2   | D     | 601 | MLI  | O8-C3-C1 | -4.31 | 109.49      | 122.08   |
| 2   | E     | 601 | MLI  | O8-C3-C1 | -4.17 | 109.90      | 122.08   |
| 2   | K     | 601 | MLI  | O7-C2-O6 | -3.97 | 113.41      | 123.30   |
| 2   | K     | 601 | MLI  | O8-C3-C1 | -3.84 | 110.86      | 122.08   |
| 2   | J     | 601 | MLI  | O9-C3-O8 | -3.83 | 113.76      | 123.30   |
| 2   | D     | 601 | MLI  | O6-C2-C1 | -3.80 | 110.98      | 122.08   |
| 2   | A     | 601 | MLI  | O7-C2-O6 | -3.77 | 113.89      | 123.30   |
| 2   | G     | 601 | MLI  | O7-C2-O6 | -3.69 | 114.09      | 123.30   |
| 2   | J     | 601 | MLI  | O7-C2-O6 | -3.68 | 114.12      | 123.30   |
| 2   | E     | 601 | MLI  | O9-C3-O8 | -3.53 | 114.49      | 123.30   |
| 2   | E     | 601 | MLI  | O7-C2-O6 | -3.40 | 114.82      | 123.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | D     | 601 | MLI  | O9-C3-O8 | -3.29 | 115.10      | 123.30   |
| 2   | A     | 601 | MLI  | O9-C3-O8 | -3.05 | 115.69      | 123.30   |
| 2   | K     | 601 | MLI  | O9-C3-O8 | -3.04 | 115.71      | 123.30   |
| 2   | G     | 601 | MLI  | O8-C3-C1 | -2.98 | 113.38      | 122.08   |
| 2   | G     | 601 | MLI  | O9-C3-C1 | -2.91 | 105.25      | 114.54   |
| 2   | J     | 601 | MLI  | O7-C2-C1 | -2.61 | 106.22      | 114.54   |
| 2   | E     | 601 | MLI  | O9-C3-C1 | -2.60 | 106.23      | 114.54   |
| 2   | K     | 601 | MLI  | O9-C3-C1 | -2.51 | 106.54      | 114.54   |
| 2   | D     | 601 | MLI  | O7-C2-C1 | -2.32 | 107.14      | 114.54   |
| 2   | A     | 601 | MLI  | O7-C2-C1 | -2.12 | 107.78      | 114.54   |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | J     | 601 | MLI  | C3-C1-C2-O7 |
| 2   | A     | 601 | MLI  | C3-C1-C2-O6 |
| 2   | D     | 601 | MLI  | C3-C1-C2-O6 |
| 2   | E     | 601 | MLI  | C2-C1-C3-O8 |
| 2   | G     | 601 | MLI  | C2-C1-C3-O8 |
| 2   | A     | 601 | MLI  | C2-C1-C3-O8 |
| 2   | D     | 601 | MLI  | C2-C1-C3-O9 |
| 2   | K     | 601 | MLI  | C3-C1-C2-O7 |
| 2   | G     | 601 | MLI  | C3-C1-C2-O7 |
| 2   | E     | 601 | MLI  | C3-C1-C2-O6 |

There are no ring outliers.

6 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | K     | 601 | MLI  | 1       | 0            |
| 2   | D     | 601 | MLI  | 4       | 0            |
| 2   | G     | 601 | MLI  | 3       | 0            |
| 2   | E     | 601 | MLI  | 5       | 0            |
| 2   | J     | 601 | MLI  | 2       | 0            |
| 2   | A     | 601 | MLI  | 2       | 0            |

## 5.7 Other polymers [\(i\)](#)

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 i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 331/337 (98%)   | -0.15  | 7 (2%) 63 62   | 28, 42, 72, 87        | 0     |
| 1   | B     | 331/337 (98%)   | 0.15   | 18 (5%) 25 22  | 31, 54, 93, 133       | 0     |
| 1   | C     | 331/337 (98%)   | 0.08   | 16 (4%) 30 27  | 31, 54, 86, 122       | 0     |
| 1   | D     | 331/337 (98%)   | -0.04  | 13 (3%) 39 36  | 28, 47, 76, 133       | 0     |
| 1   | E     | 331/337 (98%)   | -0.25  | 4 (1%) 79 79   | 29, 39, 57, 92        | 0     |
| 1   | F     | 331/337 (98%)   | -0.06  | 11 (3%) 46 42  | 32, 46, 75, 106       | 0     |
| 1   | G     | 331/337 (98%)   | -0.21  | 4 (1%) 79 79   | 27, 42, 63, 92        | 0     |
| 1   | H     | 331/337 (98%)   | -0.07  | 7 (2%) 63 62   | 30, 46, 75, 102       | 0     |
| 1   | I     | 331/337 (98%)   | 0.05   | 16 (4%) 30 27  | 33, 55, 90, 129       | 0     |
| 1   | J     | 331/337 (98%)   | -0.08  | 13 (3%) 39 36  | 32, 46, 76, 132       | 0     |
| 1   | K     | 331/337 (98%)   | -0.21  | 4 (1%) 79 79   | 29, 42, 69, 96        | 0     |
| 1   | L     | 331/337 (98%)   | 0.15   | 18 (5%) 25 22  | 30, 55, 98, 134       | 0     |
| All | All   | 3972/4044 (98%) | -0.05  | 131 (3%) 46 42 | 27, 46, 81, 134       | 0     |

All (131) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 102 | GLY  | 10.8 |
| 1   | I     | 105 | ARG  | 9.6  |
| 1   | J     | 102 | GLY  | 9.2  |
| 1   | B     | 107 | ASN  | 9.0  |
| 1   | B     | 106 | LEU  | 8.7  |
| 1   | D     | 104 | SER  | 8.4  |
| 1   | J     | 100 | GLN  | 7.1  |
| 1   | I     | 104 | SER  | 6.8  |
| 1   | L     | 106 | LEU  | 6.8  |
| 1   | D     | 100 | GLN  | 6.7  |
| 1   | B     | 103 | GLU  | 6.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 99  | GLN  | 6.2  |
| 1   | B     | 99  | GLN  | 6.1  |
| 1   | L     | 101 | GLU  | 5.9  |
| 1   | B     | 104 | SER  | 5.8  |
| 1   | D     | 105 | ARG  | 5.5  |
| 1   | L     | 102 | GLY  | 5.4  |
| 1   | B     | 102 | GLY  | 5.4  |
| 1   | D     | 101 | GLU  | 5.3  |
| 1   | L     | 107 | ASN  | 5.3  |
| 1   | B     | 101 | GLU  | 5.3  |
| 1   | I     | 103 | GLU  | 5.1  |
| 1   | L     | 100 | GLN  | 5.0  |
| 1   | C     | 107 | ASN  | 4.9  |
| 1   | B     | 331 | PHE  | 4.9  |
| 1   | J     | 101 | GLU  | 4.8  |
| 1   | J     | 105 | ARG  | 4.7  |
| 1   | D     | 99  | GLN  | 4.7  |
| 1   | C     | 105 | ARG  | 4.5  |
| 1   | J     | 99  | GLN  | 4.4  |
| 1   | D     | 98  | ARG  | 4.4  |
| 1   | B     | 100 | GLN  | 4.2  |
| 1   | L     | 331 | PHE  | 4.2  |
| 1   | L     | 98  | ARG  | 4.2  |
| 1   | I     | 99  | GLN  | 4.1  |
| 1   | B     | 98  | ARG  | 4.1  |
| 1   | J     | 107 | ASN  | 4.1  |
| 1   | C     | 104 | SER  | 4.1  |
| 1   | L     | 99  | GLN  | 4.1  |
| 1   | B     | 1   | ALA  | 4.0  |
| 1   | C     | 108 | LEU  | 3.9  |
| 1   | H     | 108 | LEU  | 3.9  |
| 1   | B     | 327 | LYS  | 3.8  |
| 1   | L     | 97  | ALA  | 3.8  |
| 1   | F     | 102 | GLY  | 3.8  |
| 1   | F     | 101 | GLU  | 3.8  |
| 1   | I     | 217 | LEU  | 3.7  |
| 1   | B     | 105 | ARG  | 3.6  |
| 1   | I     | 13  | LYS  | 3.6  |
| 1   | C     | 106 | LEU  | 3.6  |
| 1   | J     | 12  | LEU  | 3.6  |
| 1   | K     | 330 | GLN  | 3.5  |
| 1   | L     | 104 | SER  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 103 | GLU  | 3.4  |
| 1   | F     | 100 | GLN  | 3.3  |
| 1   | I     | 106 | LEU  | 3.3  |
| 1   | L     | 15  | GLU  | 3.3  |
| 1   | J     | 104 | SER  | 3.2  |
| 1   | I     | 107 | ASN  | 3.2  |
| 1   | L     | 105 | ARG  | 3.2  |
| 1   | E     | 330 | GLN  | 3.2  |
| 1   | G     | 331 | PHE  | 3.1  |
| 1   | E     | 331 | PHE  | 3.1  |
| 1   | I     | 220 | ASP  | 3.1  |
| 1   | H     | 102 | GLY  | 3.1  |
| 1   | C     | 97  | ALA  | 3.0  |
| 1   | F     | 55  | ASP  | 3.0  |
| 1   | B     | 329 | LEU  | 3.0  |
| 1   | G     | 14  | GLU  | 2.9  |
| 1   | L     | 1   | ALA  | 2.9  |
| 1   | B     | 238 | TYR  | 2.9  |
| 1   | H     | 101 | GLU  | 2.9  |
| 1   | L     | 103 | GLU  | 2.9  |
| 1   | J     | 331 | PHE  | 2.8  |
| 1   | A     | 327 | LYS  | 2.8  |
| 1   | D     | 14  | GLU  | 2.8  |
| 1   | D     | 331 | PHE  | 2.8  |
| 1   | F     | 107 | ASN  | 2.8  |
| 1   | H     | 106 | LEU  | 2.7  |
| 1   | L     | 330 | GLN  | 2.7  |
| 1   | C     | 15  | GLU  | 2.7  |
| 1   | L     | 14  | GLU  | 2.6  |
| 1   | C     | 217 | LEU  | 2.6  |
| 1   | A     | 330 | GLN  | 2.6  |
| 1   | F     | 106 | LEU  | 2.6  |
| 1   | J     | 108 | LEU  | 2.6  |
| 1   | I     | 219 | THR  | 2.5  |
| 1   | E     | 14  | GLU  | 2.5  |
| 1   | H     | 100 | GLN  | 2.5  |
| 1   | J     | 15  | GLU  | 2.5  |
| 1   | J     | 103 | GLU  | 2.5  |
| 1   | K     | 331 | PHE  | 2.5  |
| 1   | H     | 104 | SER  | 2.5  |
| 1   | F     | 242 | LYS  | 2.4  |
| 1   | A     | 328 | GLU  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 104 | SER  | 2.4  |
| 1   | D     | 106 | LEU  | 2.4  |
| 1   | A     | 221 | LYS  | 2.4  |
| 1   | G     | 160 | SER  | 2.4  |
| 1   | C     | 98  | ARG  | 2.4  |
| 1   | F     | 254 | SER  | 2.3  |
| 1   | B     | 15  | GLU  | 2.3  |
| 1   | I     | 283 | LYS  | 2.3  |
| 1   | C     | 13  | LYS  | 2.3  |
| 1   | I     | 16  | GLN  | 2.3  |
| 1   | D     | 103 | GLU  | 2.3  |
| 1   | C     | 14  | GLU  | 2.2  |
| 1   | A     | 162 | CYS  | 2.2  |
| 1   | I     | 12  | LEU  | 2.2  |
| 1   | J     | 98  | ARG  | 2.2  |
| 1   | L     | 108 | LEU  | 2.2  |
| 1   | C     | 327 | LYS  | 2.2  |
| 1   | K     | 329 | LEU  | 2.2  |
| 1   | E     | 42  | ASP  | 2.1  |
| 1   | A     | 161 | GLY  | 2.1  |
| 1   | F     | 160 | SER  | 2.1  |
| 1   | C     | 331 | PHE  | 2.1  |
| 1   | H     | 13  | LYS  | 2.1  |
| 1   | I     | 98  | ARG  | 2.1  |
| 1   | F     | 103 | GLU  | 2.1  |
| 1   | I     | 102 | GLY  | 2.1  |
| 1   | B     | 220 | ASP  | 2.1  |
| 1   | B     | 108 | LEU  | 2.0  |
| 1   | G     | 5   | ASP  | 2.0  |
| 1   | I     | 227 | LYS  | 2.0  |
| 1   | L     | 13  | LYS  | 2.0  |
| 1   | D     | 12  | LEU  | 2.0  |
| 1   | D     | 108 | LEU  | 2.0  |
| 1   | A     | 331 | PHE  | 2.0  |
| 1   | K     | 14  | GLU  | 2.0  |
| 1   | C     | 238 | TYR  | 2.0  |

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

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

### 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [\(i\)](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | MLI  | E     | 601 | 7/7   | 0.84 | 0.30 | 46,48,53,54                | 0     |
| 2   | MLI  | D     | 601 | 7/7   | 0.88 | 0.22 | 58,68,71,75                | 0     |
| 2   | MLI  | G     | 601 | 7/7   | 0.90 | 0.23 | 43,45,53,62                | 0     |
| 2   | MLI  | K     | 601 | 7/7   | 0.91 | 0.21 | 37,41,55,55                | 0     |
| 2   | MLI  | J     | 601 | 7/7   | 0.92 | 0.19 | 58,62,70,85                | 0     |
| 2   | MLI  | A     | 601 | 7/7   | 0.92 | 0.24 | 41,48,49,51                | 0     |

### 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.