



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:15 PM UTC

PDB ID : 1AQF / pdb\_00001aqf  
Title : PYRUVATE KINASE FROM RABBIT MUSCLE WITH MG, K, AND L-PHOSPHOLACTATE  
Authors : Larsen, T.M.; Benning, M.M.; Wesenberg, G.E.; Rayment, I.; Reed, G.H.  
Deposited on : 1997-07-29  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

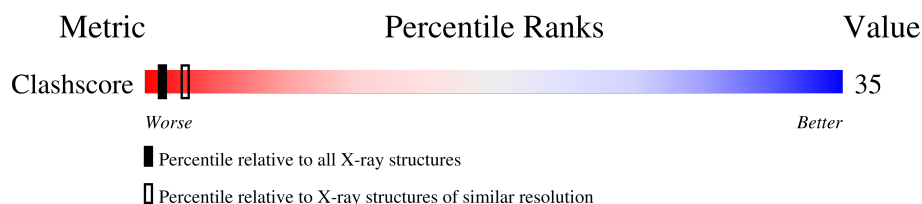
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



| Metric     | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|-------------------------------------------------------|
| Clashscore | 190562                      | 3843 (2.70-2.70)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 530    | 43% 50% 5% .     |
| 1   | B     | 530    | 41% 52% 5% .     |
| 1   | C     | 530    | 56% 36% 6% .     |
| 1   | D     | 530    | 52% 42% . .      |
| 1   | E     | 530    | 38% 38% . 20%    |
| 1   | F     | 530    | 50% 45% . .      |
| 1   | G     | 530    | 40% 52% 6% .     |
| 1   | H     | 530    | 38% 55% 5% .     |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | PEQ  | H     | 532 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31410 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 PYRUVATE KINASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3979  | 2498 | 708 | 745 | 28 |         |         |       |
| 1   | B     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3979  | 2498 | 708 | 745 | 28 |         |         |       |
| 1   | C     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3978  | 2498 | 708 | 744 | 28 |         |         |       |
| 1   | D     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3979  | 2498 | 708 | 745 | 28 |         |         |       |
| 1   | E     | 426      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3268  | 2045 | 592 | 606 | 25 |         |         |       |
| 1   | F     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3979  | 2498 | 708 | 745 | 28 |         |         |       |
| 1   | G     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3979  | 2498 | 708 | 745 | 28 |         |         |       |
| 1   | H     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3979  | 2498 | 708 | 745 | 28 |         |         |       |

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2   | A     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | B     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | C     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | D     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | E     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | F     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

*Continued on next page...*

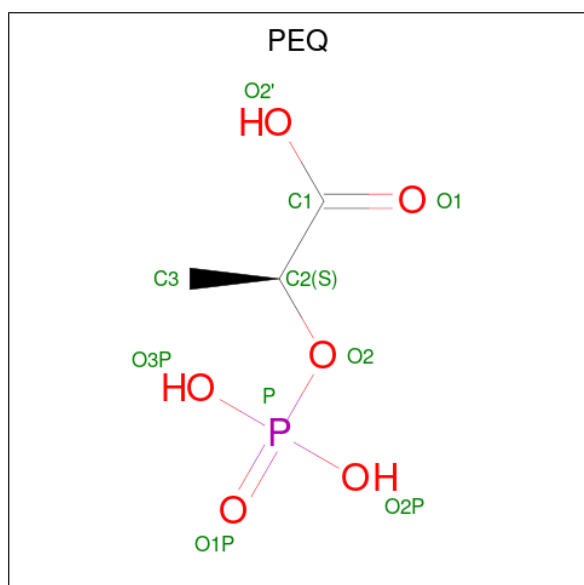
Continued from previous page...

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 2   | G     | 1        | Total K<br>1 1 | 0       | 0       |
| 2   | H     | 1        | Total K<br>1 1 | 0       | 0       |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | F     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | G     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | H     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 4 is L-PHOSPHOLACTATE (CCD ID: PEQ) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |
| 4   | B     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |
| 4   | C     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |
| 4   | D     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |
| 4   | E     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |
| 4   | F     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |
| 4   | G     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |
| 4   | H     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 10    | 3 | 6 | 1 |         |         |

- Molecule 5 is water.

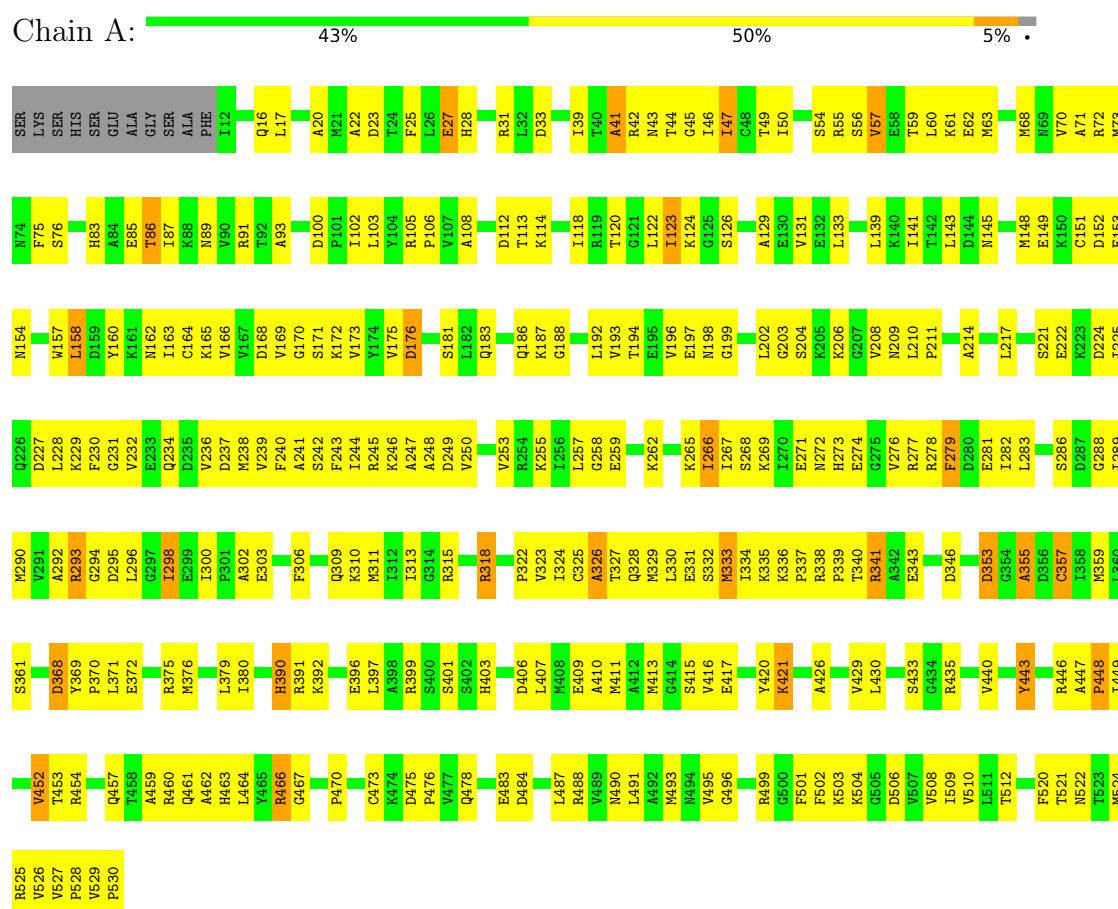
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |
| 5   | B     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 5   | C     | 35       | Total | O  | 0       | 0       |
|     |       |          | 35    | 35 |         |         |
| 5   | D     | 35       | Total | O  | 0       | 0       |
|     |       |          | 35    | 35 |         |         |
| 5   | E     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 5   | F     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 5   | G     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 5   | H     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |

### 3 Residue-property plots

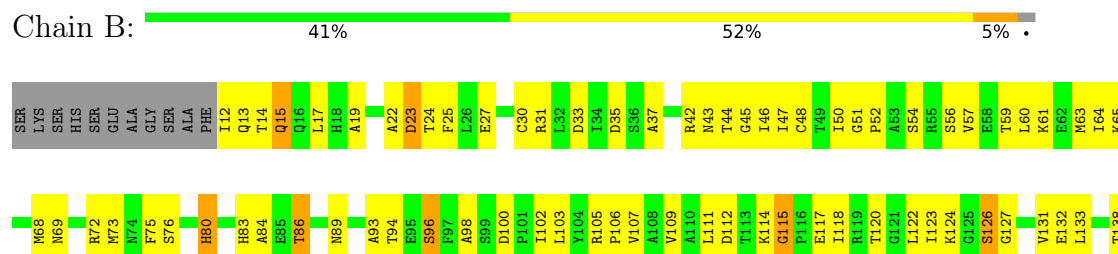
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

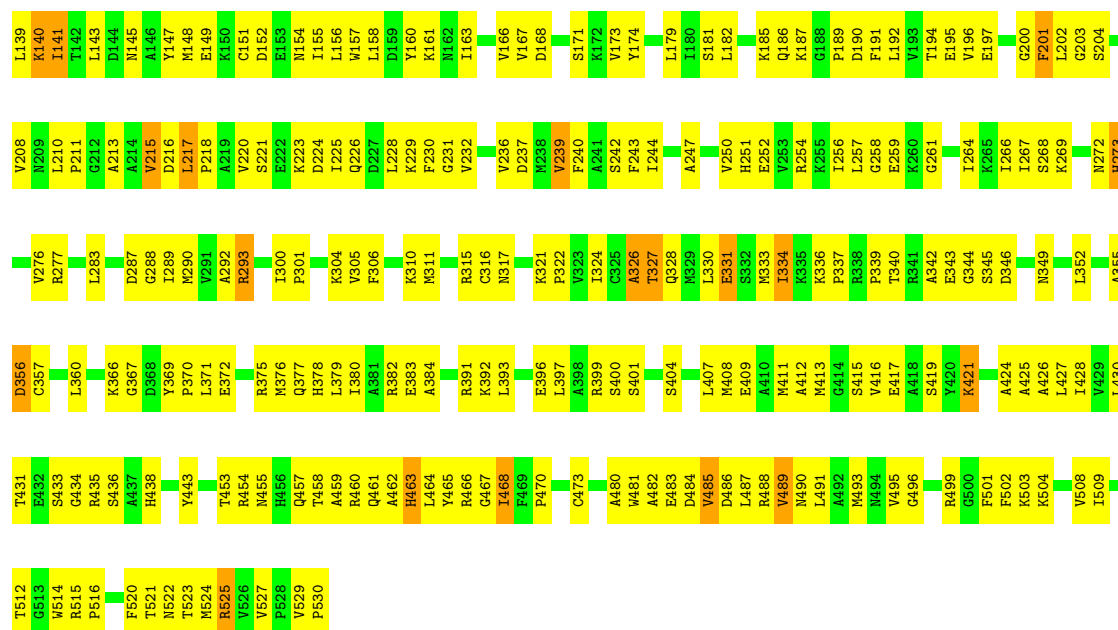
Note EDS was not executed.

#### • Molecule 1: PYRUVATE KINASE



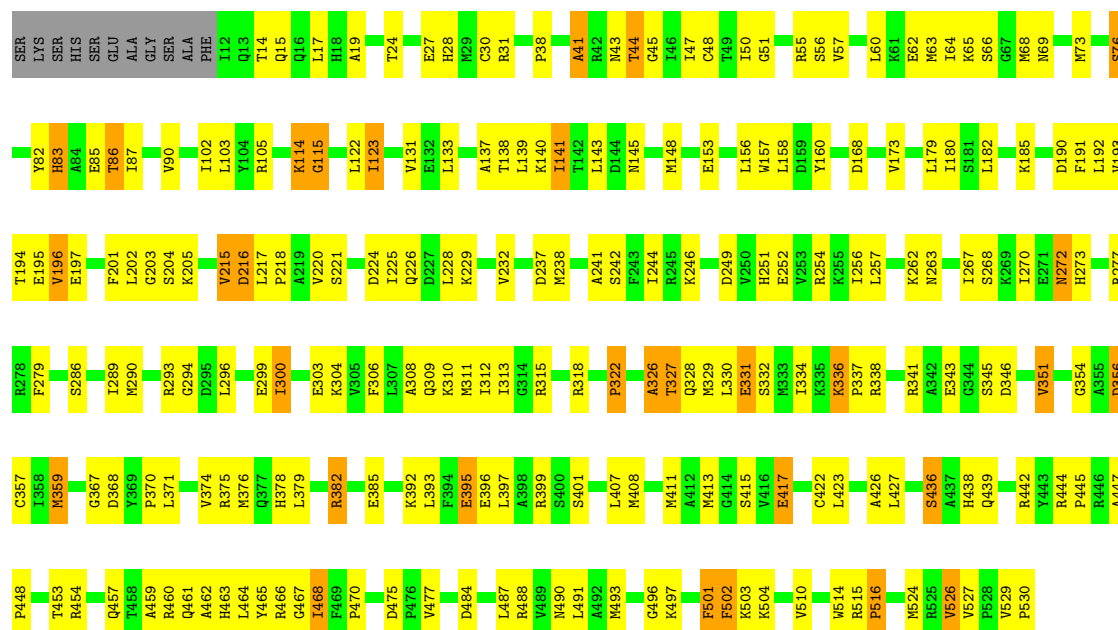
#### • Molecule 1: PYRUVATE KINASE





• Molecule 1: PYRUVATE KINASE

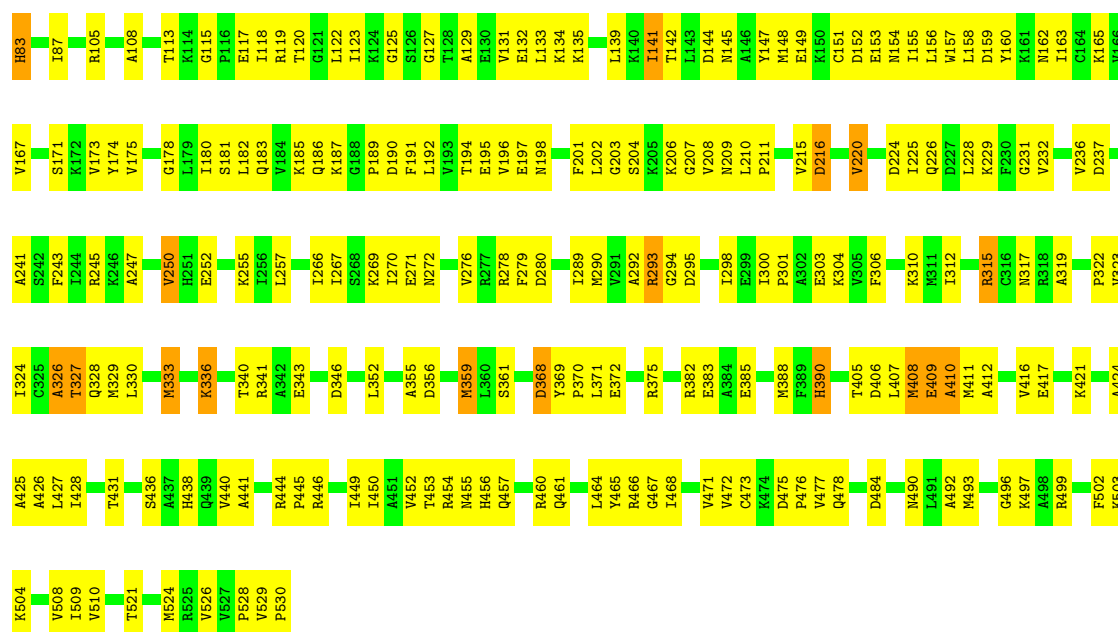
Chain C: 56% 36% 6% .



• Molecule 1: PYRUVATE KINASE

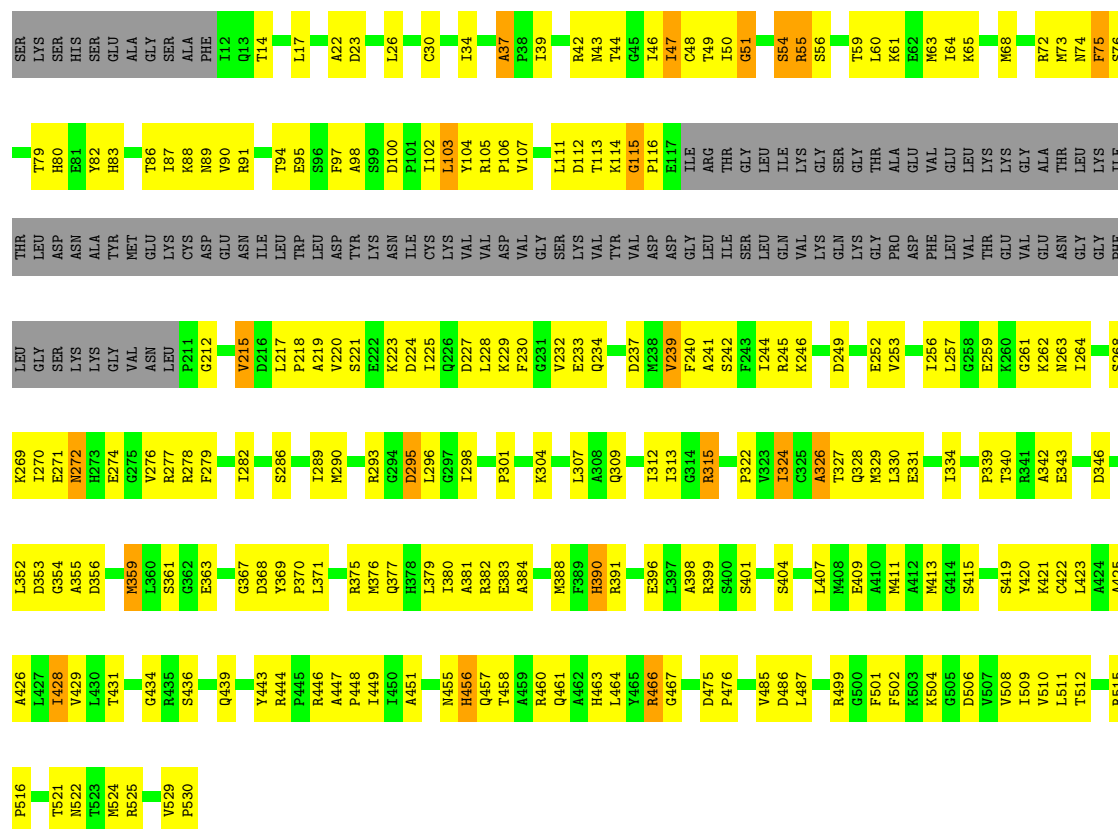
Chain D: 52% 42% . .





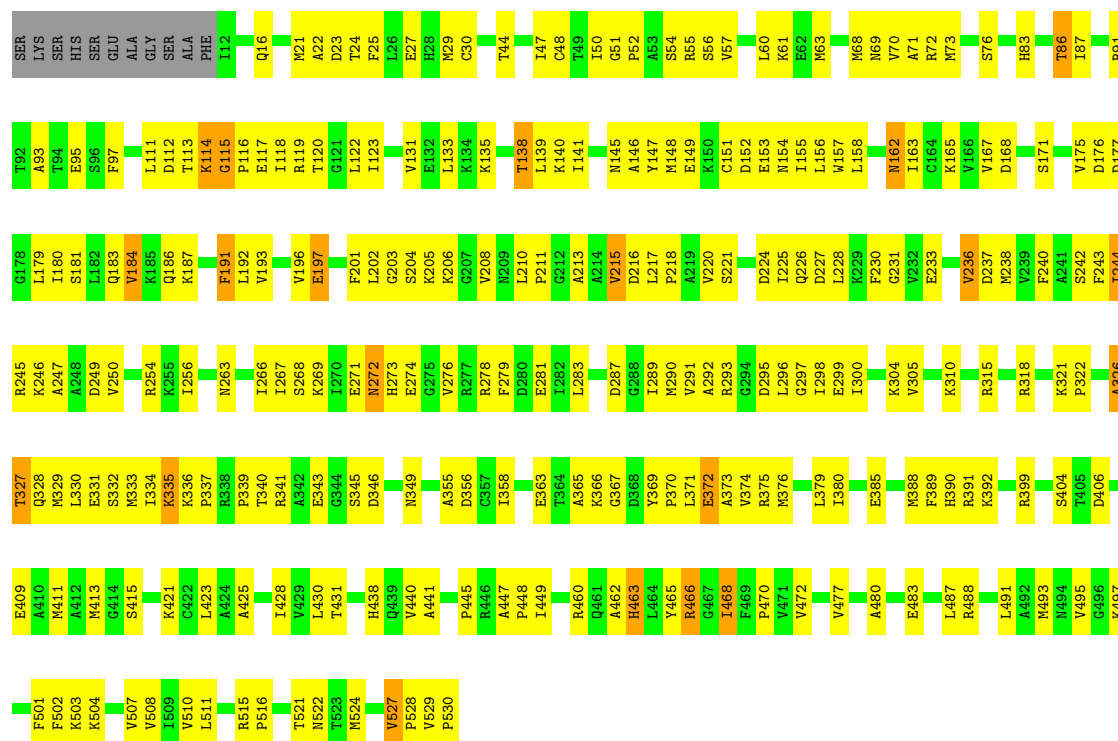
• Molecule 1: PYRUVATE KINASE

Chain E: 38% 38% 20%



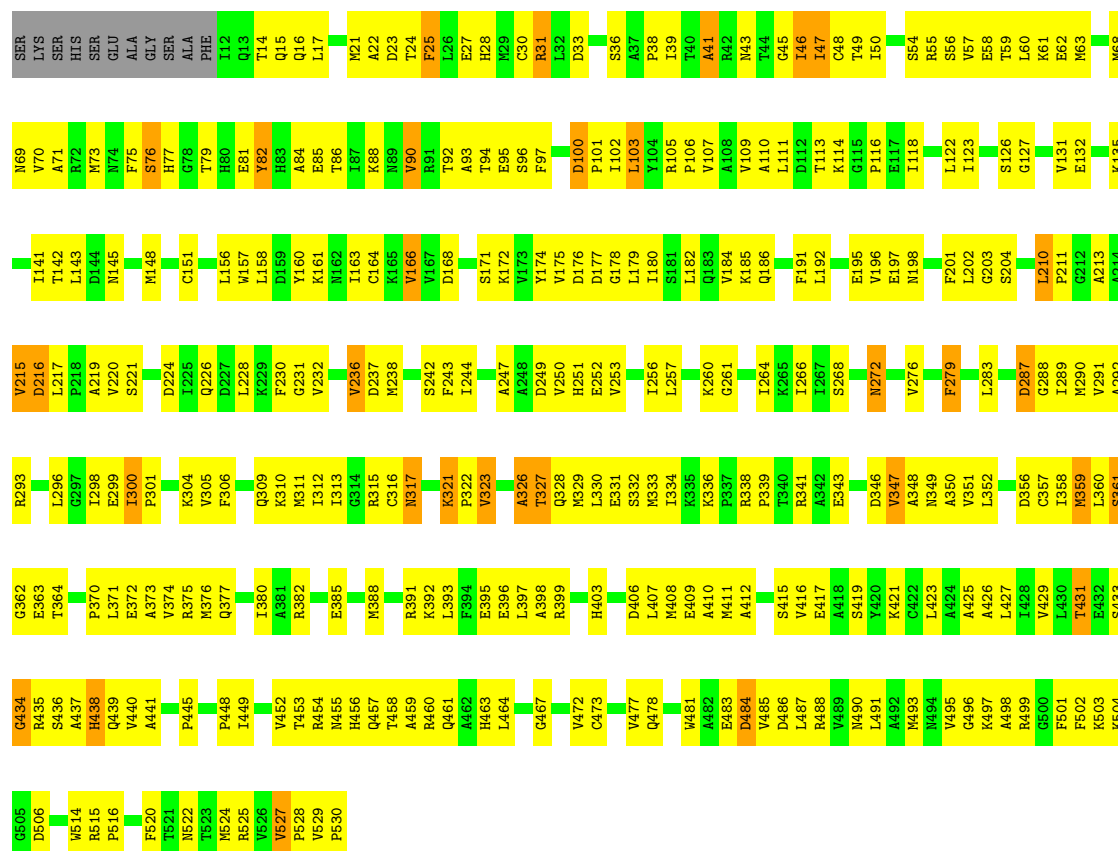
• Molecule 1: PYRUVATE KINASE

Chain F: 50% 45%



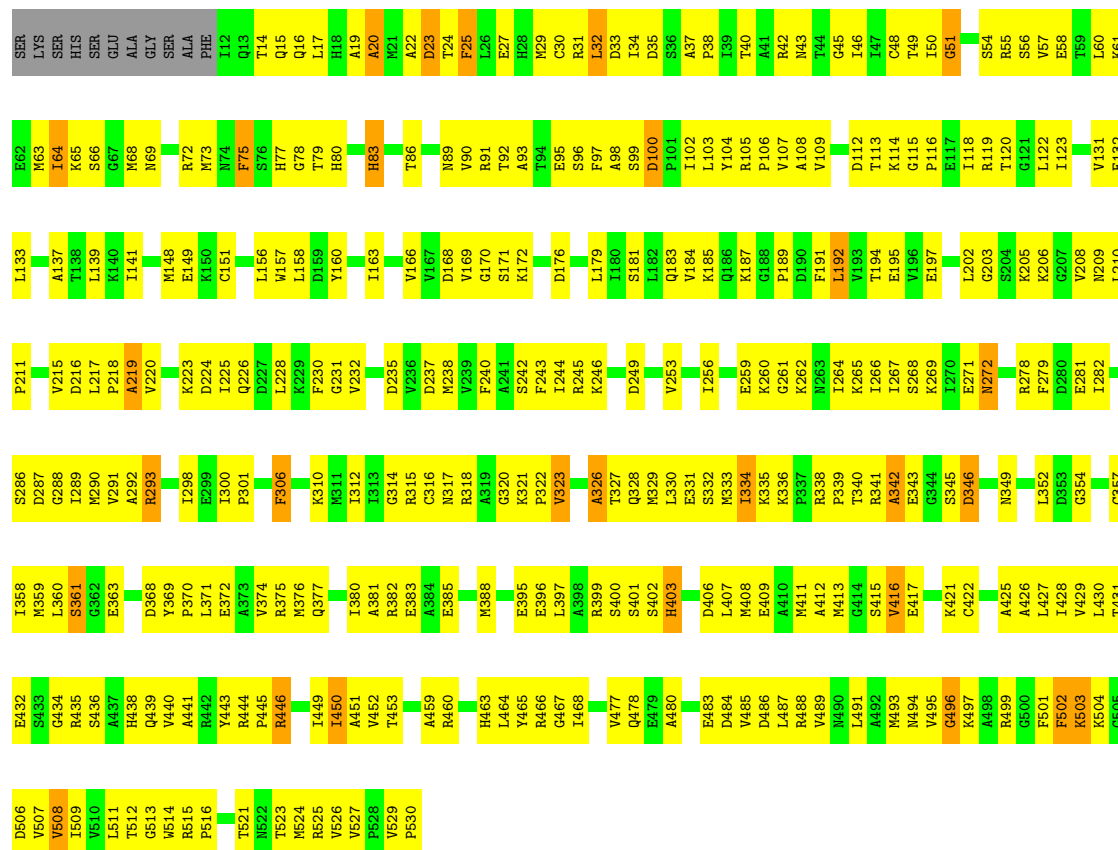
● Molecule 1: PYRUVATE KINASE

Chain G: 40% 52% 6% .



● Molecule 1: PYRUVATE KINASE

Chain H:  38% 55% 5%



## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                        | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 144.40Å 112.60Å 171.20Å<br>90.00° 93.70° 90.00° | Depositor |
| Resolution (Å)                                           | 30.00 – 2.70                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 93.0 (30.00-2.70)                               | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | TNT 5E                                          | Depositor |
| R, $R_{free}$                                            | 0.196 , (Not available)                         | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 31410                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 41.0                                            | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, PEQ

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.24         | 3/4042 (0.1%)   | 1.69        | 45/5452 (0.8%)   |
| 1   | B     | 1.26         | 1/4042 (0.0%)   | 1.70        | 51/5452 (0.9%)   |
| 1   | C     | 1.28         | 6/4041 (0.1%)   | 1.69        | 62/5452 (1.1%)   |
| 1   | D     | 1.24         | 1/4042 (0.0%)   | 1.67        | 44/5452 (0.8%)   |
| 1   | E     | 1.21         | 2/3322 (0.1%)   | 1.69        | 39/4482 (0.9%)   |
| 1   | F     | 1.22         | 3/4042 (0.1%)   | 1.69        | 49/5452 (0.9%)   |
| 1   | G     | 1.21         | 3/4042 (0.1%)   | 1.70        | 47/5452 (0.9%)   |
| 1   | H     | 1.22         | 2/4042 (0.0%)   | 1.71        | 50/5452 (0.9%)   |
| All | All   | 1.23         | 21/31615 (0.1%) | 1.69        | 387/42646 (0.9%) |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 445 | PRO  | C-N     | -7.44 | 1.22        | 1.33     |
| 1   | G     | 323 | VAL  | CA-C    | -7.25 | 1.43        | 1.52     |
| 1   | G     | 514 | TRP  | NE1-CE2 | -5.90 | 1.30        | 1.37     |
| 1   | E     | 315 | ARG  | N-CA    | -5.67 | 1.39        | 1.46     |
| 1   | F     | 495 | VAL  | CA-CB   | -5.58 | 1.47        | 1.54     |
| 1   | H     | 395 | GLU  | CD-OE1  | 5.52  | 1.35        | 1.25     |
| 1   | B     | 344 | GLY  | CA-C    | 5.43  | 1.58        | 1.52     |
| 1   | E     | 116 | PRO  | C-N     | 5.36  | 1.40        | 1.33     |
| 1   | F     | 374 | VAL  | CA-CB   | -5.33 | 1.48        | 1.54     |
| 1   | H     | 46  | ILE  | CA-CB   | -5.26 | 1.48        | 1.54     |
| 1   | A     | 27  | GLU  | CA-C    | -5.25 | 1.45        | 1.52     |
| 1   | C     | 417 | GLU  | C-N     | -5.22 | 1.26        | 1.34     |
| 1   | F     | 372 | GLU  | CD-OE1  | 5.22  | 1.35        | 1.25     |
| 1   | C     | 351 | VAL  | N-CA    | -5.19 | 1.40        | 1.46     |
| 1   | C     | 395 | GLU  | CD-OE1  | 5.18  | 1.35        | 1.25     |
| 1   | G     | 527 | VAL  | N-CA    | -5.17 | 1.42        | 1.46     |
| 1   | C     | 197 | GLU  | N-CA    | -5.14 | 1.40        | 1.46     |
| 1   | A     | 47  | ILE  | CA-CB   | -5.10 | 1.48        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 123 | ILE  | N-CA  | -5.10 | 1.40        | 1.46     |
| 1   | C     | 196 | VAL  | C-N   | -5.10 | 1.26        | 1.33     |
| 1   | D     | 336 | LYS  | C-N   | -5.08 | 1.29        | 1.33     |

All (387) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | B     | 251 | HIS  | CA-CB-CG | -13.30 | 100.50      | 113.80   |
| 1   | D     | 359 | MET  | N-CA-C   | 9.21   | 124.61      | 109.24   |
| 1   | F     | 115 | GLY  | CA-C-N   | 9.07   | 129.42      | 119.90   |
| 1   | F     | 115 | GLY  | C-N-CA   | 9.07   | 129.42      | 119.90   |
| 1   | A     | 306 | PHE  | CA-CB-CG | -8.71  | 105.08      | 113.80   |
| 1   | D     | 83  | HIS  | CA-CB-CG | -8.62  | 105.18      | 113.80   |
| 1   | C     | 201 | PHE  | CA-CB-CG | -8.51  | 105.29      | 113.80   |
| 1   | F     | 463 | HIS  | CA-CB-CG | -8.44  | 105.36      | 113.80   |
| 1   | A     | 83  | HIS  | CA-CB-CG | -8.43  | 105.37      | 113.80   |
| 1   | G     | 251 | HIS  | CA-CB-CG | -8.42  | 105.38      | 113.80   |
| 1   | B     | 86  | THR  | N-CA-C   | -8.37  | 102.11      | 111.07   |
| 1   | C     | 270 | ILE  | CB-CA-C  | 8.32   | 120.22      | 111.23   |
| 1   | E     | 390 | HIS  | N-CA-C   | 8.32   | 121.17      | 111.02   |
| 1   | D     | 326 | ALA  | N-CA-C   | 8.26   | 121.97      | 109.41   |
| 1   | E     | 295 | ASP  | CA-CB-CG | 8.13   | 120.73      | 112.60   |
| 1   | E     | 428 | ILE  | CB-CA-C  | -8.07  | 99.86       | 110.84   |
| 1   | H     | 83  | HIS  | CA-CB-CG | -8.07  | 105.73      | 113.80   |
| 1   | E     | 272 | ASN  | N-CA-C   | 8.06   | 118.88      | 108.24   |
| 1   | G     | 317 | ASN  | CB-CA-C  | -7.99  | 97.10       | 110.68   |
| 1   | C     | 141 | ILE  | N-CA-CB  | 7.90   | 122.31      | 111.41   |
| 1   | D     | 490 | ASN  | CA-CB-CG | -7.82  | 104.78      | 112.60   |
| 1   | E     | 359 | MET  | N-CA-C   | 7.75   | 122.19      | 109.24   |
| 1   | G     | 166 | VAL  | N-CA-CB  | -7.66  | 102.37      | 112.26   |
| 1   | F     | 367 | GLY  | N-CA-C   | 7.65   | 120.74      | 112.33   |
| 1   | F     | 326 | ALA  | N-CA-C   | 7.62   | 121.32      | 109.52   |
| 1   | E     | 75  | PHE  | CA-CB-CG | -7.61  | 106.19      | 113.80   |
| 1   | G     | 100 | ASP  | CB-CA-C  | -7.60  | 102.75      | 110.65   |
| 1   | B     | 115 | GLY  | CA-C-N   | 7.58   | 127.86      | 119.90   |
| 1   | B     | 115 | GLY  | C-N-CA   | 7.58   | 127.86      | 119.90   |
| 1   | G     | 300 | ILE  | N-CA-CB  | 7.51   | 119.68      | 111.64   |
| 1   | E     | 55  | ARG  | N-CA-C   | -7.50  | 104.27      | 113.50   |
| 1   | D     | 298 | ILE  | N-CA-C   | -7.47  | 104.58      | 111.67   |
| 1   | H     | 25  | PHE  | CA-CB-CG | -7.33  | 106.47      | 113.80   |
| 1   | F     | 146 | ALA  | N-CA-C   | -7.29  | 102.73      | 111.69   |
| 1   | A     | 510 | VAL  | N-CA-C   | 7.25   | 118.31      | 107.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 47  | ILE  | N-CA-CB  | -7.21 | 102.37      | 111.46   |
| 1   | C     | 196 | VAL  | N-CA-CB  | 7.16  | 119.72      | 110.13   |
| 1   | G     | 472 | VAL  | N-CA-C   | 7.13  | 118.14      | 107.51   |
| 1   | E     | 115 | GLY  | CA-C-N   | 7.12  | 127.69      | 120.14   |
| 1   | E     | 115 | GLY  | C-N-CA   | 7.12  | 127.69      | 120.14   |
| 1   | A     | 279 | PHE  | CA-CB-CG | -7.07 | 106.73      | 113.80   |
| 1   | C     | 215 | VAL  | CA-C-N   | 7.06  | 129.75      | 120.28   |
| 1   | C     | 215 | VAL  | C-N-CA   | 7.06  | 129.75      | 120.28   |
| 1   | C     | 168 | ASP  | CA-CB-CG | 7.01  | 119.61      | 112.60   |
| 1   | B     | 179 | LEU  | N-CA-C   | 6.94  | 118.85      | 111.28   |
| 1   | F     | 191 | PHE  | CA-CB-CG | 6.92  | 120.72      | 113.80   |
| 1   | D     | 117 | GLU  | N-CA-C   | 6.88  | 118.57      | 108.86   |
| 1   | E     | 326 | ALA  | N-CA-C   | 6.85  | 119.17      | 108.96   |
| 1   | B     | 35  | ASP  | CB-CA-C  | 6.83  | 121.03      | 109.55   |
| 1   | D     | 456 | HIS  | N-CA-C   | 6.82  | 118.37      | 111.07   |
| 1   | F     | 210 | LEU  | CB-CA-C  | -6.80 | 103.58      | 110.65   |
| 1   | E     | 212 | GLY  | N-CA-C   | -6.79 | 105.87      | 115.30   |
| 1   | F     | 83  | HIS  | CA-CB-CG | -6.77 | 107.03      | 113.80   |
| 1   | A     | 322 | PRO  | N-CA-CB  | 6.75  | 109.19      | 103.25   |
| 1   | B     | 201 | PHE  | N-CA-C   | 6.71  | 119.46      | 108.52   |
| 1   | C     | 300 | ILE  | N-CA-CB  | 6.69  | 116.45      | 111.83   |
| 1   | F     | 366 | LYS  | CA-C-N   | 6.69  | 127.73      | 120.44   |
| 1   | F     | 366 | LYS  | C-N-CA   | 6.69  | 127.73      | 120.44   |
| 1   | H     | 468 | ILE  | N-CA-C   | 6.69  | 117.66      | 109.30   |
| 1   | E     | 37  | ALA  | N-CA-C   | 6.68  | 118.31      | 109.83   |
| 1   | C     | 379 | LEU  | N-CA-C   | 6.66  | 118.33      | 111.14   |
| 1   | F     | 331 | GLU  | N-CA-C   | 6.66  | 119.39      | 111.33   |
| 1   | A     | 333 | MET  | N-CA-C   | 6.66  | 121.07      | 113.15   |
| 1   | D     | 141 | ILE  | N-CA-CB  | 6.65  | 119.73      | 110.56   |
| 1   | G     | 347 | VAL  | CB-CA-C  | -6.64 | 103.51      | 111.81   |
| 1   | F     | 477 | VAL  | N-CA-C   | 6.62  | 118.34      | 108.54   |
| 1   | B     | 98  | ALA  | CA-C-N   | 6.62  | 129.48      | 120.54   |
| 1   | B     | 98  | ALA  | C-N-CA   | 6.62  | 129.48      | 120.54   |
| 1   | F     | 497 | LYS  | O-C-N    | 6.56  | 128.83      | 122.07   |
| 1   | H     | 100 | ASP  | CA-CB-CG | 6.54  | 119.14      | 112.60   |
| 1   | C     | 516 | PRO  | CB-CA-C  | -6.54 | 103.25      | 111.56   |
| 1   | A     | 390 | HIS  | N-CA-C   | 6.53  | 118.99      | 111.02   |
| 1   | H     | 215 | VAL  | CA-C-N   | 6.53  | 132.57      | 121.14   |
| 1   | H     | 215 | VAL  | C-N-CA   | 6.53  | 132.57      | 121.14   |
| 1   | D     | 272 | ASN  | N-CA-C   | 6.46  | 118.37      | 108.42   |
| 1   | C     | 436 | SER  | CB-CA-C  | 6.46  | 121.02      | 110.88   |
| 1   | C     | 359 | MET  | N-CA-C   | 6.43  | 118.95      | 109.24   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 484 | ASP  | N-CA-C   | -6.43 | 103.97      | 110.97   |
| 1   | A     | 176 | ASP  | CA-CB-CG | 6.39  | 118.99      | 112.60   |
| 1   | A     | 353 | ASP  | CA-CB-CG | 6.38  | 118.98      | 112.60   |
| 1   | E     | 456 | HIS  | N-CA-C   | 6.35  | 117.99      | 111.14   |
| 1   | F     | 162 | ASN  | CA-CB-CG | 6.33  | 118.93      | 112.60   |
| 1   | D     | 37  | ALA  | O-C-N    | 6.32  | 126.93      | 121.30   |
| 1   | C     | 326 | ALA  | N-CA-C   | 6.31  | 119.00      | 109.41   |
| 1   | C     | 336 | LYS  | CA-C-N   | 6.30  | 126.84      | 120.04   |
| 1   | C     | 336 | LYS  | C-N-CA   | 6.30  | 126.84      | 120.04   |
| 1   | D     | 368 | ASP  | CA-CB-CG | 6.29  | 118.89      | 112.60   |
| 1   | D     | 427 | LEU  | CA-C-N   | -6.29 | 115.39      | 123.19   |
| 1   | D     | 427 | LEU  | C-N-CA   | -6.29 | 115.39      | 123.19   |
| 1   | C     | 368 | ASP  | CA-CB-CG | 6.29  | 118.89      | 112.60   |
| 1   | E     | 390 | HIS  | N-CA-CB  | 6.27  | 119.35      | 109.82   |
| 1   | A     | 318 | ARG  | O-C-N    | 6.24  | 129.27      | 122.15   |
| 1   | B     | 243 | PHE  | CA-CB-CG | 6.24  | 120.04      | 113.80   |
| 1   | B     | 527 | VAL  | N-CA-CB  | -6.24 | 102.48      | 111.21   |
| 1   | D     | 471 | VAL  | CB-CA-C  | -6.22 | 101.93      | 110.77   |
| 1   | D     | 220 | VAL  | N-CA-CB  | -6.21 | 102.45      | 111.52   |
| 1   | C     | 484 | ASP  | CA-CB-CG | 6.20  | 118.80      | 112.60   |
| 1   | A     | 86  | THR  | N-CA-CB  | 6.19  | 119.34      | 110.06   |
| 1   | E     | 324 | ILE  | CB-CA-C  | -6.17 | 101.63      | 110.83   |
| 1   | A     | 420 | TYR  | N-CA-C   | -6.16 | 104.48      | 111.14   |
| 1   | A     | 326 | ALA  | N-CA-C   | 6.15  | 118.41      | 109.07   |
| 1   | A     | 368 | ASP  | CA-CB-CG | 6.15  | 118.75      | 112.60   |
| 1   | E     | 501 | PHE  | CA-CB-CG | -6.13 | 107.67      | 113.80   |
| 1   | B     | 293 | ARG  | CD-NE-CZ | -6.13 | 115.82      | 124.40   |
| 1   | H     | 326 | ALA  | N-CA-C   | 6.12  | 118.72      | 109.41   |
| 1   | D     | 317 | ASN  | CA-CB-CG | 6.12  | 118.72      | 112.60   |
| 1   | H     | 298 | ILE  | N-CA-C   | -6.12 | 106.55      | 111.81   |
| 1   | G     | 326 | ALA  | N-CA-C   | 6.11  | 118.47      | 109.24   |
| 1   | A     | 188 | GLY  | C-N-CD   | -6.09 | 100.01      | 125.00   |
| 1   | B     | 83  | HIS  | CA-CB-CG | -6.09 | 107.71      | 113.80   |
| 1   | E     | 215 | VAL  | CB-CA-C  | 6.09  | 119.07      | 111.15   |
| 1   | C     | 83  | HIS  | CA-CB-CG | -6.05 | 107.75      | 113.80   |
| 1   | C     | 378 | HIS  | CA-C-N   | 6.05  | 128.67      | 120.44   |
| 1   | C     | 378 | HIS  | C-N-CA   | 6.05  | 128.67      | 120.44   |
| 1   | A     | 41  | ALA  | N-CA-C   | 6.05  | 118.58      | 110.35   |
| 1   | G     | 210 | LEU  | N-CA-CB  | -6.05 | 101.26      | 111.30   |
| 1   | E     | 420 | TYR  | CA-CB-CG | 6.04  | 124.78      | 113.90   |
| 1   | F     | 236 | VAL  | CB-CA-C  | 6.04  | 118.23      | 111.59   |
| 1   | A     | 421 | LYS  | N-CA-C   | 6.04  | 118.36      | 111.11   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 510 | VAL  | CB-CA-C  | -6.04 | 103.42      | 110.91   |
| 1   | C     | 216 | ASP  | CB-CA-C  | -6.04 | 100.77      | 110.79   |
| 1   | A     | 463 | HIS  | CA-CB-CG | -6.03 | 107.77      | 113.80   |
| 1   | B     | 421 | LYS  | N-CA-C   | 6.03  | 118.34      | 111.11   |
| 1   | D     | 250 | VAL  | N-CA-C   | -6.02 | 104.48      | 110.62   |
| 1   | F     | 331 | GLU  | N-CA-CB  | 6.02  | 119.09      | 110.06   |
| 1   | A     | 206 | LYS  | CA-C-N   | 6.01  | 126.81      | 120.43   |
| 1   | A     | 206 | LYS  | C-N-CA   | 6.01  | 126.81      | 120.43   |
| 1   | D     | 361 | SER  | CA-C-O   | 6.01  | 123.22      | 119.55   |
| 1   | A     | 331 | GLU  | N-CA-C   | 6.01  | 118.60      | 111.33   |
| 1   | A     | 33  | ASP  | CA-CB-CG | 6.00  | 118.60      | 112.60   |
| 1   | D     | 215 | VAL  | CA-C-N   | 6.00  | 129.43      | 120.31   |
| 1   | D     | 215 | VAL  | C-N-CA   | 6.00  | 129.43      | 120.31   |
| 1   | F     | 138 | THR  | N-CA-C   | 6.00  | 117.75      | 109.54   |
| 1   | A     | 401 | SER  | CA-C-N   | 5.99  | 128.80      | 120.29   |
| 1   | A     | 401 | SER  | C-N-CA   | 5.99  | 128.80      | 120.29   |
| 1   | E     | 103 | LEU  | CA-C-O   | 5.99  | 126.25      | 119.18   |
| 1   | H     | 525 | ARG  | N-CA-C   | 5.99  | 118.99      | 108.75   |
| 1   | G     | 236 | VAL  | N-CA-C   | -5.99 | 103.45      | 110.21   |
| 1   | E     | 466 | ARG  | N-CA-C   | 5.98  | 119.27      | 110.30   |
| 1   | A     | 443 | TYR  | CA-CB-CG | -5.97 | 103.15      | 113.90   |
| 1   | D     | 452 | VAL  | N-CA-C   | 5.96  | 115.32      | 106.85   |
| 1   | G     | 82  | TYR  | N-CA-C   | -5.96 | 104.35      | 111.69   |
| 1   | C     | 115 | GLY  | CA-C-N   | 5.96  | 125.90      | 119.76   |
| 1   | C     | 115 | GLY  | C-N-CA   | 5.96  | 125.90      | 119.76   |
| 1   | G     | 243 | PHE  | N-CA-C   | 5.96  | 119.41      | 111.30   |
| 1   | B     | 215 | VAL  | CA-C-N   | 5.96  | 132.98      | 121.18   |
| 1   | B     | 215 | VAL  | C-N-CA   | 5.96  | 132.98      | 121.18   |
| 1   | H     | 346 | ASP  | N-CA-CB  | 5.95  | 118.64      | 110.01   |
| 1   | A     | 341 | ARG  | N-CA-C   | -5.95 | 106.15      | 113.41   |
| 1   | E     | 113 | THR  | N-CA-CB  | -5.92 | 100.75      | 110.41   |
| 1   | H     | 329 | MET  | N-CA-C   | 5.91  | 118.20      | 111.11   |
| 1   | E     | 331 | GLU  | N-CA-C   | 5.91  | 117.52      | 111.14   |
| 1   | F     | 335 | LYS  | CB-CA-C  | 5.89  | 118.92      | 109.02   |
| 1   | G     | 161 | LYS  | N-CA-C   | 5.89  | 119.29      | 111.75   |
| 1   | H     | 334 | ILE  | CB-CA-C  | -5.89 | 104.10      | 112.22   |
| 1   | F     | 273 | HIS  | CA-CB-CG | -5.88 | 107.92      | 113.80   |
| 1   | C     | 327 | THR  | N-CA-CB  | -5.88 | 100.55      | 110.49   |
| 1   | C     | 123 | ILE  | CB-CA-C  | -5.88 | 104.20      | 111.08   |
| 1   | B     | 140 | LYS  | CA-C-N   | -5.87 | 115.44      | 123.14   |
| 1   | B     | 140 | LYS  | C-N-CA   | -5.87 | 115.44      | 123.14   |
| 1   | D     | 18  | HIS  | N-CA-C   | -5.85 | 104.82      | 111.14   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 44  | THR  | CA-C-N   | -5.84 | 114.80      | 120.34   |
| 1   | C     | 44  | THR  | C-N-CA   | -5.84 | 114.80      | 120.34   |
| 1   | D     | 390 | HIS  | N-CA-C   | 5.83  | 117.64      | 111.28   |
| 1   | A     | 448 | PRO  | CB-CA-C  | -5.83 | 104.29      | 111.64   |
| 1   | E     | 215 | VAL  | N-CA-C   | 5.83  | 116.58      | 108.89   |
| 1   | A     | 293 | ARG  | N-CA-C   | 5.81  | 118.08      | 111.11   |
| 1   | G     | 279 | PHE  | CA-CB-CG | -5.81 | 107.99      | 113.80   |
| 1   | H     | 446 | ARG  | N-CA-C   | -5.80 | 106.83      | 114.31   |
| 1   | D     | 326 | ALA  | CB-CA-C  | -5.80 | 98.82       | 110.30   |
| 1   | C     | 326 | ALA  | N-CA-CB  | -5.79 | 102.22      | 111.43   |
| 1   | D     | 293 | ARG  | N-CA-CB  | 5.79  | 119.29      | 110.14   |
| 1   | A     | 243 | PHE  | N-CA-C   | 5.79  | 119.38      | 111.39   |
| 1   | D     | 510 | VAL  | N-CA-C   | 5.78  | 116.26      | 108.17   |
| 1   | C     | 527 | VAL  | N-CA-CB  | -5.78 | 103.12      | 111.21   |
| 1   | D     | 330 | LEU  | N-CA-CB  | -5.77 | 103.57      | 111.65   |
| 1   | G     | 359 | MET  | N-CA-C   | 5.77  | 118.05      | 108.99   |
| 1   | G     | 25  | PHE  | CA-CB-CG | -5.77 | 108.03      | 113.80   |
| 1   | E     | 426 | ALA  | N-CA-C   | 5.76  | 116.16      | 108.38   |
| 1   | B     | 326 | ALA  | N-CA-C   | 5.76  | 117.72      | 109.14   |
| 1   | D     | 326 | ALA  | N-CA-CB  | -5.76 | 102.27      | 111.43   |
| 1   | G     | 438 | HIS  | N-CA-C   | -5.76 | 104.37      | 111.40   |
| 1   | F     | 390 | HIS  | N-CA-C   | 5.76  | 117.23      | 111.07   |
| 1   | C     | 445 | PRO  | O-C-N    | -5.75 | 115.95      | 122.91   |
| 1   | F     | 117 | GLU  | N-CA-C   | 5.74  | 118.13      | 109.41   |
| 1   | F     | 244 | ILE  | N-CA-CB  | 5.73  | 116.78      | 110.53   |
| 1   | B     | 80  | HIS  | CA-CB-CG | -5.73 | 108.07      | 113.80   |
| 1   | G     | 305 | VAL  | N-CA-C   | 5.73  | 116.19      | 110.23   |
| 1   | E     | 37  | ALA  | CA-C-N   | 5.72  | 125.91      | 120.31   |
| 1   | E     | 37  | ALA  | C-N-CA   | 5.72  | 125.91      | 120.31   |
| 1   | H     | 192 | LEU  | CA-C-N   | -5.68 | 115.78      | 122.93   |
| 1   | H     | 192 | LEU  | C-N-CA   | -5.68 | 115.78      | 122.93   |
| 1   | H     | 64  | ILE  | O-C-N    | 5.66  | 127.66      | 121.83   |
| 1   | B     | 117 | GLU  | N-CA-C   | 5.66  | 117.22      | 109.18   |
| 1   | H     | 20  | ALA  | N-CA-C   | 5.66  | 119.00      | 111.75   |
| 1   | B     | 525 | ARG  | N-CA-C   | 5.66  | 117.78      | 109.24   |
| 1   | D     | 315 | ARG  | N-CA-C   | 5.66  | 117.45      | 111.28   |
| 1   | G     | 38  | PRO  | CB-CA-C  | -5.66 | 102.38      | 110.75   |
| 1   | C     | 490 | ASN  | CA-CB-CG | -5.65 | 106.95      | 112.60   |
| 1   | B     | 463 | HIS  | CA-CB-CG | 5.65  | 119.45      | 113.80   |
| 1   | C     | 331 | GLU  | N-CA-C   | 5.65  | 120.63      | 111.37   |
| 1   | H     | 163 | ILE  | N-CA-C   | 5.64  | 116.38      | 110.62   |
| 1   | H     | 342 | ALA  | N-CA-C   | -5.63 | 105.05      | 111.14   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 76  | SER  | N-CA-C   | -5.62 | 106.26      | 113.01   |
| 1   | E     | 54  | SER  | N-CA-CB  | -5.62 | 103.39      | 111.54   |
| 1   | E     | 449 | ILE  | N-CA-CB  | -5.62 | 104.38      | 111.46   |
| 1   | C     | 114 | LYS  | CA-C-N   | -5.62 | 113.05      | 121.87   |
| 1   | C     | 114 | LYS  | C-N-CA   | -5.62 | 113.05      | 121.87   |
| 1   | B     | 37  | ALA  | N-CA-C   | 5.61  | 116.72      | 109.65   |
| 1   | H     | 502 | PHE  | CA-CB-CG | -5.61 | 108.19      | 113.80   |
| 1   | B     | 334 | ILE  | CB-CA-C  | -5.60 | 104.71      | 112.04   |
| 1   | G     | 215 | VAL  | CA-C-N   | 5.60  | 130.94      | 121.14   |
| 1   | G     | 215 | VAL  | C-N-CA   | 5.60  | 130.94      | 121.14   |
| 1   | C     | 86  | THR  | N-CA-CB  | 5.59  | 118.11      | 110.01   |
| 1   | G     | 90  | VAL  | N-CA-CB  | -5.59 | 104.53      | 110.62   |
| 1   | B     | 272 | ASN  | N-CA-C   | 5.58  | 116.75      | 108.60   |
| 1   | H     | 323 | VAL  | CB-CA-C  | -5.58 | 102.18      | 110.33   |
| 1   | H     | 361 | SER  | CA-C-O   | 5.58  | 122.95      | 119.77   |
| 1   | H     | 317 | ASN  | CA-C-N   | 5.57  | 127.75      | 120.28   |
| 1   | H     | 317 | ASN  | C-N-CA   | 5.57  | 127.75      | 120.28   |
| 1   | A     | 475 | ASP  | CA-CB-CG | 5.57  | 118.17      | 112.60   |
| 1   | H     | 403 | HIS  | CA-CB-CG | -5.57 | 108.23      | 113.80   |
| 1   | G     | 434 | GLY  | N-CA-C   | -5.57 | 107.27      | 113.79   |
| 1   | H     | 496 | GLY  | O-C-N    | 5.57  | 127.64      | 122.13   |
| 1   | D     | 327 | THR  | N-CA-C   | 5.56  | 122.64      | 110.80   |
| 1   | A     | 286 | SER  | N-CA-C   | 5.54  | 118.75      | 109.95   |
| 1   | G     | 272 | ASN  | CA-CB-CG | 5.52  | 118.12      | 112.60   |
| 1   | B     | 273 | HIS  | CA-CB-CG | 5.51  | 119.31      | 113.80   |
| 1   | C     | 90  | VAL  | CB-CA-C  | -5.51 | 104.92      | 111.81   |
| 1   | A     | 490 | ASN  | CA-CB-CG | -5.51 | 107.09      | 112.60   |
| 1   | C     | 50  | ILE  | N-CA-C   | 5.51  | 116.23      | 108.36   |
| 1   | C     | 69  | ASN  | CA-CB-CG | 5.51  | 118.11      | 112.60   |
| 1   | F     | 279 | PHE  | N-CA-C   | 5.51  | 117.72      | 111.11   |
| 1   | B     | 305 | VAL  | N-CA-C   | 5.50  | 115.70      | 110.42   |
| 1   | H     | 503 | LYS  | CA-C-N   | 5.50  | 128.44      | 120.79   |
| 1   | H     | 503 | LYS  | C-N-CA   | 5.50  | 128.44      | 120.79   |
| 1   | B     | 141 | ILE  | N-CA-CB  | 5.50  | 119.00      | 111.41   |
| 1   | F     | 466 | ARG  | N-CA-C   | 5.48  | 117.58      | 108.20   |
| 1   | B     | 468 | ILE  | CA-C-N   | 5.48  | 129.16      | 122.42   |
| 1   | B     | 468 | ILE  | C-N-CA   | 5.48  | 129.16      | 122.42   |
| 1   | B     | 242 | SER  | N-CA-C   | 5.48  | 118.86      | 110.20   |
| 1   | C     | 242 | SER  | N-CA-C   | 5.48  | 118.59      | 110.48   |
| 1   | D     | 216 | ASP  | CB-CA-C  | -5.47 | 100.16      | 110.67   |
| 1   | G     | 321 | LYS  | CA-C-N   | 5.47  | 125.37      | 119.85   |
| 1   | G     | 321 | LYS  | C-N-CA   | 5.47  | 125.37      | 119.85   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | H     | 48  | CYS  | N-CA-CB  | 5.47  | 120.43      | 111.08   |
| 1   | B     | 331 | GLU  | N-CA-C   | 5.46  | 116.91      | 111.07   |
| 1   | F     | 440 | VAL  | CB-CA-C  | -5.46 | 104.93      | 112.24   |
| 1   | H     | 443 | TYR  | CA-CB-CG | -5.46 | 104.08      | 113.90   |
| 1   | B     | 161 | LYS  | N-CA-C   | 5.45  | 117.93      | 111.33   |
| 1   | E     | 51  | GLY  | CA-C-N   | 5.44  | 125.11      | 119.56   |
| 1   | E     | 51  | GLY  | C-N-CA   | 5.44  | 125.11      | 119.56   |
| 1   | C     | 468 | ILE  | N-CA-CB  | 5.44  | 116.86      | 110.82   |
| 1   | B     | 23  | ASP  | CA-CB-CG | 5.44  | 118.04      | 112.60   |
| 1   | A     | 298 | ILE  | CB-CA-C  | -5.43 | 106.08      | 111.30   |
| 1   | A     | 129 | ALA  | N-CA-C   | 5.43  | 122.36      | 110.80   |
| 1   | C     | 526 | VAL  | CB-CA-C  | -5.43 | 103.64      | 111.19   |
| 1   | C     | 15  | GLN  | CB-CG-CD | -5.42 | 103.38      | 112.60   |
| 1   | B     | 217 | LEU  | CA-C-N   | 5.42  | 125.34      | 119.76   |
| 1   | B     | 217 | LEU  | C-N-CA   | 5.42  | 125.34      | 119.76   |
| 1   | G     | 349 | ASN  | CA-CB-CG | -5.42 | 107.18      | 112.60   |
| 1   | C     | 76  | SER  | N-CA-C   | -5.42 | 106.62      | 113.18   |
| 1   | H     | 185 | LYS  | CB-CA-C  | 5.41  | 118.70      | 109.24   |
| 1   | B     | 366 | LYS  | CB-CA-C  | -5.40 | 100.47      | 109.55   |
| 1   | B     | 259 | GLU  | N-CA-C   | 5.40  | 117.17      | 111.28   |
| 1   | C     | 356 | ASP  | CA-CB-CG | -5.40 | 107.20      | 112.60   |
| 1   | B     | 327 | THR  | N-CA-C   | 5.40  | 122.30      | 110.80   |
| 1   | E     | 522 | ASN  | CA-CB-CG | 5.39  | 117.99      | 112.60   |
| 1   | C     | 38  | PRO  | CA-C-N   | -5.39 | 116.39      | 122.48   |
| 1   | C     | 38  | PRO  | C-N-CA   | -5.39 | 116.39      | 122.48   |
| 1   | E     | 239 | VAL  | CA-C-N   | -5.38 | 115.85      | 122.84   |
| 1   | E     | 239 | VAL  | C-N-CA   | -5.38 | 115.85      | 122.84   |
| 1   | F     | 527 | VAL  | N-CA-CB  | -5.38 | 108.12      | 111.83   |
| 1   | C     | 322 | PRO  | N-CA-CB  | 5.37  | 107.98      | 103.25   |
| 1   | E     | 353 | ASP  | CA-CB-CG | 5.37  | 117.97      | 112.60   |
| 1   | B     | 126 | SER  | N-CA-CB  | 5.37  | 119.90      | 111.20   |
| 1   | D     | 215 | VAL  | N-CA-C   | 5.37  | 116.17      | 108.93   |
| 1   | H     | 450 | ILE  | CA-C-N   | -5.36 | 115.24      | 123.07   |
| 1   | H     | 450 | ILE  | C-N-CA   | -5.36 | 115.24      | 123.07   |
| 1   | C     | 444 | ARG  | N-CA-C   | 5.36  | 121.65      | 109.81   |
| 1   | B     | 485 | VAL  | CB-CA-C  | -5.35 | 105.12      | 111.81   |
| 1   | D     | 41  | ALA  | N-CA-C   | 5.35  | 118.26      | 109.76   |
| 1   | B     | 201 | PHE  | CA-CB-CG | -5.34 | 108.46      | 113.80   |
| 1   | H     | 75  | PHE  | CA-CB-CG | -5.34 | 108.46      | 113.80   |
| 1   | C     | 105 | ARG  | N-CA-CB  | 5.34  | 119.02      | 109.94   |
| 1   | A     | 466 | ARG  | CD-NE-CZ | -5.34 | 116.93      | 124.40   |
| 1   | H     | 51  | GLY  | O-C-N    | 5.34  | 127.11      | 121.77   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 199 | GLY  | CA-C-N    | 5.33  | 127.02      | 120.51   |
| 1   | A     | 199 | GLY  | C-N-CA    | 5.33  | 127.02      | 120.51   |
| 1   | A     | 355 | ALA  | CA-C-O    | -5.33 | 114.88      | 120.80   |
| 1   | G     | 431 | THR  | CA-CB-CG2 | -5.33 | 101.44      | 110.50   |
| 1   | F     | 197 | GLU  | N-CA-CB   | -5.32 | 102.19      | 110.55   |
| 1   | F     | 374 | VAL  | CA-CB-CG1 | -5.32 | 101.35      | 110.40   |
| 1   | B     | 96  | SER  | N-CA-C    | -5.32 | 105.48      | 111.28   |
| 1   | D     | 440 | VAL  | CB-CA-C   | -5.31 | 104.97      | 112.14   |
| 1   | G     | 216 | ASP  | CA-CB-CG  | 5.30  | 117.90      | 112.60   |
| 1   | H     | 416 | VAL  | CB-CA-C   | 5.30  | 118.75      | 111.97   |
| 1   | E     | 89  | ASN  | O-C-N     | 5.29  | 127.81      | 122.09   |
| 1   | A     | 357 | CYS  | N-CA-C    | 5.29  | 117.43      | 109.23   |
| 1   | B     | 15  | GLN  | CB-CG-CD  | -5.28 | 103.62      | 112.60   |
| 1   | E     | 44  | THR  | CA-C-N    | -5.28 | 117.24      | 122.36   |
| 1   | E     | 44  | THR  | C-N-CA    | -5.28 | 117.24      | 122.36   |
| 1   | C     | 502 | PHE  | N-CA-C    | 5.28  | 116.87      | 108.79   |
| 1   | A     | 57  | VAL  | CB-CA-C   | -5.28 | 105.00      | 111.92   |
| 1   | F     | 215 | VAL  | CA-C-N    | 5.27  | 128.31      | 120.31   |
| 1   | F     | 215 | VAL  | C-N-CA    | 5.27  | 128.31      | 120.31   |
| 1   | C     | 510 | VAL  | N-CA-C    | 5.26  | 115.48      | 108.11   |
| 1   | D     | 39  | ILE  | N-CA-CB   | 5.26  | 118.34      | 112.34   |
| 1   | D     | 410 | ALA  | N-CA-CB   | -5.26 | 102.10      | 109.94   |
| 1   | F     | 327 | THR  | N-CA-C    | 5.26  | 122.01      | 110.80   |
| 1   | D     | 333 | MET  | N-CA-C    | 5.26  | 119.19      | 112.87   |
| 1   | F     | 272 | ASN  | N-CA-C    | 5.26  | 115.08      | 108.45   |
| 1   | H     | 306 | PHE  | CA-CB-CG  | -5.26 | 108.54      | 113.80   |
| 1   | B     | 239 | VAL  | N-CA-C    | 5.25  | 116.07      | 107.24   |
| 1   | G     | 361 | SER  | CA-C-O    | 5.25  | 122.75      | 119.55   |
| 1   | F     | 510 | VAL  | N-CA-C    | 5.25  | 115.41      | 107.75   |
| 1   | A     | 266 | ILE  | N-CA-C    | 5.24  | 116.25      | 108.23   |
| 1   | G     | 287 | ASP  | N-CA-C    | -5.24 | 106.92      | 113.72   |
| 1   | A     | 379 | LEU  | O-C-N     | 5.23  | 127.47      | 122.03   |
| 1   | B     | 409 | GLU  | N-CA-C    | -5.23 | 105.48      | 111.07   |
| 1   | C     | 114 | LYS  | O-C-N     | -5.22 | 116.19      | 122.15   |
| 1   | D     | 319 | ALA  | N-CA-C    | 5.22  | 119.36      | 112.89   |
| 1   | E     | 47  | ILE  | CB-CA-C   | -5.22 | 103.82      | 110.98   |
| 1   | A     | 452 | VAL  | N-CA-C    | 5.22  | 114.81      | 106.88   |
| 1   | G     | 81  | GLU  | N-CA-CB   | 5.22  | 119.06      | 110.39   |
| 1   | C     | 140 | LYS  | CB-CA-C   | 5.21  | 118.24      | 109.48   |
| 1   | F     | 392 | LYS  | N-CA-CB   | 5.21  | 117.52      | 109.91   |
| 1   | C     | 263 | ASN  | CA-CB-CG  | -5.21 | 107.39      | 112.60   |
| 1   | C     | 327 | THR  | N-CA-C    | 5.21  | 121.89      | 110.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 114 | LYS  | CA-C-N   | -5.21 | 113.70      | 121.87   |
| 1   | F     | 114 | LYS  | C-N-CA   | -5.21 | 113.70      | 121.87   |
| 1   | G     | 46  | ILE  | N-CA-CB  | 5.20  | 118.01      | 111.46   |
| 1   | H     | 508 | VAL  | CA-C-N   | -5.20 | 114.89      | 122.68   |
| 1   | H     | 508 | VAL  | C-N-CA   | -5.20 | 114.89      | 122.68   |
| 1   | G     | 438 | HIS  | CA-C-N   | 5.19  | 127.54      | 120.54   |
| 1   | G     | 438 | HIS  | C-N-CA   | 5.19  | 127.54      | 120.54   |
| 1   | A     | 106 | PRO  | N-CA-CB  | 5.18  | 107.86      | 103.35   |
| 1   | H     | 527 | VAL  | N-CA-C   | 5.18  | 113.78      | 107.61   |
| 1   | F     | 86  | THR  | N-CA-C   | -5.18 | 105.71      | 111.36   |
| 1   | G     | 27  | GLU  | O-C-N    | 5.18  | 127.68      | 122.09   |
| 1   | A     | 158 | LEU  | CB-CA-C  | -5.18 | 99.62       | 109.66   |
| 1   | H     | 115 | GLY  | CA-C-N   | 5.17  | 125.09      | 119.76   |
| 1   | H     | 115 | GLY  | C-N-CA   | 5.17  | 125.09      | 119.76   |
| 1   | F     | 201 | PHE  | N-CA-C   | 5.17  | 117.04      | 108.20   |
| 1   | G     | 103 | LEU  | N-CA-C   | 5.17  | 119.46      | 113.20   |
| 1   | C     | 241 | ALA  | N-CA-C   | 5.17  | 117.17      | 108.96   |
| 1   | H     | 57  | VAL  | N-CA-C   | -5.16 | 105.57      | 110.42   |
| 1   | H     | 293 | ARG  | N-CA-C   | 5.16  | 117.64      | 111.71   |
| 1   | H     | 116 | PRO  | N-CA-CB  | 5.15  | 107.89      | 103.31   |
| 1   | B     | 356 | ASP  | CA-CB-CG | -5.14 | 107.46      | 112.60   |
| 1   | C     | 501 | PHE  | CA-CB-CG | -5.13 | 108.67      | 113.80   |
| 1   | B     | 489 | VAL  | CB-CA-C  | -5.13 | 105.41      | 111.97   |
| 1   | F     | 184 | VAL  | CB-CA-C  | -5.13 | 106.36      | 111.80   |
| 1   | F     | 468 | ILE  | CB-CA-C  | -5.12 | 103.70      | 111.33   |
| 1   | G     | 31  | ARG  | CB-CA-C  | -5.12 | 102.49      | 110.94   |
| 1   | H     | 346 | ASP  | O-C-N    | 5.11  | 127.33      | 122.07   |
| 1   | D     | 408 | MET  | N-CA-C   | 5.10  | 116.84      | 111.28   |
| 1   | B     | 470 | PRO  | N-CA-CB  | 5.09  | 107.84      | 103.31   |
| 1   | G     | 317 | ASN  | O-C-N    | 5.09  | 127.52      | 122.12   |
| 1   | G     | 490 | ASN  | O-C-N    | 5.08  | 127.31      | 122.07   |
| 1   | H     | 272 | ASN  | N-CA-C   | 5.07  | 116.01      | 108.86   |
| 1   | F     | 472 | VAL  | N-CA-CB  | 5.07  | 117.55      | 110.56   |
| 1   | H     | 23  | ASP  | N-CA-C   | -5.06 | 107.65      | 113.88   |
| 1   | F     | 71  | ALA  | CA-C-N   | -5.06 | 115.74      | 122.72   |
| 1   | F     | 71  | ALA  | C-N-CA   | -5.06 | 115.74      | 122.72   |
| 1   | H     | 32  | LEU  | N-CA-C   | 5.06  | 116.99      | 109.25   |
| 1   | F     | 431 | THR  | N-CA-C   | 5.06  | 117.07      | 109.23   |
| 1   | C     | 382 | ARG  | CB-CA-C  | -5.05 | 102.40      | 110.79   |
| 1   | G     | 327 | THR  | N-CA-C   | 5.05  | 121.56      | 110.80   |
| 1   | C     | 438 | HIS  | CA-CB-CG | 5.05  | 118.85      | 113.80   |
| 1   | D     | 409 | GLU  | N-CA-CB  | 5.05  | 117.54      | 110.12   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | H     | 219 | ALA  | O-C-N    | 5.05  | 127.27      | 122.07   |
| 1   | C     | 41  | ALA  | N-CA-C   | 5.04  | 118.16      | 110.20   |
| 1   | B     | 213 | ALA  | N-CA-C   | 5.03  | 117.77      | 109.72   |
| 1   | C     | 215 | VAL  | N-CA-C   | 5.03  | 115.72      | 108.93   |
| 1   | D     | 444 | ARG  | N-CA-C   | 5.03  | 120.92      | 109.81   |
| 1   | F     | 216 | ASP  | CA-CB-CG | 5.03  | 117.63      | 112.60   |
| 1   | F     | 345 | SER  | N-CA-CB  | 5.03  | 117.51      | 110.12   |
| 1   | F     | 445 | PRO  | N-CA-C   | -5.03 | 103.87      | 111.41   |
| 1   | G     | 76  | SER  | N-CA-C   | -5.03 | 106.98      | 113.01   |
| 1   | C     | 272 | ASN  | N-CA-C   | 5.03  | 114.88      | 108.24   |
| 1   | D     | 280 | ASP  | N-CA-C   | 5.03  | 117.41      | 111.33   |
| 1   | G     | 456 | HIS  | N-CA-CB  | 5.01  | 117.94      | 110.22   |
| 1   | G     | 41  | ALA  | N-CA-C   | 5.01  | 117.49      | 110.23   |
| 1   | G     | 101 | PRO  | N-CA-CB  | 5.01  | 108.51      | 103.25   |
| 1   | D     | 528 | PRO  | N-CA-CB  | 5.01  | 108.51      | 103.25   |
| 1   | G     | 47  | ILE  | N-CA-CB  | -5.00 | 105.60      | 111.90   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3979  | 0        | 4055     | 268     | 0            |
| 1   | B     | 3979  | 0        | 4055     | 323     | 0            |
| 1   | C     | 3978  | 0        | 4055     | 229     | 0            |
| 1   | D     | 3979  | 0        | 4056     | 234     | 0            |
| 1   | E     | 3268  | 0        | 3315     | 234     | 0            |
| 1   | F     | 3979  | 0        | 4055     | 284     | 0            |
| 1   | G     | 3979  | 0        | 4056     | 364     | 0            |
| 1   | H     | 3979  | 0        | 4056     | 371     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 10    | 0        | 4        | 1       | 0            |
| 4   | B     | 10    | 0        | 4        | 3       | 0            |
| 4   | C     | 10    | 0        | 4        | 1       | 0            |
| 4   | D     | 10    | 0        | 4        | 1       | 0            |
| 4   | E     | 10    | 0        | 4        | 0       | 0            |
| 4   | F     | 10    | 0        | 4        | 3       | 0            |
| 4   | G     | 10    | 0        | 4        | 0       | 0            |
| 4   | H     | 10    | 0        | 4        | 5       | 0            |
| 5   | A     | 36    | 0        | 0        | 3       | 0            |
| 5   | B     | 25    | 0        | 0        | 2       | 0            |
| 5   | C     | 35    | 0        | 0        | 7       | 0            |
| 5   | D     | 35    | 0        | 0        | 3       | 0            |
| 5   | E     | 16    | 0        | 0        | 0       | 0            |
| 5   | F     | 18    | 0        | 0        | 2       | 0            |
| 5   | G     | 14    | 0        | 0        | 1       | 0            |
| 5   | H     | 15    | 0        | 0        | 0       | 0            |
| All | All   | 31410 | 0        | 31735    | 2191    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (2191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:141:ILE:HG22 | 1:C:156:LEU:HB3  | 1.27                     | 1.13              |
| 1:F:186:GLN:HB3  | 1:F:193:VAL:HB   | 1.30                     | 1.12              |
| 1:E:47:ILE:HB    | 1:E:359:MET:HG2  | 1.27                     | 1.12              |
| 1:H:15:GLN:HB3   | 1:H:17:LEU:HD23  | 1.29                     | 1.09              |
| 1:E:391:ARG:NH1  | 1:F:399:ARG:HH21 | 1.51                     | 1.09              |
| 1:G:123:ILE:HD11 | 1:G:202:LEU:HD13 | 1.33                     | 1.06              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:493:MET:HE2  | 1:B:530:PRO:HD2  | 1.37                     | 1.05              |
| 1:E:114:LYS:HD3  | 1:E:223:LYS:HD3  | 1.37                     | 1.05              |
| 1:H:24:THR:HG22  | 1:H:27:GLU:H     | 1.12                     | 1.04              |
| 1:G:43:ASN:HB3   | 1:G:467:GLY:HA2  | 1.36                     | 1.04              |
| 1:C:145:ASN:H    | 1:C:145:ASN:ND2  | 1.55                     | 1.03              |
| 1:C:145:ASN:HD22 | 1:C:145:ASN:N    | 1.57                     | 1.01              |
| 1:F:215:VAL:HG11 | 1:F:217:LEU:HD12 | 1.39                     | 1.01              |
| 1:H:55:ARG:HG3   | 1:H:86:THR:HG23  | 1.40                     | 1.01              |
| 1:E:220:VAL:HG22 | 1:E:224:ASP:HB2  | 1.43                     | 1.00              |
| 1:E:257:LEU:HD21 | 1:E:264:ILE:HD12 | 1.44                     | 0.99              |
| 1:C:273:HIS:HB3  | 1:C:277:ARG:HH11 | 1.26                     | 0.99              |
| 1:H:105:ARG:HE   | 1:H:499:ARG:HH21 | 1.10                     | 0.99              |
| 1:B:63:MET:HG3   | 1:B:371:LEU:HD23 | 1.45                     | 0.97              |
| 1:G:272:ASN:HB2  | 1:G:299:GLU:HG2  | 1.47                     | 0.96              |
| 1:H:187:LYS:HA   | 1:H:192:LEU:HD12 | 1.48                     | 0.95              |
| 1:D:122:LEU:HD11 | 1:D:127:GLY:HA2  | 1.46                     | 0.94              |
| 1:F:333:MET:HE2  | 1:F:373:ALA:HA   | 1.46                     | 0.94              |
| 1:G:23:ASP:HB3   | 1:H:399:ARG:HH12 | 1.30                     | 0.93              |
| 1:H:122:LEU:HB2  | 1:H:149:GLU:HA   | 1.49                     | 0.93              |
| 1:F:328:GLN:HE21 | 1:H:341:ARG:H    | 1.16                     | 0.93              |
| 1:A:328:GLN:HE21 | 1:C:341:ARG:H    | 1.03                     | 0.92              |
| 1:H:43:ASN:HB3   | 1:H:467:GLY:HA2  | 1.51                     | 0.92              |
| 1:D:493:MET:HE2  | 1:D:529:VAL:HA   | 1.49                     | 0.91              |
| 1:H:123:ILE:HD13 | 1:H:131:VAL:HG23 | 1.51                     | 0.91              |
| 1:H:24:THR:HG22  | 1:H:27:GLU:N     | 1.85                     | 0.91              |
| 1:F:511:LEU:HB3  | 1:F:521:THR:HG21 | 1.51                     | 0.90              |
| 1:A:406:ASP:HB3  | 1:A:409:GLU:HG3  | 1.50                     | 0.90              |
| 1:G:69:ASN:HB3   | 1:G:463:HIS:CD2  | 2.05                     | 0.90              |
| 1:H:480:ALA:HB3  | 1:H:483:GLU:HG3  | 1.52                     | 0.89              |
| 1:G:323:VAL:H    | 1:G:356:ASP:HB2  | 1.36                     | 0.89              |
| 1:G:406:ASP:HB3  | 1:G:409:GLU:HB2  | 1.53                     | 0.89              |
| 1:A:328:GLN:NE2  | 1:C:341:ARG:H    | 1.70                     | 0.89              |
| 1:A:509:ILE:CD1  | 1:A:526:VAL:HG22 | 2.03                     | 0.89              |
| 1:G:61:LYS:HG2   | 1:G:93:ALA:HB1   | 1.54                     | 0.89              |
| 1:H:69:ASN:HB3   | 1:H:463:HIS:CD2  | 2.06                     | 0.89              |
| 1:A:145:ASN:HB3  | 1:A:148:MET:HE3  | 1.54                     | 0.88              |
| 1:B:453:THR:HG21 | 1:B:459:ALA:HB2  | 1.56                     | 0.88              |
| 1:E:328:GLN:HE21 | 1:G:341:ARG:H    | 1.22                     | 0.87              |
| 1:B:379:LEU:HB3  | 1:D:303:GLU:HG2  | 1.56                     | 0.87              |
| 1:G:454:ARG:NH1  | 1:G:477:VAL:HG22 | 1.88                     | 0.87              |
| 1:B:50:ILE:HB    | 1:B:73:MET:HE1   | 1.53                     | 0.87              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:102:ILE:HG22 | 1:B:103:LEU:HD12 | 1.57                     | 0.86              |
| 1:H:15:GLN:HB3   | 1:H:17:LEU:CD2   | 2.04                     | 0.86              |
| 1:A:145:ASN:HD22 | 1:A:145:ASN:H    | 1.21                     | 0.86              |
| 1:H:430:LEU:CD1  | 1:H:452:VAL:HB   | 2.05                     | 0.86              |
| 1:H:63:MET:HG3   | 1:H:371:LEU:HD23 | 1.57                     | 0.86              |
| 1:A:493:MET:HE2  | 1:A:530:PRO:HD2  | 1.57                     | 0.86              |
| 1:B:57:VAL:HG22  | 1:B:89:ASN:HB3   | 1.56                     | 0.86              |
| 1:B:428:ILE:HD12 | 1:B:508:VAL:HG11 | 1.58                     | 0.86              |
| 1:G:110:ALA:HB2  | 1:G:238:MET:HE2  | 1.57                     | 0.86              |
| 1:H:60:LEU:HD21  | 1:H:90:VAL:HG23  | 1.57                     | 0.86              |
| 1:A:493:MET:HE2  | 1:A:529:VAL:HA   | 1.56                     | 0.86              |
| 1:E:391:ARG:HH12 | 1:F:399:ARG:HH21 | 1.17                     | 0.86              |
| 1:B:63:MET:HG3   | 1:B:371:LEU:CD2  | 2.06                     | 0.86              |
| 1:H:25:PHE:CE2   | 1:H:29:MET:HE2   | 2.10                     | 0.85              |
| 1:A:340:THR:HB   | 1:C:328:GLN:HE21 | 1.42                     | 0.85              |
| 1:E:47:ILE:CD1   | 1:E:324:ILE:HD13 | 2.06                     | 0.85              |
| 1:F:133:LEU:HD13 | 1:F:139:LEU:HD13 | 1.57                     | 0.85              |
| 1:D:123:ILE:HG22 | 1:D:129:ALA:HB3  | 1.59                     | 0.85              |
| 1:A:145:ASN:HD22 | 1:A:145:ASN:N    | 1.74                     | 0.84              |
| 1:C:139:LEU:HD21 | 1:C:156:LEU:HB2  | 1.59                     | 0.84              |
| 1:G:440:VAL:HG12 | 1:G:449:ILE:HD13 | 1.59                     | 0.84              |
| 1:D:154:ASN:HB2  | 1:D:155:ILE:HD12 | 1.59                     | 0.84              |
| 1:H:63:MET:HG3   | 1:H:371:LEU:CD2  | 2.07                     | 0.84              |
| 1:H:63:MET:HB3   | 1:H:68:MET:HE3   | 1.59                     | 0.84              |
| 1:A:493:MET:CE   | 1:A:529:VAL:HA   | 2.06                     | 0.84              |
| 1:G:46:ILE:HG23  | 1:G:377:GLN:NE2  | 1.93                     | 0.84              |
| 1:A:43:ASN:HB3   | 1:A:467:GLY:HA2  | 1.59                     | 0.84              |
| 1:F:242:SER:HA   | 1:F:269:LYS:HE2  | 1.59                     | 0.84              |
| 1:F:493:MET:HE2  | 1:F:529:VAL:HA   | 1.60                     | 0.84              |
| 1:G:102:ILE:HG22 | 1:G:103:LEU:HD12 | 1.60                     | 0.84              |
| 1:C:123:ILE:HD12 | 1:C:131:VAL:CG2  | 2.08                     | 0.84              |
| 1:B:145:ASN:HD22 | 1:B:145:ASN:N    | 1.75                     | 0.83              |
| 1:G:382:ARG:HB2  | 1:G:382:ARG:HH11 | 1.41                     | 0.83              |
| 1:A:493:MET:HE2  | 1:A:530:PRO:CD   | 2.07                     | 0.83              |
| 1:G:23:ASP:HB3   | 1:H:399:ARG:NH1  | 1.92                     | 0.83              |
| 1:G:43:ASN:HB3   | 1:G:467:GLY:CA   | 2.06                     | 0.83              |
| 1:H:496:GLY:HA3  | 1:H:502:PHE:CZ   | 2.13                     | 0.83              |
| 1:D:132:GLU:HG3  | 1:D:201:PHE:HE1  | 1.42                     | 0.83              |
| 1:A:273:HIS:CD2  | 1:A:277:ARG:HE   | 1.94                     | 0.83              |
| 1:A:520:PHE:CE1  | 1:A:522:ASN:HB3  | 2.14                     | 0.83              |
| 1:C:141:ILE:CG2  | 1:C:156:LEU:HB3  | 2.09                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:34:ILE:CD1   | 1:G:276:VAL:HG11 | 2.09                     | 0.83              |
| 1:B:43:ASN:HB3   | 1:B:467:GLY:HA2  | 1.59                     | 0.82              |
| 1:B:292:ALA:HB1  | 4:B:532:PEQ:H21  | 1.61                     | 0.82              |
| 1:E:511:LEU:HB3  | 1:E:521:THR:HG21 | 1.62                     | 0.82              |
| 1:F:247:ALA:HB2  | 1:F:281:GLU:HG3  | 1.59                     | 0.82              |
| 1:B:215:VAL:CG1  | 1:B:217:LEU:HD12 | 2.10                     | 0.82              |
| 1:G:185:LYS:HG3  | 1:G:195:GLU:HB2  | 1.61                     | 0.82              |
| 1:A:493:MET:HE3  | 1:A:529:VAL:HG13 | 1.61                     | 0.82              |
| 1:G:499:ARG:HD2  | 1:G:501:PHE:CZ   | 2.15                     | 0.82              |
| 1:D:131:VAL:CG2  | 1:D:153:GLU:HB3  | 2.09                     | 0.82              |
| 1:B:132:GLU:HG3  | 1:B:201:PHE:CE1  | 2.15                     | 0.81              |
| 1:G:62:GLU:HB3   | 1:G:371:LEU:HD11 | 1.61                     | 0.81              |
| 1:D:123:ILE:HG22 | 1:D:129:ALA:CB   | 2.10                     | 0.81              |
| 1:H:55:ARG:CG    | 1:H:86:THR:HG23  | 2.09                     | 0.81              |
| 1:A:266:ILE:C    | 1:A:267:ILE:HD13 | 2.06                     | 0.81              |
| 1:C:493:MET:HE1  | 1:C:529:VAL:HG22 | 1.62                     | 0.81              |
| 1:C:524:MET:HE3  | 1:D:524:MET:HE3  | 1.63                     | 0.81              |
| 1:E:47:ILE:HD11  | 1:E:324:ILE:HD13 | 1.60                     | 0.81              |
| 1:E:301:PRO:HG2  | 1:E:304:LYS:HD2  | 1.63                     | 0.81              |
| 1:C:515:ARG:HB3  | 1:C:516:PRO:HD2  | 1.63                     | 0.80              |
| 1:E:46:ILE:HG23  | 1:E:377:GLN:NE2  | 1.96                     | 0.80              |
| 1:H:43:ASN:HB3   | 1:H:467:GLY:CA   | 2.11                     | 0.80              |
| 1:A:145:ASN:HB3  | 1:A:148:MET:CE   | 2.11                     | 0.80              |
| 1:B:503:LYS:HG2  | 1:B:504:LYS:H    | 1.44                     | 0.80              |
| 1:C:426:ALA:C    | 1:C:427:LEU:HD12 | 2.06                     | 0.80              |
| 1:G:343:GLU:O    | 1:G:347:VAL:HG23 | 1.82                     | 0.80              |
| 1:A:328:GLN:NE2  | 1:C:341:ARG:HG2  | 1.97                     | 0.80              |
| 1:C:290:MET:HE2  | 1:C:326:ALA:CB   | 2.12                     | 0.80              |
| 1:F:328:GLN:NE2  | 1:H:341:ARG:H    | 1.80                     | 0.80              |
| 1:B:43:ASN:HB3   | 1:B:467:GLY:CA   | 2.12                     | 0.79              |
| 1:G:61:LYS:HG2   | 1:G:93:ALA:CB    | 2.11                     | 0.79              |
| 1:H:242:SER:HA   | 1:H:269:LYS:HE2  | 1.64                     | 0.79              |
| 1:F:511:LEU:HD22 | 1:F:521:THR:HG22 | 1.64                     | 0.79              |
| 1:F:511:LEU:HB3  | 1:F:521:THR:CG2  | 2.12                     | 0.79              |
| 1:G:524:MET:HG2  | 1:G:525:ARG:N    | 1.96                     | 0.79              |
| 1:B:57:VAL:CG2   | 1:B:89:ASN:HB3   | 2.12                     | 0.79              |
| 1:E:105:ARG:NE   | 1:E:499:ARG:HH12 | 1.80                     | 0.79              |
| 1:B:261:GLY:CA   | 1:B:264:ILE:HG13 | 2.12                     | 0.79              |
| 1:E:241:ALA:HB1  | 1:E:244:ILE:HD11 | 1.65                     | 0.79              |
| 1:G:376:MET:O    | 1:G:380:ILE:HG13 | 1.83                     | 0.79              |
| 1:G:360:LEU:HB3  | 1:G:363:GLU:HB2  | 1.65                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:465:TYR:HB2  | 1:C:468:ILE:HD12 | 1.64                     | 0.78              |
| 1:A:241:ALA:HB1  | 1:A:244:ILE:HD11 | 1.65                     | 0.78              |
| 1:B:328:GLN:HE21 | 1:D:340:THR:HB   | 1.46                     | 0.78              |
| 1:G:382:ARG:HH11 | 1:G:382:ARG:CB   | 1.95                     | 0.78              |
| 1:E:257:LEU:CD2  | 1:E:264:ILE:HD12 | 2.12                     | 0.78              |
| 1:H:105:ARG:HE   | 1:H:499:ARG:NH2  | 1.81                     | 0.78              |
| 1:B:393:LEU:HG   | 1:B:397:LEU:HD22 | 1.64                     | 0.78              |
| 1:B:426:ALA:C    | 1:B:427:LEU:HD12 | 2.09                     | 0.78              |
| 1:F:247:ALA:O    | 1:F:250:VAL:HG23 | 1.84                     | 0.78              |
| 1:A:237:ASP:OD2  | 1:A:460:ARG:HD2  | 1.83                     | 0.78              |
| 1:E:376:MET:O    | 1:E:380:ILE:HG13 | 1.82                     | 0.78              |
| 1:E:221:SER:O    | 1:E:225:ILE:HG13 | 1.83                     | 0.78              |
| 1:B:102:ILE:HG22 | 1:B:103:LEU:CD1  | 2.13                     | 0.78              |
| 1:B:428:ILE:HD12 | 1:B:508:VAL:CG1  | 2.14                     | 0.78              |
| 1:C:131:VAL:CG1  | 1:C:153:GLU:HB3  | 2.13                     | 0.78              |
| 1:C:141:ILE:HG22 | 1:C:156:LEU:CB   | 2.10                     | 0.78              |
| 1:A:273:HIS:HD2  | 1:A:277:ARG:HE   | 1.30                     | 0.78              |
| 1:B:342:ALA:HB1  | 1:D:346:ASP:HB2  | 1.65                     | 0.78              |
| 1:D:247:ALA:O    | 1:D:250:VAL:HG23 | 1.84                     | 0.78              |
| 1:A:457:GLN:O    | 1:A:461:GLN:HG3  | 1.85                     | 0.77              |
| 1:D:24:THR:HG23  | 1:D:27:GLU:H     | 1.48                     | 0.77              |
| 1:F:371:LEU:O    | 1:F:375:ARG:HG3  | 1.85                     | 0.77              |
| 1:B:411:MET:HG2  | 1:B:521:THR:O    | 1.84                     | 0.77              |
| 1:F:315:ARG:HD2  | 1:H:30:CYS:HB3   | 1.67                     | 0.77              |
| 1:F:493:MET:HG2  | 1:F:530:PRO:HD2  | 1.67                     | 0.77              |
| 1:H:503:LYS:HG2  | 1:H:504:LYS:H    | 1.50                     | 0.77              |
| 1:D:132:GLU:HG3  | 1:D:201:PHE:CE1  | 2.19                     | 0.77              |
| 1:G:524:MET:CE   | 1:H:524:MET:HE3  | 2.14                     | 0.77              |
| 1:B:221:SER:H    | 1:B:224:ASP:HB2  | 1.50                     | 0.76              |
| 1:D:226:GLN:HA   | 1:D:229:LYS:HE2  | 1.68                     | 0.76              |
| 1:A:87:ILE:O     | 1:A:91:ARG:HG3   | 1.85                     | 0.76              |
| 1:B:173:VAL:HB   | 1:B:182:LEU:HD12 | 1.65                     | 0.76              |
| 1:G:21:MET:HE2   | 1:G:21:MET:HA    | 1.66                     | 0.76              |
| 1:C:462:ALA:HB1  | 1:C:468:ILE:HG21 | 1.68                     | 0.76              |
| 1:F:187:LYS:HA   | 1:F:192:LEU:CD1  | 2.15                     | 0.76              |
| 1:E:237:ASP:OD2  | 1:E:460:ARG:HD2  | 1.86                     | 0.76              |
| 1:H:408:MET:HE2  | 1:H:436:SER:O    | 1.85                     | 0.76              |
| 1:D:228:LEU:O    | 1:D:232:VAL:HG23 | 1.84                     | 0.76              |
| 1:E:105:ARG:CZ   | 1:E:499:ARG:HH12 | 1.99                     | 0.76              |
| 1:H:399:ARG:O    | 1:H:402:SER:HB3  | 1.86                     | 0.76              |
| 1:C:237:ASP:OD1  | 1:C:460:ARG:HD2  | 1.85                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:391:ARG:NH1  | 1:F:399:ARG:NH2  | 2.33                     | 0.76              |
| 1:G:61:LYS:HD3   | 1:G:93:ALA:HA    | 1.67                     | 0.76              |
| 1:G:86:THR:O     | 1:G:90:VAL:HG23  | 1.86                     | 0.76              |
| 1:G:412:ALA:O    | 1:G:416:VAL:HG23 | 1.86                     | 0.75              |
| 1:B:261:GLY:HA3  | 1:B:264:ILE:HG13 | 1.66                     | 0.75              |
| 1:H:426:ALA:C    | 1:H:427:LEU:HD12 | 2.10                     | 0.75              |
| 1:A:433:SER:HB2  | 1:A:435:ARG:HG3  | 1.68                     | 0.75              |
| 1:C:43:ASN:HB3   | 1:C:467:GLY:HA2  | 1.68                     | 0.75              |
| 1:B:220:VAL:HG22 | 1:B:224:ASP:HB3  | 1.67                     | 0.75              |
| 1:B:496:GLY:HA3  | 1:B:502:PHE:CZ   | 2.22                     | 0.75              |
| 1:G:94:THR:HG22  | 1:G:95:GLU:HG2   | 1.68                     | 0.75              |
| 1:G:338:ARG:HH22 | 1:G:341:ARG:HH22 | 1.34                     | 0.75              |
| 1:E:224:ASP:O    | 1:E:228:LEU:HG   | 1.86                     | 0.75              |
| 1:B:43:ASN:HB3   | 1:B:467:GLY:N    | 2.00                     | 0.75              |
| 1:F:154:ASN:C    | 1:F:155:ILE:HD12 | 2.11                     | 0.75              |
| 1:H:103:LEU:HA   | 1:H:499:ARG:HH12 | 1.51                     | 0.75              |
| 1:G:73:MET:HE2   | 1:G:86:THR:HG21  | 1.69                     | 0.75              |
| 1:G:416:VAL:HG13 | 1:G:445:PRO:HB3  | 1.69                     | 0.75              |
| 1:A:302:ALA:HB3  | 1:C:376:MET:HE1  | 1.69                     | 0.74              |
| 1:F:237:ASP:OD2  | 1:F:460:ARG:HD2  | 1.86                     | 0.74              |
| 1:G:328:GLN:HA   | 1:G:331:GLU:HG2  | 1.69                     | 0.74              |
| 1:E:87:ILE:O     | 1:E:91:ARG:HG3   | 1.86                     | 0.74              |
| 1:H:430:LEU:HD11 | 1:H:452:VAL:HB   | 1.70                     | 0.74              |
| 1:B:141:ILE:CD1  | 1:B:192:LEU:HB2  | 2.18                     | 0.74              |
| 1:E:413:MET:HE2  | 1:E:443:TYR:CE1  | 2.23                     | 0.74              |
| 1:H:376:MET:O    | 1:H:380:ILE:HG13 | 1.87                     | 0.74              |
| 1:B:151:CYS:HB3  | 1:B:156:LEU:CD2  | 2.18                     | 0.74              |
| 1:B:393:LEU:O    | 1:B:397:LEU:HB2  | 1.88                     | 0.74              |
| 1:E:46:ILE:HG23  | 1:E:377:GLN:HE22 | 1.52                     | 0.74              |
| 1:H:412:ALA:O    | 1:H:416:VAL:HG23 | 1.87                     | 0.74              |
| 1:E:102:ILE:C    | 1:E:103:LEU:HD12 | 2.13                     | 0.73              |
| 1:F:76:SER:HA    | 1:F:114:LYS:HB2  | 1.69                     | 0.73              |
| 1:F:515:ARG:HB3  | 1:F:516:PRO:HD2  | 1.69                     | 0.73              |
| 1:H:19:ALA:HA    | 1:H:31:ARG:HB3   | 1.70                     | 0.73              |
| 1:H:430:LEU:HD12 | 1:H:452:VAL:HB   | 1.70                     | 0.73              |
| 1:H:54:SER:O     | 1:H:60:LEU:HD13  | 1.87                     | 0.73              |
| 1:D:406:ASP:HB3  | 1:D:409:GLU:HG3  | 1.69                     | 0.73              |
| 1:E:115:GLY:HA2  | 1:E:224:ASP:OD2  | 1.89                     | 0.73              |
| 1:G:288:GLY:O    | 1:G:289:ILE:HG12 | 1.87                     | 0.73              |
| 1:H:25:PHE:HE2   | 1:H:29:MET:HE2   | 1.51                     | 0.73              |
| 1:H:328:GLN:HA   | 1:H:331:GLU:HG3  | 1.69                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:504:LYS:HG3  | 1:B:530:PRO:OXT  | 1.87                     | 0.73              |
| 1:H:102:ILE:HG12 | 1:H:103:LEU:N    | 2.03                     | 0.73              |
| 1:E:60:LEU:HD23  | 1:E:90:VAL:HA    | 1.69                     | 0.73              |
| 1:G:440:VAL:CG1  | 1:G:449:ILE:HD13 | 2.19                     | 0.73              |
| 1:H:209:ASN:O    | 1:H:211:PRO:HD3  | 1.88                     | 0.73              |
| 1:B:151:CYS:HB3  | 1:B:156:LEU:HD23 | 1.68                     | 0.73              |
| 1:B:382:ARG:HB2  | 1:B:382:ARG:HH11 | 1.52                     | 0.73              |
| 1:C:300:ILE:HD12 | 1:C:304:LYS:HB2  | 1.70                     | 0.73              |
| 1:H:246:LYS:HE2  | 1:H:249:ASP:OD1  | 1.88                     | 0.73              |
| 1:G:293:ARG:HD3  | 1:G:326:ALA:O    | 1.89                     | 0.73              |
| 1:H:360:LEU:HD11 | 1:H:377:GLN:CD   | 2.13                     | 0.73              |
| 1:D:24:THR:CG2   | 1:D:27:GLU:HB2   | 2.19                     | 0.72              |
| 1:G:454:ARG:HG2  | 1:G:473:CYS:O    | 1.89                     | 0.72              |
| 1:G:329:MET:O    | 1:G:343:GLU:HG2  | 1.89                     | 0.72              |
| 1:F:296:LEU:HD12 | 1:F:296:LEU:O    | 1.89                     | 0.72              |
| 1:G:63:MET:HG2   | 1:G:371:LEU:HD21 | 1.71                     | 0.72              |
| 1:H:202:LEU:HD22 | 1:H:203:GLY:N    | 2.04                     | 0.72              |
| 1:G:123:ILE:HD11 | 1:G:202:LEU:CD1  | 2.16                     | 0.72              |
| 1:H:328:GLN:HA   | 1:H:331:GLU:CG   | 2.19                     | 0.72              |
| 1:H:503:LYS:HG2  | 1:H:504:LYS:N    | 2.04                     | 0.72              |
| 1:B:408:MET:O    | 1:B:408:MET:HE3  | 1.87                     | 0.72              |
| 1:C:55:ARG:HG3   | 1:C:86:THR:HG23  | 1.71                     | 0.72              |
| 1:F:215:VAL:CG1  | 1:F:217:LEU:HD12 | 2.18                     | 0.72              |
| 1:G:399:ARG:NH1  | 1:H:23:ASP:HB3   | 2.03                     | 0.72              |
| 1:A:122:LEU:HD12 | 1:A:126:SER:O    | 1.89                     | 0.72              |
| 1:C:370:PRO:O    | 1:C:374:VAL:HG23 | 1.90                     | 0.72              |
| 1:G:49:THR:OG1   | 1:G:361:SER:HA   | 1.90                     | 0.72              |
| 1:A:55:ARG:CG    | 1:A:86:THR:HG23  | 2.20                     | 0.72              |
| 1:A:271:GLU:HG3  | 1:A:292:ALA:CB   | 2.19                     | 0.72              |
| 1:D:160:TYR:OH   | 1:D:216:ASP:HB2  | 1.88                     | 0.72              |
| 1:G:371:LEU:O    | 1:G:375:ARG:HD2  | 1.89                     | 0.72              |
| 1:C:290:MET:HE1  | 1:C:359:MET:HE1  | 1.71                     | 0.72              |
| 1:E:49:THR:HG23  | 1:E:72:ARG:HD3   | 1.71                     | 0.72              |
| 1:E:391:ARG:HH12 | 1:F:399:ARG:NH2  | 1.86                     | 0.72              |
| 1:G:322:PRO:HA   | 1:G:356:ASP:OD2  | 1.88                     | 0.72              |
| 1:G:56:SER:OG    | 1:G:58:GLU:HB2   | 1.90                     | 0.72              |
| 1:A:309:GLN:O    | 1:A:313:ILE:HD12 | 1.90                     | 0.71              |
| 1:G:113:THR:HG22 | 1:G:242:SER:HB2  | 1.72                     | 0.71              |
| 1:A:145:ASN:N    | 1:A:145:ASN:ND2  | 2.38                     | 0.71              |
| 1:B:76:SER:HA    | 1:B:114:LYS:HB2  | 1.71                     | 0.71              |
| 1:D:123:ILE:CD1  | 1:D:131:VAL:HB   | 2.21                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:504:LYS:HG3  | 1:E:530:PRO:O    | 1.89                     | 0.71              |
| 1:G:202:LEU:HD22 | 1:G:203:GLY:N    | 2.04                     | 0.71              |
| 1:C:290:MET:HE2  | 1:C:326:ALA:HB2  | 1.70                     | 0.71              |
| 1:E:352:LEU:HD22 | 1:E:384:ALA:HB1  | 1.71                     | 0.71              |
| 1:G:452:VAL:HG11 | 1:G:488:ARG:HB3  | 1.71                     | 0.71              |
| 1:B:493:MET:HE2  | 1:B:530:PRO:CD   | 2.20                     | 0.71              |
| 1:D:131:VAL:HG21 | 1:D:153:GLU:HB3  | 1.71                     | 0.71              |
| 1:G:493:MET:CE   | 1:G:529:VAL:HG13 | 2.20                     | 0.71              |
| 1:C:83:HIS:O     | 1:C:87:ILE:HG13  | 1.90                     | 0.71              |
| 1:B:369:TYR:HB3  | 1:B:372:GLU:HB2  | 1.72                     | 0.71              |
| 1:C:123:ILE:HD12 | 1:C:131:VAL:HG23 | 1.72                     | 0.71              |
| 1:D:461:GLN:O    | 1:D:464:LEU:HB2  | 1.91                     | 0.71              |
| 1:E:421:LYS:HD3  | 1:F:413:MET:SD   | 2.31                     | 0.71              |
| 1:H:123:ILE:HD13 | 1:H:131:VAL:CG2  | 2.21                     | 0.71              |
| 1:H:330:LEU:HD12 | 1:H:339:PRO:HB3  | 1.71                     | 0.71              |
| 1:B:412:ALA:O    | 1:B:416:VAL:HG23 | 1.90                     | 0.71              |
| 1:H:63:MET:HE2   | 1:H:68:MET:HE2   | 1.73                     | 0.71              |
| 1:H:245:ARG:O    | 1:H:282:ILE:HD11 | 1.91                     | 0.70              |
| 1:C:102:ILE:HG22 | 1:C:103:LEU:HD12 | 1.73                     | 0.70              |
| 1:D:382:ARG:NH1  | 5:D:6191:HOH:O   | 2.25                     | 0.70              |
| 1:E:102:ILE:HG22 | 1:E:103:LEU:CD1  | 2.21                     | 0.70              |
| 1:F:179:LEU:HD13 | 1:H:338:ARG:NH2  | 2.06                     | 0.70              |
| 1:A:415:SER:HA   | 1:A:524:MET:HE2  | 1.72                     | 0.70              |
| 1:G:410:ALA:HA   | 1:H:421:LYS:HG2  | 1.73                     | 0.70              |
| 1:A:133:LEU:HD11 | 1:A:139:LEU:HD13 | 1.74                     | 0.70              |
| 1:C:392:LYS:O    | 1:C:396:GLU:HG3  | 1.91                     | 0.70              |
| 1:G:290:MET:HE1  | 1:G:359:MET:HE1  | 1.74                     | 0.70              |
| 1:G:440:VAL:HG12 | 1:G:449:ILE:CD1  | 2.21                     | 0.70              |
| 1:B:493:MET:CE   | 1:B:529:VAL:HG13 | 2.21                     | 0.70              |
| 1:E:340:THR:HB   | 1:G:328:GLN:HE21 | 1.57                     | 0.70              |
| 1:F:376:MET:HA   | 1:F:376:MET:HE3  | 1.73                     | 0.70              |
| 1:F:376:MET:HE2  | 1:F:380:ILE:HD11 | 1.73                     | 0.70              |
| 1:G:524:MET:HE3  | 1:H:524:MET:HE3  | 1.73                     | 0.70              |
| 1:B:328:GLN:HG2  | 1:B:331:GLU:HG3  | 1.74                     | 0.70              |
| 1:B:480:ALA:HB3  | 1:B:483:GLU:HG3  | 1.72                     | 0.70              |
| 1:F:202:LEU:HD23 | 1:F:203:GLY:H    | 1.56                     | 0.70              |
| 1:A:89:ASN:HD22  | 1:A:89:ASN:N     | 1.86                     | 0.70              |
| 1:E:330:LEU:HD12 | 1:E:343:GLU:HB3  | 1.74                     | 0.70              |
| 1:E:515:ARG:HB3  | 1:E:516:PRO:HD2  | 1.74                     | 0.70              |
| 1:G:338:ARG:NH2  | 1:G:341:ARG:HH12 | 1.89                     | 0.70              |
| 1:A:27:GLU:O     | 1:A:31:ARG:HG3   | 1.91                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:338:ARG:NH2  | 1:G:341:ARG:HH22 | 1.89                     | 0.69              |
| 1:B:160:TYR:O    | 1:B:163:ILE:HG22 | 1.92                     | 0.69              |
| 1:B:433:SER:HB2  | 1:B:435:ARG:CD   | 2.22                     | 0.69              |
| 1:C:156:LEU:HD22 | 1:C:157:TRP:N    | 2.07                     | 0.69              |
| 1:G:43:ASN:CB    | 1:G:467:GLY:HA2  | 2.18                     | 0.69              |
| 1:H:316:CYS:HB2  | 1:H:323:VAL:HG22 | 1.75                     | 0.69              |
| 1:A:122:LEU:O    | 1:A:151:CYS:HB2  | 1.91                     | 0.69              |
| 1:A:491:LEU:O    | 1:A:495:VAL:HG23 | 1.92                     | 0.69              |
| 1:C:273:HIS:ND1  | 1:C:277:ARG:NH1  | 2.39                     | 0.69              |
| 1:B:514:TRP:C    | 1:B:515:ARG:HG2  | 2.17                     | 0.69              |
| 1:F:50:ILE:HB    | 1:F:73:MET:HE1   | 1.74                     | 0.69              |
| 1:F:141:ILE:HG22 | 1:F:156:LEU:HB2  | 1.75                     | 0.69              |
| 1:E:103:LEU:HD12 | 1:E:103:LEU:N    | 2.08                     | 0.69              |
| 1:A:269:LYS:HD2  | 1:A:290:MET:SD   | 2.31                     | 0.69              |
| 1:B:167:VAL:HG13 | 1:B:171:SER:CB   | 2.22                     | 0.69              |
| 1:C:308:ALA:O    | 1:C:312:ILE:HD12 | 1.93                     | 0.69              |
| 1:F:145:ASN:HD22 | 1:F:145:ASN:N    | 1.91                     | 0.69              |
| 1:F:145:ASN:HB3  | 1:F:148:MET:CE   | 2.23                     | 0.69              |
| 1:G:47:ILE:HB    | 1:G:359:MET:HB2  | 1.73                     | 0.69              |
| 1:B:453:THR:CG2  | 1:B:459:ALA:HB2  | 2.23                     | 0.69              |
| 1:A:328:GLN:HE21 | 1:C:341:ARG:N    | 1.87                     | 0.69              |
| 1:B:210:LEU:HD12 | 1:B:210:LEU:N    | 2.07                     | 0.69              |
| 1:E:34:ILE:HD13  | 1:G:276:VAL:HG11 | 1.73                     | 0.69              |
| 1:G:411:MET:SD   | 1:H:526:VAL:HG23 | 2.33                     | 0.69              |
| 1:H:160:TYR:OH   | 1:H:216:ASP:HB2  | 1.93                     | 0.69              |
| 1:H:267:ILE:HD13 | 1:H:267:ILE:N    | 2.08                     | 0.69              |
| 1:B:141:ILE:HG13 | 1:B:158:LEU:CD2  | 2.23                     | 0.68              |
| 1:C:328:GLN:HA   | 1:C:331:GLU:HG3  | 1.74                     | 0.68              |
| 1:F:50:ILE:HB    | 1:F:73:MET:CE    | 2.23                     | 0.68              |
| 1:G:132:GLU:HG3  | 1:G:201:PHE:CE1  | 2.28                     | 0.68              |
| 1:B:244:ILE:HG13 | 1:B:268:SER:OG   | 1.93                     | 0.68              |
| 1:C:76:SER:HA    | 1:C:114:LYS:HB2  | 1.74                     | 0.68              |
| 1:C:123:ILE:HD12 | 1:C:131:VAL:HG21 | 1.75                     | 0.68              |
| 1:H:358:ILE:HG13 | 1:H:377:GLN:NE2  | 2.08                     | 0.68              |
| 1:A:42:ARG:NH1   | 1:A:46:ILE:HG13  | 2.08                     | 0.68              |
| 1:E:51:GLY:O     | 1:E:55:ARG:HB2   | 1.92                     | 0.68              |
| 1:H:72:ARG:NH2   | 4:H:532:PEQ:O1P  | 2.26                     | 0.68              |
| 1:G:57:VAL:HG13  | 1:G:93:ALA:HB2   | 1.75                     | 0.68              |
| 1:G:92:THR:HG22  | 1:G:93:ALA:N     | 2.08                     | 0.68              |
| 1:H:529:VAL:HG13 | 1:H:530:PRO:HD2  | 1.74                     | 0.68              |
| 1:A:447:ALA:HB1  | 1:A:448:PRO:HD2  | 1.74                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:141:ILE:HD13 | 1:B:192:LEU:HB2  | 1.75                     | 0.68              |
| 1:H:328:GLN:HG2  | 1:H:331:GLU:HG3  | 1.74                     | 0.68              |
| 1:D:187:LYS:HA   | 1:D:192:LEU:CD1  | 2.23                     | 0.68              |
| 1:F:118:ILE:CG2  | 1:F:208:VAL:HB   | 2.24                     | 0.68              |
| 1:F:293:ARG:HD3  | 1:F:326:ALA:O    | 1.93                     | 0.68              |
| 1:H:406:ASP:HB3  | 1:H:409:GLU:HB2  | 1.75                     | 0.68              |
| 1:A:158:LEU:HD23 | 1:A:163:ILE:HD12 | 1.76                     | 0.68              |
| 1:B:226:GLN:HA   | 1:B:229:LYS:HE2  | 1.74                     | 0.68              |
| 1:B:489:VAL:O    | 1:B:493:MET:HG2  | 1.94                     | 0.68              |
| 1:E:76:SER:HA    | 1:E:114:LYS:HB2  | 1.76                     | 0.68              |
| 1:E:355:ALA:O    | 1:E:466:ARG:NH1  | 2.27                     | 0.68              |
| 1:F:376:MET:HE3  | 1:F:376:MET:O    | 1.94                     | 0.68              |
| 1:G:455:ASN:HB3  | 1:G:458:THR:HB   | 1.76                     | 0.68              |
| 1:H:316:CYS:CB   | 1:H:323:VAL:HG22 | 2.24                     | 0.68              |
| 1:H:370:PRO:O    | 1:H:374:VAL:HG23 | 1.94                     | 0.68              |
| 1:B:328:GLN:NE2  | 1:D:341:ARG:H    | 1.92                     | 0.67              |
| 1:E:75:PHE:HB2   | 1:E:112:ASP:O    | 1.94                     | 0.67              |
| 1:E:431:THR:HG21 | 1:E:434:GLY:HA2  | 1.75                     | 0.67              |
| 1:H:249:ASP:O    | 1:H:253:VAL:HG23 | 1.94                     | 0.67              |
| 1:A:340:THR:HB   | 1:C:328:GLN:NE2  | 2.09                     | 0.67              |
| 1:B:218:PRO:HB2  | 1:B:220:VAL:O    | 1.93                     | 0.67              |
| 1:D:241:ALA:O    | 1:D:269:LYS:HG3  | 1.94                     | 0.67              |
| 1:D:290:MET:HE3  | 1:D:326:ALA:HB2  | 1.75                     | 0.67              |
| 1:E:309:GLN:O    | 1:E:313:ILE:HG13 | 1.94                     | 0.67              |
| 1:E:329:MET:O    | 1:E:343:GLU:HB3  | 1.95                     | 0.67              |
| 1:G:116:PRO:HB2  | 1:G:217:LEU:HD23 | 1.77                     | 0.67              |
| 1:B:14:THR:O     | 1:B:17:LEU:HG    | 1.95                     | 0.67              |
| 1:B:293:ARG:HH22 | 1:B:346:ASP:CG   | 2.02                     | 0.67              |
| 1:C:131:VAL:HG13 | 1:C:153:GLU:OE1  | 1.95                     | 0.67              |
| 1:E:270:ILE:HD12 | 1:E:270:ILE:N    | 2.10                     | 0.67              |
| 1:E:295:ASP:O    | 1:E:298:ILE:HB   | 1.94                     | 0.67              |
| 1:E:425:ALA:HB1  | 1:E:502:PHE:HB3  | 1.77                     | 0.67              |
| 1:F:140:LYS:HB2  | 1:F:193:VAL:HG22 | 1.76                     | 0.67              |
| 1:H:43:ASN:CB    | 1:H:467:GLY:HA2  | 2.24                     | 0.67              |
| 1:F:119:ARG:O    | 1:F:158:LEU:HD12 | 1.95                     | 0.67              |
| 1:F:333:MET:HE1  | 1:F:376:MET:HB2  | 1.77                     | 0.67              |
| 1:A:524:MET:HG2  | 1:A:525:ARG:N    | 2.07                     | 0.67              |
| 1:D:293:ARG:HD3  | 1:D:326:ALA:O    | 1.95                     | 0.67              |
| 1:F:406:ASP:HB3  | 1:F:409:GLU:HG3  | 1.75                     | 0.67              |
| 1:H:360:LEU:N    | 1:H:360:LEU:HD12 | 2.10                     | 0.67              |
| 1:B:54:SER:HA    | 1:B:59:THR:HG21  | 1.77                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:504:LYS:O    | 1:B:529:VAL:HB   | 1.95                     | 0.67              |
| 1:E:457:GLN:HG2  | 1:E:461:GLN:HE21 | 1.59                     | 0.67              |
| 1:G:135:LYS:HG3  | 1:G:198:ASN:H    | 1.59                     | 0.67              |
| 1:H:512:THR:CA   | 1:H:521:THR:HG22 | 2.25                     | 0.67              |
| 1:D:493:MET:HE3  | 1:D:529:VAL:HG22 | 1.77                     | 0.67              |
| 1:C:273:HIS:HB3  | 1:C:277:ARG:NH1  | 2.03                     | 0.66              |
| 1:D:225:ILE:O    | 1:D:229:LYS:HG3  | 1.94                     | 0.66              |
| 1:E:224:ASP:O    | 1:E:227:ASP:HB2  | 1.95                     | 0.66              |
| 1:E:256:ILE:HG22 | 1:E:257:LEU:N    | 2.10                     | 0.66              |
| 1:G:56:SER:HB3   | 1:G:59:THR:OG1   | 1.95                     | 0.66              |
| 1:H:484:ASP:O    | 1:H:487:LEU:HB3  | 1.94                     | 0.66              |
| 1:H:512:THR:N    | 1:H:521:THR:HG22 | 2.10                     | 0.66              |
| 1:B:428:ILE:CD1  | 1:B:508:VAL:HG11 | 2.25                     | 0.66              |
| 1:C:43:ASN:HB3   | 1:C:467:GLY:N    | 2.10                     | 0.66              |
| 1:D:155:ILE:HD12 | 1:D:155:ILE:N    | 2.10                     | 0.66              |
| 1:D:228:LEU:HD22 | 1:D:257:LEU:CD1  | 2.25                     | 0.66              |
| 1:H:118:ILE:CG2  | 1:H:208:VAL:HB   | 2.25                     | 0.66              |
| 1:H:118:ILE:HG22 | 1:H:208:VAL:HB   | 1.77                     | 0.66              |
| 1:D:119:ARG:HH11 | 1:D:207:GLY:N    | 1.93                     | 0.66              |
| 1:D:167:VAL:HG13 | 1:D:171:SER:OG   | 1.96                     | 0.66              |
| 1:G:46:ILE:HG23  | 1:G:377:GLN:HE21 | 1.60                     | 0.66              |
| 1:H:132:GLU:C    | 1:H:133:LEU:HD23 | 2.20                     | 0.66              |
| 1:A:244:ILE:HG13 | 1:A:268:SER:HB3  | 1.77                     | 0.66              |
| 1:B:355:ALA:O    | 1:B:466:ARG:NH1  | 2.28                     | 0.66              |
| 1:D:118:ILE:O    | 1:D:207:GLY:HA2  | 1.95                     | 0.66              |
| 1:E:22:ALA:O     | 1:E:391:ARG:NH2  | 2.29                     | 0.66              |
| 1:G:15:GLN:HG3   | 1:G:39:ILE:HG23  | 1.76                     | 0.66              |
| 1:B:47:ILE:CD1   | 1:B:324:ILE:HD13 | 2.25                     | 0.66              |
| 1:B:433:SER:HB2  | 1:B:435:ARG:HD2  | 1.78                     | 0.66              |
| 1:B:515:ARG:HB3  | 1:B:516:PRO:HD2  | 1.77                     | 0.66              |
| 1:C:43:ASN:HB3   | 1:C:467:GLY:CA   | 2.24                     | 0.66              |
| 1:F:163:ILE:O    | 1:F:167:VAL:HG23 | 1.95                     | 0.66              |
| 1:E:220:VAL:CG1  | 1:E:225:ILE:HD11 | 2.26                     | 0.66              |
| 1:F:349:ASN:HD21 | 1:H:310:LYS:NZ   | 1.93                     | 0.66              |
| 1:B:202:LEU:HD22 | 1:B:203:GLY:O    | 1.96                     | 0.66              |
| 1:H:220:VAL:HG13 | 1:H:224:ASP:HB2  | 1.76                     | 0.66              |
| 1:B:304:LYS:NZ   | 1:D:383:GLU:OE2  | 2.29                     | 0.66              |
| 1:C:160:TYR:OH   | 1:C:216:ASP:HB2  | 1.95                     | 0.66              |
| 1:D:122:LEU:HD12 | 1:D:123:ILE:H    | 1.58                     | 0.66              |
| 1:F:329:MET:O    | 1:F:343:GLU:HB3  | 1.96                     | 0.66              |
| 1:H:515:ARG:HB3  | 1:H:516:PRO:HD2  | 1.78                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:333:MET:CE   | 1:B:339:PRO:HD3  | 2.26                     | 0.66              |
| 1:D:63:MET:HG3   | 1:D:371:LEU:CD2  | 2.26                     | 0.66              |
| 1:D:123:ILE:HB   | 1:D:204:SER:OG   | 1.96                     | 0.66              |
| 1:E:220:VAL:HG22 | 1:E:224:ASP:CB   | 2.23                     | 0.66              |
| 1:E:220:VAL:HG11 | 1:E:225:ILE:HD11 | 1.77                     | 0.66              |
| 1:E:457:GLN:O    | 1:E:461:GLN:HG3  | 1.96                     | 0.65              |
| 1:G:309:GLN:O    | 1:G:313:ILE:HG13 | 1.96                     | 0.65              |
| 1:A:452:VAL:HG11 | 1:A:488:ARG:HB3  | 1.78                     | 0.65              |
| 1:B:457:GLN:O    | 1:B:461:GLN:HG3  | 1.97                     | 0.65              |
| 1:C:415:SER:HA   | 1:C:524:MET:HE2  | 1.78                     | 0.65              |
| 1:E:249:ASP:O    | 1:E:253:VAL:HG23 | 1.96                     | 0.65              |
| 1:A:271:GLU:HG3  | 1:A:292:ALA:HB3  | 1.78                     | 0.65              |
| 1:B:427:LEU:HD12 | 1:B:427:LEU:N    | 2.11                     | 0.65              |
| 1:G:54:SER:O     | 1:G:60:LEU:HD11  | 1.97                     | 0.65              |
| 1:H:266:ILE:C    | 1:H:267:ILE:HD13 | 2.21                     | 0.65              |
| 1:A:328:GLN:NE2  | 1:C:341:ARG:N    | 2.42                     | 0.65              |
| 1:C:131:VAL:HG12 | 1:C:153:GLU:HB3  | 1.77                     | 0.65              |
| 1:F:409:GLU:O    | 1:F:413:MET:HG3  | 1.96                     | 0.65              |
| 1:H:176:ASP:O    | 1:H:179:LEU:HB2  | 1.96                     | 0.65              |
| 1:C:252:GLU:O    | 1:C:256:ILE:HG12 | 1.97                     | 0.65              |
| 1:C:296:LEU:O    | 1:C:296:LEU:HD12 | 1.97                     | 0.65              |
| 1:E:220:VAL:HG13 | 1:E:221:SER:N    | 2.11                     | 0.65              |
| 1:E:298:ILE:HD13 | 1:E:298:ILE:N    | 2.12                     | 0.65              |
| 1:F:227:ASP:O    | 1:F:230:PHE:HB3  | 1.95                     | 0.65              |
| 1:H:330:LEU:CD2  | 1:H:377:GLN:HG2  | 2.27                     | 0.65              |
| 1:A:266:ILE:O    | 1:A:267:ILE:HD13 | 1.95                     | 0.65              |
| 1:B:123:ILE:HD11 | 1:B:202:LEU:HD13 | 1.78                     | 0.65              |
| 1:E:240:PHE:CD2  | 1:E:290:MET:HE1  | 2.32                     | 0.65              |
| 1:F:25:PHE:N     | 1:H:396:GLU:OE2  | 2.29                     | 0.65              |
| 1:F:247:ALA:CB   | 1:F:281:GLU:HG3  | 2.26                     | 0.65              |
| 1:A:288:GLY:O    | 1:A:289:ILE:HG12 | 1.95                     | 0.65              |
| 1:B:54:SER:O     | 1:B:60:LEU:HD11  | 1.96                     | 0.65              |
| 1:G:392:LYS:O    | 1:G:396:GLU:HG3  | 1.97                     | 0.65              |
| 1:C:27:GLU:O     | 1:C:31:ARG:HG3   | 1.96                     | 0.65              |
| 1:G:220:VAL:HG22 | 1:G:224:ASP:HB3  | 1.78                     | 0.65              |
| 1:H:64:ILE:HD13  | 1:H:107:VAL:HG21 | 1.78                     | 0.65              |
| 1:E:485:VAL:HG12 | 1:E:486:ASP:N    | 2.11                     | 0.65              |
| 1:F:118:ILE:HG22 | 1:F:208:VAL:CG2  | 2.26                     | 0.65              |
| 1:F:507:VAL:HG12 | 1:F:508:VAL:H    | 1.62                     | 0.65              |
| 1:F:511:LEU:HD22 | 1:F:521:THR:CG2  | 2.27                     | 0.65              |
| 1:H:361:SER:N    | 1:H:363:GLU:OE1  | 2.28                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:306:PHE:O    | 1:D:310:LYS:HG3  | 1.97                     | 0.64              |
| 1:E:411:MET:HE1  | 1:F:524:MET:SD   | 2.38                     | 0.64              |
| 1:F:154:ASN:O    | 1:F:155:ILE:HD12 | 1.97                     | 0.64              |
| 1:H:23:ASP:OD1   | 1:H:23:ASP:N     | 2.30                     | 0.64              |
| 1:A:278:ARG:O    | 1:A:282:ILE:HG13 | 1.96                     | 0.64              |
| 1:B:156:LEU:HD22 | 1:B:157:TRP:H    | 1.62                     | 0.64              |
| 1:C:493:MET:CE   | 1:C:529:VAL:HG13 | 2.28                     | 0.64              |
| 1:E:47:ILE:HB    | 1:E:359:MET:CG   | 2.16                     | 0.64              |
| 1:G:416:VAL:O    | 1:G:419:SER:HB3  | 1.96                     | 0.64              |
| 1:A:315:ARG:NH1  | 1:C:30:CYS:O     | 2.30                     | 0.64              |
| 1:F:186:GLN:O    | 1:F:192:LEU:HD12 | 1.98                     | 0.64              |
| 1:F:336:LYS:HB3  | 1:F:337:PRO:HD2  | 1.80                     | 0.64              |
| 1:B:141:ILE:HG13 | 1:B:158:LEU:HD21 | 1.78                     | 0.64              |
| 1:F:191:PHE:O    | 1:F:192:LEU:HD13 | 1.97                     | 0.64              |
| 1:G:485:VAL:HG12 | 1:G:486:ASP:N    | 2.10                     | 0.64              |
| 1:E:246:LYS:HG2  | 1:E:249:ASP:OD2  | 1.97                     | 0.64              |
| 1:G:496:GLY:HA3  | 1:G:502:PHE:CZ   | 2.33                     | 0.64              |
| 1:G:497:LYS:NZ   | 1:G:530:PRO:O    | 2.30                     | 0.64              |
| 1:H:381:ALA:HB1  | 1:H:385:GLU:OE2  | 1.96                     | 0.64              |
| 1:A:293:ARG:HD3  | 1:A:326:ALA:O    | 1.98                     | 0.64              |
| 1:B:43:ASN:CB    | 1:B:467:GLY:HA2  | 2.27                     | 0.64              |
| 1:B:69:ASN:HB3   | 1:B:463:HIS:CD2  | 2.33                     | 0.64              |
| 1:G:70:VAL:HG11  | 1:G:238:MET:HE1  | 1.79                     | 0.64              |
| 1:F:50:ILE:HG21  | 1:F:86:THR:CG2   | 2.27                     | 0.64              |
| 1:A:43:ASN:HB3   | 1:A:467:GLY:CA   | 2.27                     | 0.64              |
| 1:A:293:ARG:HH22 | 1:A:346:ASP:CG   | 2.05                     | 0.64              |
| 1:D:267:ILE:HD12 | 1:D:267:ILE:N    | 2.12                     | 0.64              |
| 1:F:304:LYS:NZ   | 1:H:383:GLU:OE2  | 2.30                     | 0.64              |
| 1:H:493:MET:O    | 1:H:497:LYS:HB2  | 1.98                     | 0.64              |
| 1:A:102:ILE:HG22 | 1:A:103:LEU:HD12 | 1.79                     | 0.64              |
| 1:G:48:CYS:HB3   | 1:G:364:THR:HG21 | 1.80                     | 0.64              |
| 1:G:266:ILE:O    | 1:G:287:ASP:HB2  | 1.98                     | 0.64              |
| 1:H:493:MET:HE2  | 1:H:529:VAL:HA   | 1.80                     | 0.64              |
| 1:A:288:GLY:C    | 1:A:289:ILE:HG12 | 2.23                     | 0.64              |
| 1:C:225:ILE:O    | 1:C:229:LYS:HG3  | 1.97                     | 0.64              |
| 1:E:328:GLN:NE2  | 1:G:341:ARG:H    | 1.94                     | 0.64              |
| 1:G:288:GLY:C    | 1:G:289:ILE:HG12 | 2.23                     | 0.64              |
| 1:G:393:LEU:HG   | 1:G:397:LEU:HD22 | 1.80                     | 0.64              |
| 1:G:215:VAL:CG1  | 1:G:217:LEU:HB2  | 2.28                     | 0.63              |
| 1:H:55:ARG:CD    | 1:H:86:THR:HG23  | 2.27                     | 0.63              |
| 1:D:202:LEU:HD22 | 1:D:203:GLY:O    | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:431:THR:HG21 | 1:G:434:GLY:HA2  | 1.78                     | 0.63              |
| 1:H:60:LEU:HD21  | 1:H:90:VAL:CG2   | 2.26                     | 0.63              |
| 1:B:160:TYR:CD2  | 1:B:163:ILE:HB   | 2.33                     | 0.63              |
| 1:C:217:LEU:HD23 | 1:C:218:PRO:HD2  | 1.78                     | 0.63              |
| 1:D:185:LYS:HD3  | 1:D:195:GLU:HB3  | 1.79                     | 0.63              |
| 1:D:243:PHE:N    | 1:D:271:GLU:OE1  | 2.29                     | 0.63              |
| 1:F:217:LEU:HB3  | 1:F:218:PRO:HD2  | 1.79                     | 0.63              |
| 1:F:507:VAL:HG12 | 1:F:508:VAL:N    | 2.13                     | 0.63              |
| 1:G:57:VAL:HG11  | 1:G:92:THR:HG22  | 1.79                     | 0.63              |
| 1:H:435:ARG:O    | 1:H:438:HIS:N    | 2.31                     | 0.63              |
| 1:H:503:LYS:O    | 1:H:506:ASP:HB2  | 1.98                     | 0.63              |
| 1:A:241:ALA:CB   | 1:A:244:ILE:HD11 | 2.27                     | 0.63              |
| 1:B:254:ARG:CZ   | 1:B:266:ILE:HD12 | 2.29                     | 0.63              |
| 1:C:279:PHE:HE2  | 1:C:315:ARG:HB3  | 1.63                     | 0.63              |
| 1:C:293:ARG:NH2  | 1:C:346:ASP:OD1  | 2.30                     | 0.63              |
| 1:E:105:ARG:NE   | 1:E:499:ARG:NH1  | 2.46                     | 0.63              |
| 1:E:383:GLU:OE2  | 1:G:304:LYS:NZ   | 2.30                     | 0.63              |
| 1:G:63:MET:HA    | 1:G:371:LEU:HD21 | 1.81                     | 0.63              |
| 1:G:429:VAL:HG11 | 1:G:437:ALA:HB2  | 1.80                     | 0.63              |
| 1:A:181:SER:HB3  | 1:A:198:ASN:HB2  | 1.79                     | 0.63              |
| 1:E:56:SER:O     | 1:E:60:LEU:HD13  | 1.97                     | 0.63              |
| 1:F:30:CYS:O     | 1:H:315:ARG:NH1  | 2.30                     | 0.63              |
| 1:G:68:MET:O     | 1:G:69:ASN:ND2   | 2.31                     | 0.63              |
| 1:G:431:THR:HG21 | 1:G:434:GLY:CA   | 2.28                     | 0.63              |
| 1:C:279:PHE:HE1  | 1:C:289:ILE:HD12 | 1.64                     | 0.63              |
| 1:D:329:MET:O    | 1:D:343:GLU:HB3  | 1.97                     | 0.63              |
| 1:G:45:GLY:CA    | 1:G:357:CYS:HB3  | 2.29                     | 0.63              |
| 1:H:382:ARG:HH11 | 1:H:382:ARG:HG3  | 1.62                     | 0.63              |
| 1:A:221:SER:O    | 1:A:224:ASP:HB2  | 1.98                     | 0.63              |
| 1:D:148:MET:HG2  | 1:D:148:MET:O    | 1.99                     | 0.63              |
| 1:E:61:LYS:O     | 1:E:65:LYS:HB2   | 1.99                     | 0.63              |
| 1:G:57:VAL:HG11  | 1:G:92:THR:CG2   | 2.29                     | 0.63              |
| 1:C:293:ARG:HH22 | 1:C:346:ASP:CG   | 2.06                     | 0.63              |
| 1:A:25:PHE:O     | 1:A:28:HIS:HB3   | 1.99                     | 0.63              |
| 1:B:231:GLY:O    | 1:B:236:VAL:HG22 | 1.99                     | 0.63              |
| 1:C:427:LEU:HD12 | 1:C:427:LEU:N    | 2.13                     | 0.63              |
| 1:H:148:MET:HG3  | 1:H:157:TRP:CZ3  | 2.34                     | 0.63              |
| 1:D:123:ILE:O    | 1:D:129:ALA:HB3  | 1.99                     | 0.62              |
| 1:G:60:LEU:HD23  | 1:G:90:VAL:HA    | 1.80                     | 0.62              |
| 1:E:511:LEU:HB3  | 1:E:521:THR:CG2  | 2.28                     | 0.62              |
| 1:D:187:LYS:HB2  | 1:D:192:LEU:HD11 | 1.80                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:292:ALA:HB1  | 4:H:532:PEQ:C1   | 2.28                     | 0.62              |
| 1:B:47:ILE:HD11  | 1:B:324:ILE:HD13 | 1.81                     | 0.62              |
| 1:F:246:LYS:HG2  | 1:F:249:ASP:OD2  | 2.00                     | 0.62              |
| 1:F:333:MET:HE2  | 1:F:373:ALA:CA   | 2.24                     | 0.62              |
| 1:G:403:HIS:H    | 1:G:403:HIS:CD2  | 2.15                     | 0.62              |
| 1:B:22:ALA:O     | 1:B:391:ARG:NH2  | 2.29                     | 0.62              |
| 1:B:50:ILE:HB    | 1:B:73:MET:CE    | 2.26                     | 0.62              |
| 1:B:376:MET:HG3  | 1:B:376:MET:O    | 1.99                     | 0.62              |
| 1:G:493:MET:HE2  | 1:G:529:VAL:HG13 | 1.81                     | 0.62              |
| 1:B:45:GLY:O     | 1:B:357:CYS:HB3  | 2.00                     | 0.62              |
| 1:F:328:GLN:HE22 | 1:H:340:THR:HA   | 1.64                     | 0.62              |
| 1:G:221:SER:O    | 1:G:224:ASP:HB2  | 2.00                     | 0.62              |
| 1:H:217:LEU:HB3  | 1:H:218:PRO:HD2  | 1.81                     | 0.62              |
| 1:B:13:GLN:HG2   | 1:B:17:LEU:HB2   | 1.80                     | 0.62              |
| 1:D:24:THR:HG23  | 1:D:27:GLU:HB2   | 1.80                     | 0.62              |
| 1:H:133:LEU:HD23 | 1:H:133:LEU:N    | 2.15                     | 0.62              |
| 1:B:292:ALA:CB   | 4:B:532:PEQ:H21  | 2.29                     | 0.62              |
| 1:D:131:VAL:HG12 | 1:D:202:LEU:HB3  | 1.82                     | 0.62              |
| 1:A:230:PHE:CE2  | 1:A:234:GLN:HG3  | 2.35                     | 0.62              |
| 1:B:167:VAL:HG13 | 1:B:171:SER:HB2  | 1.82                     | 0.62              |
| 1:E:252:GLU:O    | 1:E:256:ILE:HD13 | 2.00                     | 0.62              |
| 1:G:228:LEU:O    | 1:G:231:GLY:N    | 2.33                     | 0.62              |
| 1:A:22:ALA:O     | 1:A:391:ARG:NH2  | 2.32                     | 0.62              |
| 1:C:244:ILE:HG13 | 1:C:268:SER:OG   | 1.99                     | 0.62              |
| 1:H:485:VAL:HG12 | 1:H:486:ASP:N    | 2.13                     | 0.62              |
| 1:A:54:SER:HA    | 1:A:59:THR:HG21  | 1.81                     | 0.61              |
| 1:D:131:VAL:HG22 | 1:D:153:GLU:HB3  | 1.82                     | 0.61              |
| 1:G:197:GLU:O    | 1:G:197:GLU:HG2  | 1.98                     | 0.61              |
| 1:F:376:MET:HE3  | 1:F:376:MET:CA   | 2.30                     | 0.61              |
| 1:H:139:LEU:HD21 | 1:H:156:LEU:HB2  | 1.82                     | 0.61              |
| 1:B:217:LEU:HD23 | 1:B:218:PRO:HD2  | 1.82                     | 0.61              |
| 1:E:14:THR:HG22  | 1:E:37:ALA:O     | 2.00                     | 0.61              |
| 1:E:47:ILE:HD13  | 1:E:324:ILE:HD13 | 1.81                     | 0.61              |
| 1:A:186:GLN:O    | 1:A:192:LEU:HD12 | 2.01                     | 0.61              |
| 1:D:173:VAL:HB   | 1:D:182:LEU:HD12 | 1.83                     | 0.61              |
| 1:A:45:GLY:C     | 1:A:357:CYS:HB3  | 2.25                     | 0.61              |
| 1:C:408:MET:HE2  | 1:C:436:SER:O    | 2.01                     | 0.61              |
| 1:D:189:PRO:HD2  | 1:D:191:PHE:CD1  | 2.35                     | 0.61              |
| 1:E:102:ILE:HG22 | 1:E:103:LEU:HD12 | 1.81                     | 0.61              |
| 1:E:399:ARG:HH12 | 1:F:23:ASP:HB3   | 1.64                     | 0.61              |
| 1:F:340:THR:H    | 1:F:343:GLU:HG3  | 1.65                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:341:ARG:H    | 1:H:328:GLN:NE2  | 1.98                     | 0.61              |
| 1:H:416:VAL:CG1  | 1:H:445:PRO:HA   | 2.31                     | 0.61              |
| 1:A:240:PHE:HB3  | 1:A:269:LYS:HD3  | 1.83                     | 0.61              |
| 1:B:400:SER:OG   | 1:B:401:SER:N    | 2.29                     | 0.61              |
| 1:H:63:MET:HE2   | 1:H:68:MET:CE    | 2.30                     | 0.61              |
| 1:H:92:THR:HG22  | 1:H:93:ALA:N     | 2.14                     | 0.61              |
| 1:G:219:ALA:HB3  | 1:G:252:GLU:CD   | 2.25                     | 0.61              |
| 1:A:318:ARG:NH2  | 1:C:27:GLU:OE2   | 2.34                     | 0.61              |
| 1:F:51:GLY:O     | 1:F:55:ARG:HB2   | 1.99                     | 0.61              |
| 1:H:224:ASP:O    | 1:H:228:LEU:N    | 2.30                     | 0.61              |
| 1:F:24:THR:OG1   | 1:H:396:GLU:HG2  | 2.01                     | 0.61              |
| 1:H:43:ASN:HB3   | 1:H:467:GLY:N    | 2.16                     | 0.61              |
| 1:H:493:MET:HE3  | 1:H:529:VAL:HG22 | 1.83                     | 0.61              |
| 1:A:493:MET:HE2  | 1:A:530:PRO:HD3  | 1.83                     | 0.60              |
| 1:G:219:ALA:HB2  | 1:G:249:ASP:OD1  | 1.99                     | 0.60              |
| 1:A:55:ARG:HG2   | 1:A:86:THR:HG23  | 1.83                     | 0.60              |
| 1:A:392:LYS:O    | 1:A:396:GLU:HG3  | 2.01                     | 0.60              |
| 1:B:221:SER:O    | 1:B:224:ASP:HB2  | 2.01                     | 0.60              |
| 1:C:226:GLN:HB3  | 5:C:6127:HOH:O   | 2.01                     | 0.60              |
| 1:C:256:ILE:HD13 | 1:C:256:ILE:N    | 2.16                     | 0.60              |
| 1:D:446:ARG:HD3  | 5:D:6142:HOH:O   | 1.99                     | 0.60              |
| 1:E:436:SER:HB3  | 1:E:521:THR:OG1  | 2.01                     | 0.60              |
| 1:F:63:MET:HG2   | 1:F:371:LEU:CD2  | 2.31                     | 0.60              |
| 1:F:73:MET:HE2   | 1:F:86:THR:HG21  | 1.83                     | 0.60              |
| 1:F:339:PRO:HG3  | 1:F:376:MET:HG2  | 1.83                     | 0.60              |
| 1:G:135:LYS:CG   | 1:G:198:ASN:H    | 2.14                     | 0.60              |
| 1:G:219:ALA:HB3  | 1:G:252:GLU:OE2  | 2.00                     | 0.60              |
| 1:B:215:VAL:HG11 | 1:B:217:LEU:HD12 | 1.83                     | 0.60              |
| 1:B:360:LEU:HD11 | 1:B:377:GLN:NE2  | 2.16                     | 0.60              |
| 1:C:179:LEU:HB3  | 1:C:180:ILE:HD12 | 1.83                     | 0.60              |
| 1:E:245:ARG:HB2  | 1:E:246:LYS:HE2  | 1.83                     | 0.60              |
| 1:G:399:ARG:HH12 | 1:H:23:ASP:HB3   | 1.66                     | 0.60              |
| 1:G:408:MET:HE2  | 1:G:436:SER:O    | 2.01                     | 0.60              |
| 1:H:157:TRP:C    | 1:H:158:LEU:HD13 | 2.25                     | 0.60              |
| 1:A:49:THR:OG1   | 1:A:361:SER:HA   | 2.00                     | 0.60              |
| 1:B:232:VAL:HG23 | 1:B:257:LEU:HD23 | 1.82                     | 0.60              |
| 1:F:176:ASP:HB3  | 1:F:179:LEU:HB2  | 1.83                     | 0.60              |
| 1:G:358:ILE:HG13 | 1:G:377:GLN:NE2  | 2.16                     | 0.60              |
| 1:G:395:GLU:O    | 1:G:398:ALA:HB3  | 2.01                     | 0.60              |
| 1:E:245:ARG:O    | 1:E:278:ARG:HD3  | 2.02                     | 0.60              |
| 1:H:55:ARG:HG3   | 1:H:86:THR:CG2   | 2.25                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:187:LYS:HA   | 1:H:192:LEU:CD1  | 2.28                     | 0.60              |
| 1:H:354:GLY:C    | 1:H:466:ARG:HH12 | 2.09                     | 0.60              |
| 1:A:503:LYS:N    | 1:A:506:ASP:OD2  | 2.34                     | 0.60              |
| 1:C:202:LEU:HD22 | 1:C:203:GLY:N    | 2.16                     | 0.60              |
| 1:D:123:ILE:N    | 1:D:204:SER:OG   | 2.35                     | 0.60              |
| 1:G:481:TRP:O    | 1:G:484:ASP:N    | 2.35                     | 0.60              |
| 1:A:55:ARG:HG3   | 1:A:86:THR:HG23  | 1.82                     | 0.60              |
| 1:G:122:LEU:O    | 1:G:151:CYS:HB2  | 2.01                     | 0.60              |
| 1:C:173:VAL:HB   | 1:C:182:LEU:HD12 | 1.83                     | 0.60              |
| 1:E:49:THR:OG1   | 1:E:361:SER:HA   | 2.02                     | 0.60              |
| 1:C:351:VAL:O    | 1:C:354:GLY:N    | 2.32                     | 0.60              |
| 1:D:123:ILE:HD11 | 1:D:131:VAL:CG1  | 2.32                     | 0.60              |
| 1:G:15:GLN:HB3   | 1:G:17:LEU:HD21  | 1.83                     | 0.60              |
| 1:H:220:VAL:HG13 | 1:H:224:ASP:CB   | 2.32                     | 0.60              |
| 1:G:109:VAL:N    | 1:G:237:ASP:OD2  | 2.29                     | 0.60              |
| 1:G:110:ALA:HA   | 1:G:238:MET:O    | 2.01                     | 0.60              |
| 1:A:496:GLY:HA3  | 1:A:502:PHE:CZ   | 2.38                     | 0.59              |
| 1:D:24:THR:HG22  | 1:D:27:GLU:HB2   | 1.83                     | 0.59              |
| 1:E:279:PHE:CZ   | 1:E:312:ILE:HG23 | 2.36                     | 0.59              |
| 1:E:506:ASP:O    | 1:E:529:VAL:HG23 | 2.02                     | 0.59              |
| 1:H:105:ARG:NE   | 1:H:499:ARG:HH21 | 1.91                     | 0.59              |
| 1:B:336:LYS:HG2  | 1:B:337:PRO:HD2  | 1.84                     | 0.59              |
| 1:D:208:VAL:HG12 | 1:D:209:ASN:N    | 2.17                     | 0.59              |
| 1:E:322:PRO:HB3  | 1:E:464:LEU:O    | 2.01                     | 0.59              |
| 1:B:424:ALA:CB   | 1:B:509:ILE:HD13 | 2.32                     | 0.59              |
| 1:E:230:PHE:O    | 1:E:234:GLN:HG2  | 2.01                     | 0.59              |
| 1:H:56:SER:O     | 1:H:60:LEU:HB2   | 2.02                     | 0.59              |
| 1:H:382:ARG:HH11 | 1:H:382:ARG:CG   | 2.15                     | 0.59              |
| 1:A:133:LEU:HD13 | 1:A:196:VAL:HG21 | 1.84                     | 0.59              |
| 1:A:403:HIS:H    | 1:A:403:HIS:CD2  | 2.20                     | 0.59              |
| 1:B:292:ALA:HB1  | 4:B:532:PEQ:C2   | 2.30                     | 0.59              |
| 1:F:254:ARG:NH2  | 1:F:287:ASP:OD2  | 2.35                     | 0.59              |
| 1:D:47:ILE:HB    | 1:D:359:MET:HB2  | 1.83                     | 0.59              |
| 1:F:63:MET:CG    | 1:F:371:LEU:HD21 | 2.33                     | 0.59              |
| 1:A:45:GLY:O     | 1:A:357:CYS:HB3  | 2.03                     | 0.59              |
| 1:A:166:VAL:HG21 | 1:A:214:ALA:O    | 2.02                     | 0.59              |
| 1:G:316:CYS:SG   | 1:G:323:VAL:HG22 | 2.43                     | 0.59              |
| 1:C:504:LYS:HG3  | 1:C:530:PRO:O    | 2.01                     | 0.59              |
| 1:D:50:ILE:HB    | 1:D:73:MET:CE    | 2.33                     | 0.59              |
| 1:B:64:ILE:CD1   | 1:B:107:VAL:HG21 | 2.32                     | 0.59              |
| 1:C:306:PHE:O    | 1:C:310:LYS:HG2  | 2.03                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:55:ARG:HG3   | 1:E:86:THR:HG23  | 1.84                     | 0.59              |
| 1:A:23:ASP:OD2   | 1:B:399:ARG:NH1  | 2.36                     | 0.59              |
| 1:B:485:VAL:HG12 | 1:B:486:ASP:N    | 2.15                     | 0.59              |
| 1:D:372:GLU:N    | 1:D:372:GLU:OE1  | 2.35                     | 0.59              |
| 1:F:168:ASP:HA   | 1:F:187:LYS:HE2  | 1.84                     | 0.59              |
| 1:F:369:TYR:HB3  | 1:F:372:GLU:HB2  | 1.84                     | 0.59              |
| 1:G:50:ILE:HG21  | 1:G:86:THR:CG2   | 2.33                     | 0.59              |
| 1:G:306:PHE:O    | 1:G:310:LYS:HG3  | 2.03                     | 0.59              |
| 1:G:491:LEU:O    | 1:G:495:VAL:HG23 | 2.01                     | 0.59              |
| 1:D:436:SER:CB   | 1:D:521:THR:HG23 | 2.33                     | 0.59              |
| 1:D:411:MET:CE   | 1:D:524:MET:HB2  | 2.33                     | 0.58              |
| 1:E:263:ASN:N    | 1:E:263:ASN:OD1  | 2.36                     | 0.58              |
| 1:H:507:VAL:HG12 | 1:H:508:VAL:N    | 2.17                     | 0.58              |
| 4:A:532:PEQ:O1P  | 4:A:532:PEQ:H33  | 2.03                     | 0.58              |
| 1:E:48:CYS:SG    | 1:E:68:MET:HG3   | 2.43                     | 0.58              |
| 1:E:30:CYS:O     | 1:G:315:ARG:NH1  | 2.29                     | 0.58              |
| 1:H:259:GLU:O    | 1:H:262:LYS:HG2  | 2.03                     | 0.58              |
| 1:B:50:ILE:HG23  | 1:B:54:SER:O     | 2.03                     | 0.58              |
| 1:F:118:ILE:HG21 | 1:F:208:VAL:HB   | 1.86                     | 0.58              |
| 1:G:63:MET:HG2   | 1:G:371:LEU:CD2  | 2.32                     | 0.58              |
| 1:H:172:LYS:O    | 1:H:211:PRO:HD2  | 2.03                     | 0.58              |
| 1:A:410:ALA:HA   | 1:B:421:LYS:HG2  | 1.84                     | 0.58              |
| 1:G:50:ILE:HG21  | 1:G:86:THR:HG23  | 1.85                     | 0.58              |
| 1:B:232:VAL:CG2  | 1:B:257:LEU:HD23 | 2.33                     | 0.58              |
| 1:B:382:ARG:HH11 | 1:B:382:ARG:CB   | 2.15                     | 0.58              |
| 1:C:182:LEU:HD13 | 1:C:194:THR:HG21 | 1.86                     | 0.58              |
| 1:D:141:ILE:HG12 | 1:D:142:THR:N    | 2.18                     | 0.58              |
| 1:E:293:ARG:HD3  | 1:E:326:ALA:O    | 2.03                     | 0.58              |
| 1:G:63:MET:CG    | 1:G:371:LEU:HD21 | 2.33                     | 0.58              |
| 1:A:89:ASN:N     | 1:A:89:ASN:ND2   | 2.52                     | 0.58              |
| 1:B:43:ASN:HB3   | 1:B:467:GLY:H    | 1.69                     | 0.58              |
| 1:B:182:LEU:HB2  | 1:B:194:THR:HB   | 1.85                     | 0.58              |
| 1:D:12:ILE:HG21  | 1:D:33:ASP:OD2   | 2.03                     | 0.58              |
| 1:D:174:TYR:HB3  | 1:D:178:GLY:HA2  | 1.84                     | 0.58              |
| 1:E:421:LYS:O    | 1:E:421:LYS:HG3  | 2.00                     | 0.58              |
| 1:F:181:SER:O    | 1:F:197:GLU:HB3  | 2.04                     | 0.58              |
| 1:F:187:LYS:HA   | 1:F:192:LEU:HD11 | 1.84                     | 0.58              |
| 1:G:261:GLY:HA2  | 1:G:264:ILE:HG13 | 1.86                     | 0.58              |
| 1:B:383:GLU:OE2  | 1:D:304:LYS:HE2  | 2.03                     | 0.58              |
| 1:C:268:SER:HB2  | 1:C:286:SER:OG   | 2.04                     | 0.58              |
| 1:F:215:VAL:HG11 | 1:F:217:LEU:CD1  | 2.26                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:22:ALA:HB1   | 1:H:27:GLU:HB3   | 1.85                     | 0.58              |
| 1:H:105:ARG:NE   | 1:H:499:ARG:NH2  | 2.50                     | 0.58              |
| 1:H:202:LEU:HD22 | 1:H:203:GLY:H    | 1.67                     | 0.58              |
| 1:D:63:MET:HG3   | 1:D:371:LEU:HD21 | 1.84                     | 0.58              |
| 1:H:243:PHE:N    | 1:H:271:GLU:OE2  | 2.35                     | 0.58              |
| 1:H:439:GLN:CA   | 1:H:439:GLN:HE21 | 2.14                     | 0.58              |
| 1:A:102:ILE:CG2  | 1:A:103:LEU:HD12 | 2.34                     | 0.58              |
| 1:B:126:SER:OG   | 1:B:127:GLY:N    | 2.35                     | 0.58              |
| 1:C:19:ALA:O     | 1:C:28:HIS:HD2   | 1.86                     | 0.57              |
| 1:H:210:LEU:HD13 | 1:H:210:LEU:N    | 2.18                     | 0.57              |
| 1:H:293:ARG:HD3  | 1:H:326:ALA:O    | 2.04                     | 0.57              |
| 1:A:63:MET:HG3   | 1:A:371:LEU:CD2  | 2.34                     | 0.57              |
| 1:B:23:ASP:OD1   | 1:B:23:ASP:N     | 2.30                     | 0.57              |
| 1:F:167:VAL:HG11 | 1:F:184:VAL:HG21 | 1.84                     | 0.57              |
| 1:G:15:GLN:CG    | 1:G:39:ILE:HG23  | 2.34                     | 0.57              |
| 1:H:369:TYR:HB3  | 1:H:372:GLU:HB2  | 1.86                     | 0.57              |
| 1:C:51:GLY:O     | 1:C:55:ARG:HB2   | 2.04                     | 0.57              |
| 1:E:220:VAL:HG22 | 1:E:221:SER:H    | 1.69                     | 0.57              |
| 1:B:237:ASP:CG   | 1:B:460:ARG:HD2  | 2.29                     | 0.57              |
| 1:D:54:SER:O     | 1:D:60:LEU:HD13  | 2.04                     | 0.57              |
| 1:H:16:GLN:HG2   | 1:H:32:LEU:CD2   | 2.34                     | 0.57              |
| 1:A:113:THR:HG22 | 1:A:114:LYS:N    | 2.20                     | 0.57              |
| 1:C:156:LEU:HD22 | 1:C:157:TRP:H    | 1.68                     | 0.57              |
| 1:C:336:LYS:HB3  | 1:C:337:PRO:HD2  | 1.86                     | 0.57              |
| 1:A:493:MET:CE   | 1:A:530:PRO:HD2  | 2.33                     | 0.57              |
| 1:E:368:ASP:C    | 1:E:370:PRO:HD3  | 2.29                     | 0.57              |
| 1:G:22:ALA:O     | 1:G:391:ARG:NH2  | 2.37                     | 0.57              |
| 1:G:172:LYS:O    | 1:G:211:PRO:HD2  | 2.05                     | 0.57              |
| 1:A:75:PHE:HB2   | 1:A:112:ASP:O    | 2.05                     | 0.57              |
| 1:D:189:PRO:HG2  | 1:D:190:ASP:OD1  | 2.05                     | 0.57              |
| 1:G:175:VAL:HG12 | 1:G:176:ASP:N    | 2.19                     | 0.57              |
| 1:D:424:ALA:HB2  | 1:D:509:ILE:CD1  | 2.35                     | 0.57              |
| 1:F:507:VAL:O    | 1:F:508:VAL:HG23 | 2.04                     | 0.57              |
| 1:G:477:VAL:HG12 | 1:G:478:GLN:N    | 2.19                     | 0.57              |
| 1:H:322:PRO:HB3  | 1:H:464:LEU:O    | 2.05                     | 0.57              |
| 1:B:228:LEU:O    | 1:B:231:GLY:N    | 2.38                     | 0.57              |
| 1:E:272:ASN:O    | 1:E:276:VAL:HG23 | 2.05                     | 0.57              |
| 1:H:14:THR:O     | 1:H:17:LEU:HB2   | 2.04                     | 0.57              |
| 1:A:512:THR:HG21 | 1:A:525:ARG:HH21 | 1.69                     | 0.57              |
| 1:F:87:ILE:O     | 1:F:91:ARG:HG3   | 2.05                     | 0.57              |
| 1:G:45:GLY:HA3   | 1:G:357:CYS:HB3  | 1.86                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:202:LEU:HD22 | 1:G:203:GLY:H    | 1.68                     | 0.57              |
| 1:A:164:CYS:O    | 1:A:187:LYS:HE3  | 2.05                     | 0.56              |
| 1:E:114:LYS:HD3  | 1:E:223:LYS:CD   | 2.25                     | 0.56              |
| 1:E:220:VAL:HG11 | 1:E:225:ILE:CD1  | 2.35                     | 0.56              |
| 1:E:322:PRO:HA   | 1:E:356:ASP:OD2  | 2.05                     | 0.56              |
| 1:H:97:PHE:C     | 1:H:99:SER:H     | 2.11                     | 0.56              |
| 1:A:334:ILE:HG22 | 1:A:335:LYS:HG2  | 1.87                     | 0.56              |
| 1:A:509:ILE:HD13 | 1:A:526:VAL:HG22 | 1.84                     | 0.56              |
| 1:A:141:ILE:HD12 | 1:A:194:THR:HG21 | 1.87                     | 0.56              |
| 1:A:292:ALA:O    | 1:A:296:LEU:HB2  | 2.05                     | 0.56              |
| 1:D:266:ILE:C    | 1:D:267:ILE:HD12 | 2.31                     | 0.56              |
| 1:E:304:LYS:O    | 1:E:307:LEU:HB2  | 2.05                     | 0.56              |
| 1:E:399:ARG:NH1  | 1:F:23:ASP:HB3   | 2.19                     | 0.56              |
| 1:E:512:THR:N    | 1:E:521:THR:HG22 | 2.20                     | 0.56              |
| 1:F:30:CYS:HB3   | 1:H:318:ARG:NH2  | 2.20                     | 0.56              |
| 1:F:123:ILE:N    | 1:F:204:SER:OG   | 2.39                     | 0.56              |
| 1:F:315:ARG:CD   | 1:H:30:CYS:HB3   | 2.35                     | 0.56              |
| 1:G:55:ARG:NH2   | 1:G:82:TYR:O     | 2.38                     | 0.56              |
| 1:G:164:CYS:SG   | 1:G:192:LEU:HD13 | 2.45                     | 0.56              |
| 1:G:483:GLU:O    | 1:G:487:LEU:HB3  | 2.05                     | 0.56              |
| 1:H:148:MET:O    | 1:H:148:MET:HG2  | 2.04                     | 0.56              |
| 1:H:491:LEU:O    | 1:H:495:VAL:HG23 | 2.05                     | 0.56              |
| 1:H:493:MET:HE2  | 1:H:530:PRO:HD3  | 1.85                     | 0.56              |
| 1:A:341:ARG:H    | 1:C:328:GLN:HE21 | 1.51                     | 0.56              |
| 1:B:84:ALA:HB2   | 1:B:230:PHE:HZ   | 1.68                     | 0.56              |
| 1:G:63:MET:O     | 1:G:68:MET:HB2   | 2.05                     | 0.56              |
| 1:A:158:LEU:HD23 | 1:A:163:ILE:CD1  | 2.35                     | 0.56              |
| 1:F:268:SER:HB2  | 1:F:289:ILE:CD1  | 2.36                     | 0.56              |
| 1:G:485:VAL:HG12 | 1:G:486:ASP:OD1  | 2.04                     | 0.56              |
| 1:B:75:PHE:CD1   | 1:B:111:LEU:HG   | 2.40                     | 0.56              |
| 1:D:122:LEU:HD12 | 1:D:204:SER:OG   | 2.05                     | 0.56              |
| 1:D:189:PRO:CD   | 1:D:190:ASP:H    | 2.19                     | 0.56              |
| 1:D:220:VAL:HG23 | 1:D:224:ASP:HB3  | 1.87                     | 0.56              |
| 1:A:421:LYS:HD2  | 1:B:404:SER:O    | 2.05                     | 0.56              |
| 1:F:204:SER:O    | 1:F:206:LYS:HD3  | 2.05                     | 0.56              |
| 1:F:333:MET:CE   | 1:F:373:ALA:HA   | 2.28                     | 0.56              |
| 1:B:293:ARG:HD2  | 1:B:326:ALA:O    | 2.04                     | 0.56              |
| 1:B:328:GLN:NE2  | 1:D:340:THR:HB   | 2.19                     | 0.56              |
| 1:B:391:ARG:HG2  | 1:B:391:ARG:HH11 | 1.71                     | 0.56              |
| 1:B:482:ALA:O    | 1:B:486:ASP:HB2  | 2.05                     | 0.56              |
| 1:C:45:GLY:O     | 1:C:357:CYS:HB2  | 2.05                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:220:VAL:HG23 | 1:D:224:ASP:CB   | 2.36                     | 0.56              |
| 1:D:326:ALA:O    | 1:D:327:THR:HB   | 2.04                     | 0.56              |
| 1:F:315:ARG:HG3  | 1:H:30:CYS:HB3   | 1.86                     | 0.56              |
| 1:G:228:LEU:HD12 | 1:G:256:ILE:HG21 | 1.88                     | 0.56              |
| 1:H:316:CYS:HB2  | 1:H:323:VAL:CG2  | 2.36                     | 0.56              |
| 1:A:332:SER:HB3  | 1:A:343:GLU:OE1  | 2.06                     | 0.56              |
| 1:A:509:ILE:HD11 | 1:A:526:VAL:HG22 | 1.87                     | 0.56              |
| 1:F:215:VAL:HG12 | 1:F:217:LEU:H    | 1.71                     | 0.56              |
| 1:A:173:VAL:HG22 | 1:A:210:LEU:CD2  | 2.36                     | 0.56              |
| 1:B:424:ALA:HB2  | 1:B:509:ILE:HD13 | 1.87                     | 0.56              |
| 1:E:457:GLN:HG2  | 1:E:461:GLN:NE2  | 2.21                     | 0.56              |
| 1:G:338:ARG:HH22 | 1:G:341:ARG:NH2  | 2.02                     | 0.56              |
| 1:G:477:VAL:HG13 | 1:G:484:ASP:OD2  | 2.06                     | 0.56              |
| 1:G:495:VAL:O    | 1:G:498:ALA:HB3  | 2.06                     | 0.56              |
| 1:C:215:VAL:CG1  | 1:C:217:LEU:HD12 | 2.35                     | 0.55              |
| 1:F:221:SER:O    | 1:F:224:ASP:HB2  | 2.06                     | 0.55              |
| 1:G:73:MET:HE2   | 1:G:86:THR:CG2   | 2.36                     | 0.55              |
| 1:G:105:ARG:HD3  | 1:G:499:ARG:HH21 | 1.71                     | 0.55              |
| 1:G:323:VAL:N    | 1:G:356:ASP:HB2  | 2.14                     | 0.55              |
| 1:G:382:ARG:HH11 | 1:G:382:ARG:CG   | 2.19                     | 0.55              |
| 1:B:223:LYS:HA   | 1:B:226:GLN:OE1  | 2.06                     | 0.55              |
| 1:C:139:LEU:HD23 | 1:C:139:LEU:C    | 2.31                     | 0.55              |
| 1:C:220:VAL:HG13 | 1:C:224:ASP:HB2  | 1.88                     | 0.55              |
| 1:C:246:LYS:HE2  | 1:C:249:ASP:OD1  | 2.07                     | 0.55              |
| 1:D:83:HIS:O     | 1:D:87:ILE:HG13  | 2.06                     | 0.55              |
| 1:G:515:ARG:HB2  | 1:G:516:PRO:HD2  | 1.89                     | 0.55              |
| 1:H:272:ASN:HD22 | 1:H:272:ASN:H    | 1.55                     | 0.55              |
| 1:B:138:THR:HG23 | 1:B:139:LEU:N    | 2.21                     | 0.55              |
| 1:C:526:VAL:HG23 | 1:D:411:MET:SD   | 2.45                     | 0.55              |
| 1:F:56:SER:O     | 1:F:60:LEU:HD22  | 2.06                     | 0.55              |
| 1:F:293:ARG:HH22 | 1:F:346:ASP:CG   | 2.11                     | 0.55              |
| 1:H:15:GLN:CB    | 1:H:17:LEU:HD23  | 2.21                     | 0.55              |
| 1:H:512:THR:OG1  | 1:H:513:GLY:N    | 2.35                     | 0.55              |
| 1:B:56:SER:OG    | 1:B:59:THR:HB    | 2.06                     | 0.55              |
| 1:F:16:GLN:NE2   | 5:F:6168:HOH:O   | 2.30                     | 0.55              |
| 1:F:24:THR:HG22  | 1:F:27:GLU:HB2   | 1.88                     | 0.55              |
| 1:F:175:VAL:HB   | 1:F:180:ILE:HB   | 1.88                     | 0.55              |
| 1:F:231:GLY:O    | 1:F:236:VAL:HG22 | 2.06                     | 0.55              |
| 1:H:73:MET:HE2   | 1:H:86:THR:HB    | 1.87                     | 0.55              |
| 1:A:131:VAL:HG12 | 1:A:202:LEU:HB3  | 1.89                     | 0.55              |
| 1:A:341:ARG:N    | 1:C:328:GLN:NE2  | 2.55                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:215:VAL:HG13 | 1:B:217:LEU:HD12 | 1.85                     | 0.55              |
| 1:C:73:MET:HE2   | 1:C:86:THR:HB    | 1.88                     | 0.55              |
| 1:F:202:LEU:HD23 | 1:F:203:GLY:N    | 2.21                     | 0.55              |
| 1:F:376:MET:O    | 1:F:380:ILE:HG13 | 2.06                     | 0.55              |
| 1:F:428:ILE:HD12 | 1:F:508:VAL:CG1  | 2.36                     | 0.55              |
| 1:H:265:LYS:HA   | 1:H:287:ASP:OD2  | 2.06                     | 0.55              |
| 1:A:454:ARG:NH2  | 1:A:484:ASP:OD1  | 2.31                     | 0.55              |
| 1:B:109:VAL:HG12 | 1:B:236:VAL:HG12 | 1.89                     | 0.55              |
| 1:B:122:LEU:HA   | 1:B:204:SER:OG   | 2.07                     | 0.55              |
| 1:A:186:GLN:HB2  | 1:A:193:VAL:HB   | 1.87                     | 0.55              |
| 1:A:259:GLU:O    | 1:A:262:LYS:HG2  | 2.06                     | 0.55              |
| 1:D:151:CYS:HB3  | 1:D:156:LEU:HD23 | 1.89                     | 0.55              |
| 1:E:269:LYS:HD2  | 1:E:290:MET:SD   | 2.46                     | 0.55              |
| 1:D:155:ILE:HG22 | 1:D:156:LEU:N    | 2.22                     | 0.55              |
| 1:E:334:ILE:HD13 | 1:E:363:GLU:HA   | 1.89                     | 0.55              |
| 1:G:160:TYR:OH   | 1:G:216:ASP:HB2  | 2.07                     | 0.55              |
| 1:C:457:GLN:O    | 1:C:461:GLN:HG3  | 2.06                     | 0.55              |
| 1:D:189:PRO:HD2  | 1:D:190:ASP:H    | 1.72                     | 0.55              |
| 1:F:122:LEU:O    | 1:F:151:CYS:HB2  | 2.06                     | 0.55              |
| 1:A:453:THR:CG2  | 1:A:459:ALA:HB2  | 2.37                     | 0.55              |
| 1:A:484:ASP:O    | 1:A:488:ARG:HG3  | 2.06                     | 0.55              |
| 1:B:105:ARG:HG2  | 5:B:6110:HOH:O   | 2.06                     | 0.55              |
| 1:B:145:ASN:N    | 1:B:145:ASN:ND2  | 2.49                     | 0.55              |
| 1:B:237:ASP:OD1  | 1:B:460:ARG:NH1  | 2.30                     | 0.55              |
| 1:F:428:ILE:HD12 | 1:F:508:VAL:HG11 | 1.89                     | 0.55              |
| 1:G:292:ALA:O    | 1:G:296:LEU:HB2  | 2.05                     | 0.55              |
| 1:H:290:MET:HE3  | 1:H:326:ALA:CB   | 2.37                     | 0.55              |
| 1:H:429:VAL:O    | 1:H:451:ALA:HA   | 2.05                     | 0.55              |
| 1:F:237:ASP:OD2  | 1:F:460:ARG:NH1  | 2.29                     | 0.54              |
| 1:G:416:VAL:CG1  | 1:G:445:PRO:HA   | 2.36                     | 0.54              |
| 1:D:18:HIS:HB2   | 5:D:6141:HOH:O   | 2.07                     | 0.54              |
| 1:H:63:MET:HG3   | 1:H:371:LEU:HD21 | 1.87                     | 0.54              |
| 1:A:267:ILE:HD12 | 1:A:288:GLY:HA3  | 1.89                     | 0.54              |
| 1:E:431:THR:CG2  | 1:E:434:GLY:HA2  | 2.36                     | 0.54              |
| 1:F:225:ILE:HG22 | 1:F:226:GLN:N    | 2.21                     | 0.54              |
| 1:G:135:LYS:HG3  | 1:G:198:ASN:N    | 2.21                     | 0.54              |
| 1:G:410:ALA:HB2  | 1:H:421:LYS:HG3  | 1.88                     | 0.54              |
| 1:A:168:ASP:O    | 1:A:171:SER:HB2  | 2.07                     | 0.54              |
| 1:B:30:CYS:O     | 1:D:315:ARG:NH1  | 2.36                     | 0.54              |
| 1:B:61:LYS:O     | 1:B:65:LYS:HB2   | 2.07                     | 0.54              |
| 1:B:433:SER:HB2  | 1:B:435:ARG:HD3  | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:292:ALA:HB1  | 4:D:532:PEQ:C1   | 2.37                     | 0.54              |
| 1:G:132:GLU:HG3  | 1:G:201:PHE:CZ   | 2.42                     | 0.54              |
| 1:G:347:VAL:O    | 1:G:350:ALA:HB3  | 2.08                     | 0.54              |
| 1:A:63:MET:HG3   | 1:A:371:LEU:HD21 | 1.90                     | 0.54              |
| 1:A:73:MET:HB3   | 1:A:75:PHE:HE1   | 1.72                     | 0.54              |
| 1:B:454:ARG:HG3  | 1:B:473:CYS:HB3  | 1.89                     | 0.54              |
| 1:D:293:ARG:HH22 | 1:D:346:ASP:CG   | 2.15                     | 0.54              |
| 1:D:438:HIS:O    | 1:D:441:ALA:HB3  | 2.08                     | 0.54              |
| 1:E:315:ARG:NH1  | 1:G:30:CYS:O     | 2.41                     | 0.54              |
| 1:F:376:MET:HE3  | 1:F:376:MET:C    | 2.33                     | 0.54              |
| 1:G:25:PHE:O     | 1:G:28:HIS:HB3   | 2.07                     | 0.54              |
| 1:G:76:SER:HA    | 1:G:114:LYS:HB2  | 1.90                     | 0.54              |
| 1:G:370:PRO:O    | 1:G:374:VAL:HG23 | 2.07                     | 0.54              |
| 1:B:19:ALA:HA    | 1:B:31:ARG:HD3   | 1.89                     | 0.54              |
| 1:B:167:VAL:CG2  | 1:B:210:LEU:HD23 | 2.38                     | 0.54              |
| 1:B:322:PRO:HA   | 1:B:356:ASP:OD2  | 2.08                     | 0.54              |
| 1:C:43:ASN:CB    | 1:C:467:GLY:HA2  | 2.37                     | 0.54              |
| 1:G:410:ALA:HA   | 1:H:421:LYS:CG   | 2.36                     | 0.54              |
| 1:G:410:ALA:HB2  | 1:H:422:CYS:HB3  | 1.88                     | 0.54              |
| 1:H:382:ARG:HB2  | 1:H:382:ARG:NH1  | 2.23                     | 0.54              |
| 1:B:352:LEU:HD22 | 1:B:384:ALA:HB1  | 1.90                     | 0.54              |
| 1:B:512:THR:N    | 1:B:521:THR:HG22 | 2.23                     | 0.54              |
| 1:C:122:LEU:HD12 | 1:C:204:SER:OG   | 2.07                     | 0.54              |
| 1:G:220:VAL:HG22 | 1:G:224:ASP:CB   | 2.37                     | 0.54              |
| 1:G:493:MET:HE3  | 1:G:529:VAL:HG13 | 1.90                     | 0.54              |
| 1:H:330:LEU:HG   | 1:H:333:MET:SD   | 2.48                     | 0.54              |
| 1:H:453:THR:CG2  | 1:H:459:ALA:HB2  | 2.38                     | 0.54              |
| 1:B:111:LEU:HD23 | 1:B:111:LEU:C    | 2.32                     | 0.54              |
| 1:B:283:LEU:HD22 | 1:B:321:LYS:HD3  | 1.89                     | 0.54              |
| 1:B:407:LEU:HB3  | 1:B:520:PHE:CZ   | 2.43                     | 0.54              |
| 1:B:433:SER:OG   | 5:B:6001:HOH:O   | 2.18                     | 0.54              |
| 1:D:50:ILE:HD13  | 1:D:50:ILE:N     | 2.23                     | 0.54              |
| 1:G:316:CYS:HB2  | 1:G:323:VAL:CG2  | 2.38                     | 0.54              |
| 1:A:330:LEU:O    | 1:A:333:MET:HB2  | 2.07                     | 0.54              |
| 1:B:154:ASN:O    | 1:B:155:ILE:HG13 | 2.08                     | 0.54              |
| 1:F:292:ALA:CB   | 4:F:532:PEQ:H21  | 2.38                     | 0.54              |
| 1:G:334:ILE:HD11 | 1:G:362:GLY:C    | 2.33                     | 0.54              |
| 1:A:525:ARG:HA   | 1:B:522:ASN:O    | 2.08                     | 0.53              |
| 1:B:524:MET:HG2  | 1:B:525:ARG:N    | 2.21                     | 0.53              |
| 1:D:175:VAL:CG2  | 1:D:182:LEU:HD11 | 2.38                     | 0.53              |
| 1:F:332:SER:O    | 1:F:334:ILE:N    | 2.41                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:109:VAL:HG12 | 1:G:236:VAL:HG12 | 1.90                     | 0.53              |
| 1:G:182:LEU:CD2  | 1:G:196:VAL:HG22 | 2.38                     | 0.53              |
| 1:G:322:PRO:HA   | 1:G:356:ASP:CG   | 2.33                     | 0.53              |
| 1:G:473:CYS:HB2  | 1:G:491:LEU:HD23 | 1.89                     | 0.53              |
| 1:H:91:ARG:NH2   | 1:H:235:ASP:O    | 2.42                     | 0.53              |
| 1:H:123:ILE:HD11 | 1:H:202:LEU:HD13 | 1.90                     | 0.53              |
| 1:H:496:GLY:HA3  | 1:H:502:PHE:CE1  | 2.42                     | 0.53              |
| 1:C:251:HIS:O    | 1:C:254:ARG:HB3  | 2.08                     | 0.53              |
| 1:E:106:PRO:O    | 1:E:463:HIS:HE1  | 1.91                     | 0.53              |
| 1:F:145:ASN:N    | 1:F:145:ASN:ND2  | 2.56                     | 0.53              |
| 1:G:70:VAL:HG12  | 1:G:71:ALA:N     | 2.21                     | 0.53              |
| 1:A:102:ILE:HG22 | 1:A:103:LEU:CD1  | 2.37                     | 0.53              |
| 1:B:512:THR:O    | 1:B:523:THR:HB   | 2.09                     | 0.53              |
| 1:D:196:VAL:O    | 1:D:196:VAL:HG12 | 2.08                     | 0.53              |
| 1:F:73:MET:HE2   | 1:F:86:THR:CG2   | 2.38                     | 0.53              |
| 1:G:15:GLN:C     | 1:G:17:LEU:HD23  | 2.33                     | 0.53              |
| 1:H:58:GLU:O     | 1:H:61:LYS:HB2   | 2.09                     | 0.53              |
| 1:H:428:ILE:HD12 | 1:H:508:VAL:HG11 | 1.90                     | 0.53              |
| 1:A:341:ARG:H    | 1:C:328:GLN:NE2  | 2.06                     | 0.53              |
| 1:G:109:VAL:HG23 | 1:G:237:ASP:OD2  | 2.08                     | 0.53              |
| 1:H:328:GLN:HA   | 1:H:331:GLU:HG2  | 1.89                     | 0.53              |
| 1:H:358:ILE:HG13 | 1:H:377:GLN:HE22 | 1.73                     | 0.53              |
| 1:C:411:MET:SD   | 1:D:526:VAL:HG23 | 2.48                     | 0.53              |
| 1:D:119:ARG:N    | 1:D:159:ASP:OD1  | 2.33                     | 0.53              |
| 1:E:327:THR:HG22 | 1:E:328:GLN:HG3  | 1.90                     | 0.53              |
| 1:E:415:SER:HA   | 1:E:524:MET:HE2  | 1.90                     | 0.53              |
| 1:F:292:ALA:HB1  | 4:F:532:PEQ:H21  | 1.89                     | 0.53              |
| 1:F:328:GLN:NE2  | 1:H:341:ARG:N    | 2.53                     | 0.53              |
| 1:G:43:ASN:H     | 1:G:385:GLU:CD   | 2.15                     | 0.53              |
| 1:G:293:ARG:NH1  | 1:G:327:THR:O    | 2.42                     | 0.53              |
| 1:B:131:VAL:HG13 | 1:B:132:GLU:N    | 2.24                     | 0.53              |
| 1:B:465:TYR:HB2  | 1:B:468:ILE:HD12 | 1.91                     | 0.53              |
| 1:C:143:LEU:HD12 | 1:C:190:ASP:HA   | 1.90                     | 0.53              |
| 1:C:493:MET:HE2  | 1:C:529:VAL:HG13 | 1.89                     | 0.53              |
| 1:D:141:ILE:HB   | 1:D:156:LEU:HB3  | 1.91                     | 0.53              |
| 1:D:431:THR:O    | 1:D:453:THR:HB   | 2.08                     | 0.53              |
| 1:E:270:ILE:HD11 | 1:E:289:ILE:HD12 | 1.91                     | 0.53              |
| 1:G:17:LEU:HD23  | 1:G:17:LEU:N     | 2.24                     | 0.53              |
| 1:G:237:ASP:OD1  | 1:G:460:ARG:NH1  | 2.30                     | 0.53              |
| 1:C:417:GLU:OE1  | 1:D:417:GLU:OE1  | 2.27                     | 0.53              |
| 1:F:515:ARG:HB3  | 1:F:516:PRO:CD   | 2.36                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:45:GLY:C     | 1:G:357:CYS:HB3  | 2.34                     | 0.53              |
| 1:H:65:LYS:HA    | 1:H:105:ARG:NH1  | 2.23                     | 0.53              |
| 1:D:154:ASN:HB2  | 1:D:155:ILE:CD1  | 2.37                     | 0.53              |
| 1:D:202:LEU:HD22 | 1:D:202:LEU:C    | 2.34                     | 0.53              |
| 1:E:111:LEU:HB3  | 1:E:239:VAL:HG22 | 1.91                     | 0.53              |
| 1:G:312:ILE:HG22 | 1:G:313:ILE:N    | 2.23                     | 0.53              |
| 1:A:333:MET:HA   | 1:A:336:LYS:O    | 2.09                     | 0.53              |
| 1:G:179:LEU:C    | 1:G:180:ILE:HD13 | 2.33                     | 0.53              |
| 1:A:376:MET:O    | 1:A:380:ILE:HG13 | 2.08                     | 0.53              |
| 1:A:503:LYS:O    | 1:A:529:VAL:HB   | 2.09                     | 0.53              |
| 1:F:138:THR:HG22 | 1:F:138:THR:O    | 2.09                     | 0.53              |
| 1:G:493:MET:HE2  | 1:G:529:VAL:HA   | 1.91                     | 0.53              |
| 1:A:175:VAL:HG12 | 1:A:176:ASP:N    | 2.24                     | 0.52              |
| 1:A:224:ASP:O    | 1:A:227:ASP:HB2  | 2.08                     | 0.52              |
| 1:A:506:ASP:HB2  | 1:A:529:VAL:HG21 | 1.91                     | 0.52              |
| 1:D:118:ILE:CG2  | 1:D:208:VAL:HB   | 2.38                     | 0.52              |
| 1:F:296:LEU:HD12 | 1:F:296:LEU:C    | 2.30                     | 0.52              |
| 1:G:61:LYS:HD3   | 1:G:93:ALA:CA    | 2.37                     | 0.52              |
| 1:G:111:LEU:HD23 | 1:G:111:LEU:C    | 2.34                     | 0.52              |
| 1:H:220:VAL:CG1  | 1:H:224:ASP:HB2  | 2.39                     | 0.52              |
| 1:B:154:ASN:C    | 1:B:155:ILE:HG13 | 2.33                     | 0.52              |
| 1:E:54:SER:O     | 1:E:60:LEU:HD11  | 2.08                     | 0.52              |
| 1:E:274:GLU:O    | 1:E:277:ARG:N    | 2.42                     | 0.52              |
| 1:F:263:ASN:OD1  | 1:F:263:ASN:N    | 2.40                     | 0.52              |
| 1:G:457:GLN:O    | 1:G:460:ARG:N    | 2.30                     | 0.52              |
| 1:H:328:GLN:CA   | 1:H:331:GLU:HG3  | 2.38                     | 0.52              |
| 1:A:123:ILE:HA   | 1:A:151:CYS:O    | 2.08                     | 0.52              |
| 1:A:415:SER:HA   | 1:A:524:MET:CE   | 2.40                     | 0.52              |
| 1:B:228:LEU:HD12 | 1:B:256:ILE:HG21 | 1.91                     | 0.52              |
| 1:G:453:THR:CG2  | 1:G:459:ALA:HB2  | 2.39                     | 0.52              |
| 1:B:42:ARG:HD2   | 1:B:44:THR:O     | 2.09                     | 0.52              |
| 1:B:167:VAL:CG1  | 1:B:171:SER:HB2  | 2.39                     | 0.52              |
| 1:D:139:LEU:HD11 | 1:D:153:GLU:O    | 2.09                     | 0.52              |
| 1:D:202:LEU:HD22 | 1:D:203:GLY:N    | 2.24                     | 0.52              |
| 1:E:328:GLN:NE2  | 1:G:341:ARG:HG2  | 2.25                     | 0.52              |
| 1:E:339:PRO:CG   | 1:E:376:MET:HE2  | 2.40                     | 0.52              |
| 1:G:126:SER:OG   | 1:G:127:GLY:N    | 2.40                     | 0.52              |
| 1:G:261:GLY:CA   | 1:G:264:ILE:HG13 | 2.39                     | 0.52              |
| 1:G:272:ASN:ND2  | 5:G:6179:HOH:O   | 2.43                     | 0.52              |
| 1:G:290:MET:HE2  | 1:G:326:ALA:CB   | 2.39                     | 0.52              |
| 1:H:122:LEU:HD23 | 1:H:149:GLU:HG3  | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:LYS:NZ   | 1:A:197:GLU:OE1  | 2.40                     | 0.52              |
| 1:A:253:VAL:O    | 1:A:257:LEU:HB2  | 2.10                     | 0.52              |
| 1:B:328:GLN:CG   | 1:B:331:GLU:HG3  | 2.38                     | 0.52              |
| 1:C:103:LEU:HD12 | 1:C:103:LEU:N    | 2.24                     | 0.52              |
| 1:D:70:VAL:HG22  | 1:D:108:ALA:HB3  | 1.92                     | 0.52              |
| 1:F:113:THR:O    | 1:F:242:SER:OG   | 2.25                     | 0.52              |
| 1:H:316:CYS:HB3  | 1:H:321:LYS:O    | 2.09                     | 0.52              |
| 1:H:512:THR:C    | 1:H:521:THR:HG22 | 2.34                     | 0.52              |
| 1:B:316:CYS:HB3  | 1:B:321:LYS:O    | 2.09                     | 0.52              |
| 1:C:334:ILE:HG23 | 1:C:367:GLY:HA2  | 1.92                     | 0.52              |
| 1:C:439:GLN:O    | 1:C:442:ARG:HB3  | 2.10                     | 0.52              |
| 1:E:54:SER:HA    | 1:E:59:THR:HG21  | 1.91                     | 0.52              |
| 1:F:297:GLY:HA2  | 1:F:305:VAL:HG21 | 1.91                     | 0.52              |
| 1:H:95:GLU:OE1   | 1:H:98:ALA:HB2   | 2.09                     | 0.52              |
| 1:A:311:MET:SD   | 1:A:315:ARG:HD3  | 2.49                     | 0.52              |
| 1:B:455:ASN:HB3  | 1:B:458:THR:HB   | 1.91                     | 0.52              |
| 1:A:50:ILE:HG13  | 1:A:71:ALA:HB1   | 1.92                     | 0.52              |
| 1:B:122:LEU:HB2  | 1:B:149:GLU:HA   | 1.92                     | 0.52              |
| 1:B:145:ASN:HD22 | 1:B:145:ASN:H    | 1.53                     | 0.52              |
| 1:G:141:ILE:HG21 | 1:G:158:LEU:HD22 | 1.92                     | 0.52              |
| 1:A:103:LEU:HD12 | 1:A:103:LEU:N    | 2.24                     | 0.52              |
| 1:A:504:LYS:O    | 1:A:529:VAL:O    | 2.28                     | 0.52              |
| 1:B:152:ASP:C    | 1:B:154:ASN:H    | 2.18                     | 0.52              |
| 1:D:133:LEU:HD12 | 1:D:180:ILE:HG21 | 1.92                     | 0.52              |
| 1:F:211:PRO:C    | 1:F:213:ALA:H    | 2.17                     | 0.52              |
| 1:F:339:PRO:HG3  | 1:F:376:MET:CG   | 2.40                     | 0.52              |
| 1:F:487:LEU:C    | 1:F:487:LEU:HD12 | 2.35                     | 0.52              |
| 1:G:360:LEU:HA   | 1:G:363:GLU:OE1  | 2.09                     | 0.52              |
| 1:H:334:ILE:HG22 | 1:H:335:LYS:HG3  | 1.90                     | 0.52              |
| 1:A:228:LEU:HD22 | 1:A:257:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:250:VAL:O    | 1:A:250:VAL:HG12 | 2.10                     | 0.52              |
| 1:E:369:TYR:N    | 1:E:370:PRO:HD3  | 2.25                     | 0.52              |
| 1:G:385:GLU:O    | 1:G:388:MET:HG3  | 2.11                     | 0.52              |
| 1:H:170:GLY:N    | 1:H:184:VAL:O    | 2.32                     | 0.52              |
| 1:H:360:LEU:HD11 | 1:H:377:GLN:NE2  | 2.25                     | 0.52              |
| 1:E:326:ALA:CB   | 1:E:359:MET:HE2  | 2.39                     | 0.51              |
| 1:F:521:THR:HG22 | 1:F:521:THR:O    | 2.10                     | 0.51              |
| 1:G:85:GLU:O     | 1:G:88:LYS:HB3   | 2.10                     | 0.51              |
| 1:A:267:ILE:HD12 | 1:A:288:GLY:CA   | 2.39                     | 0.51              |
| 1:F:274:GLU:OE2  | 1:F:278:ARG:HD2  | 2.10                     | 0.51              |
| 1:G:290:MET:CE   | 1:G:359:MET:HE1  | 2.38                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:143:LEU:HG   | 1:B:190:ASP:O    | 2.10                     | 0.51              |
| 1:B:283:LEU:CD2  | 1:B:321:LYS:HD3  | 2.40                     | 0.51              |
| 1:G:21:MET:HA    | 1:G:21:MET:CE    | 2.36                     | 0.51              |
| 1:H:45:GLY:O     | 1:H:357:CYS:HB3  | 2.10                     | 0.51              |
| 1:H:169:VAL:HA   | 1:H:184:VAL:HG12 | 1.91                     | 0.51              |
| 1:A:123:ILE:N    | 1:A:204:SER:OG   | 2.33                     | 0.51              |
| 1:A:426:ALA:O    | 1:A:508:VAL:HG22 | 2.11                     | 0.51              |
| 1:B:493:MET:CE   | 1:B:530:PRO:HD2  | 2.25                     | 0.51              |
| 1:C:115:GLY:HA2  | 1:C:224:ASP:OD2  | 2.09                     | 0.51              |
| 1:F:283:LEU:CD2  | 1:F:321:LYS:HD2  | 2.40                     | 0.51              |
| 1:G:16:GLN:OE1   | 1:G:33:ASP:O     | 2.28                     | 0.51              |
| 1:H:427:LEU:HD12 | 1:H:427:LEU:N    | 2.25                     | 0.51              |
| 1:A:160:TYR:CE1  | 1:A:217:LEU:HD11 | 2.46                     | 0.51              |
| 1:B:173:VAL:HB   | 1:B:182:LEU:CD1  | 2.38                     | 0.51              |
| 1:C:393:LEU:O    | 1:C:397:LEU:HB2  | 2.11                     | 0.51              |
| 1:E:390:HIS:NE2  | 1:E:446:ARG:HG3  | 2.26                     | 0.51              |
| 1:H:16:GLN:O     | 1:H:20:ALA:HB2   | 2.10                     | 0.51              |
| 1:H:292:ALA:HB1  | 4:H:532:PEQ:H21  | 1.92                     | 0.51              |
| 1:A:162:ASN:HB3  | 1:A:165:LYS:HE3  | 1.92                     | 0.51              |
| 1:A:246:LYS:HD2  | 1:A:248:ALA:HB3  | 1.92                     | 0.51              |
| 1:A:281:GLU:HG3  | 1:A:282:ILE:N    | 2.24                     | 0.51              |
| 1:A:355:ALA:O    | 1:A:466:ARG:NH1  | 2.44                     | 0.51              |
| 1:C:48:CYS:SG    | 1:C:68:MET:HG3   | 2.50                     | 0.51              |
| 1:C:215:VAL:HG11 | 1:C:217:LEU:HD12 | 1.93                     | 0.51              |
| 1:E:220:VAL:HG11 | 1:E:225:ILE:CG1  | 2.41                     | 0.51              |
| 1:F:157:TRP:O    | 1:F:158:LEU:HD13 | 2.10                     | 0.51              |
| 1:F:310:LYS:NZ   | 1:H:349:ASN:HD21 | 2.09                     | 0.51              |
| 1:F:327:THR:HG22 | 1:F:328:GLN:HG3  | 1.92                     | 0.51              |
| 1:G:47:ILE:HG12  | 1:G:70:VAL:HB    | 1.92                     | 0.51              |
| 1:G:417:GLU:OE1  | 1:H:417:GLU:OE1  | 2.29                     | 0.51              |
| 1:G:504:LYS:O    | 1:G:529:VAL:O    | 2.29                     | 0.51              |
| 1:H:66:SER:OG    | 1:H:375:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:421:LYS:NZ   | 1:B:404:SER:O    | 2.41                     | 0.51              |
| 1:A:499:ARG:HB3  | 1:A:501:PHE:CE1  | 2.46                     | 0.51              |
| 1:D:157:TRP:O    | 1:D:158:LEU:HD12 | 2.11                     | 0.51              |
| 1:E:259:GLU:O    | 1:E:262:LYS:HG2  | 2.10                     | 0.51              |
| 1:F:220:VAL:HG22 | 1:F:224:ASP:HB2  | 1.93                     | 0.51              |
| 1:G:156:LEU:HD23 | 1:G:157:TRP:H    | 1.74                     | 0.51              |
| 1:H:268:SER:HB2  | 1:H:286:SER:OG   | 2.10                     | 0.51              |
| 1:H:485:VAL:O    | 1:H:489:VAL:HG23 | 2.11                     | 0.51              |
| 1:H:504:LYS:O    | 1:H:529:VAL:O    | 2.29                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:483:GLU:O    | 1:A:487:LEU:HB2  | 2.11                     | 0.51              |
| 1:B:276:VAL:HG11 | 1:D:34:ILE:HD13  | 1.93                     | 0.51              |
| 1:B:333:MET:HA   | 1:B:336:LYS:O    | 2.10                     | 0.51              |
| 1:F:141:ILE:HG22 | 1:F:156:LEU:CB   | 2.39                     | 0.51              |
| 1:F:272:ASN:HB2  | 1:F:299:GLU:HG2  | 1.93                     | 0.51              |
| 1:G:419:SER:HB2  | 1:G:427:LEU:HD11 | 1.92                     | 0.51              |
| 1:H:56:SER:O     | 1:H:60:LEU:HD22  | 2.11                     | 0.51              |
| 1:B:123:ILE:O    | 1:B:124:LYS:HB2  | 2.11                     | 0.51              |
| 1:C:224:ASP:O    | 1:C:228:LEU:HG   | 2.11                     | 0.51              |
| 1:F:72:ARG:NH2   | 4:F:532:PEQ:O1P  | 2.42                     | 0.51              |
| 1:G:61:LYS:CG    | 1:G:93:ALA:HB1   | 2.35                     | 0.51              |
| 1:H:242:SER:CA   | 1:H:269:LYS:HE2  | 2.37                     | 0.51              |
| 1:H:328:GLN:HG2  | 1:H:331:GLU:CG   | 2.41                     | 0.51              |
| 1:B:462:ALA:HB1  | 1:B:468:ILE:HG21 | 1.92                     | 0.51              |
| 1:C:326:ALA:O    | 1:C:327:THR:HB   | 2.10                     | 0.51              |
| 1:D:323:VAL:O    | 1:D:356:ASP:HB2  | 2.11                     | 0.51              |
| 1:G:110:ALA:CB   | 1:G:238:MET:HE2  | 2.36                     | 0.51              |
| 1:G:123:ILE:HB   | 1:G:204:SER:OG   | 2.10                     | 0.51              |
| 1:G:333:MET:HE2  | 1:G:373:ALA:HA   | 1.93                     | 0.51              |
| 1:G:411:MET:O    | 1:G:415:SER:OG   | 2.29                     | 0.51              |
| 1:H:15:GLN:OE1   | 1:H:446:ARG:HD2  | 2.10                     | 0.51              |
| 1:H:290:MET:HE3  | 1:H:326:ALA:HB2  | 1.93                     | 0.51              |
| 1:B:73:MET:HE2   | 1:B:86:THR:HG21  | 1.93                     | 0.50              |
| 1:C:138:THR:HG22 | 1:C:138:THR:O    | 2.10                     | 0.50              |
| 1:E:55:ARG:NE    | 1:E:82:TYR:CE1   | 2.79                     | 0.50              |
| 1:G:118:ILE:HG23 | 1:G:160:TYR:HB2  | 1.92                     | 0.50              |
| 1:G:291:VAL:HG12 | 1:G:293:ARG:HG3  | 1.93                     | 0.50              |
| 1:G:504:LYS:HG3  | 1:G:530:PRO:OXT  | 2.11                     | 0.50              |
| 1:H:181:SER:O    | 1:H:197:GLU:O    | 2.30                     | 0.50              |
| 1:B:186:GLN:HG3  | 1:B:187:LYS:O    | 2.11                     | 0.50              |
| 1:B:224:ASP:O    | 1:B:228:LEU:HG   | 2.11                     | 0.50              |
| 1:C:27:GLU:OE1   | 1:C:31:ARG:NH2   | 2.43                     | 0.50              |
| 1:C:220:VAL:HG11 | 1:C:225:ILE:HG12 | 1.93                     | 0.50              |
| 1:E:217:LEU:HB3  | 1:E:218:PRO:HD2  | 1.93                     | 0.50              |
| 1:G:113:THR:HG22 | 1:G:242:SER:H    | 1.76                     | 0.50              |
| 1:G:524:MET:HE1  | 1:H:524:MET:HE3  | 1.90                     | 0.50              |
| 1:H:291:VAL:HG22 | 1:H:312:ILE:HG21 | 1.93                     | 0.50              |
| 1:F:167:VAL:HG12 | 1:F:168:ASP:N    | 2.26                     | 0.50              |
| 1:G:339:PRO:CG   | 1:G:376:MET:HE2  | 2.41                     | 0.50              |
| 1:H:237:ASP:HB2  | 1:H:238:MET:HE2  | 1.94                     | 0.50              |
| 1:B:283:LEU:HD22 | 1:B:321:LYS:CD   | 2.40                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:395:GLU:O    | 1:C:399:ARG:HG2  | 2.11                     | 0.50              |
| 1:C:401:SER:O    | 1:D:421:LYS:NZ   | 2.45                     | 0.50              |
| 1:E:390:HIS:CD2  | 1:E:446:ARG:NH1  | 2.80                     | 0.50              |
| 1:E:487:LEU:HD23 | 1:E:487:LEU:C    | 2.37                     | 0.50              |
| 1:F:318:ARG:NH2  | 1:H:27:GLU:OE2   | 2.40                     | 0.50              |
| 1:F:333:MET:HE1  | 1:F:376:MET:CB   | 2.41                     | 0.50              |
| 1:G:300:ILE:HB   | 1:G:301:PRO:HD2  | 1.92                     | 0.50              |
| 1:H:503:LYS:N    | 1:H:506:ASP:OD2  | 2.38                     | 0.50              |
| 1:B:239:VAL:O    | 1:B:239:VAL:HG12 | 2.11                     | 0.50              |
| 1:D:181:SER:O    | 1:D:197:GLU:O    | 2.30                     | 0.50              |
| 1:D:237:ASP:OD2  | 1:D:460:ARG:HD2  | 2.12                     | 0.50              |
| 1:D:333:MET:HA   | 1:D:336:LYS:O    | 2.12                     | 0.50              |
| 1:H:286:SER:HB2  | 1:H:288:GLY:O    | 2.12                     | 0.50              |
| 1:B:118:ILE:HB   | 1:B:208:VAL:HB   | 1.94                     | 0.50              |
| 1:B:181:SER:O    | 1:B:197:GLU:O    | 2.29                     | 0.50              |
| 1:E:42:ARG:HG3   | 1:E:381:ALA:HB3  | 1.93                     | 0.50              |
| 1:E:334:ILE:HD11 | 1:E:363:GLU:N    | 2.26                     | 0.50              |
| 1:A:289:ILE:O    | 1:A:323:VAL:HA   | 2.11                     | 0.50              |
| 1:B:93:ALA:O     | 1:B:96:SER:HB3   | 2.10                     | 0.50              |
| 1:B:340:THR:HA   | 1:D:328:GLN:OE1  | 2.11                     | 0.50              |
| 1:E:227:ASP:O    | 1:E:230:PHE:HB3  | 2.12                     | 0.50              |
| 1:F:349:ASN:HD21 | 1:H:310:LYS:HZ2  | 1.57                     | 0.50              |
| 1:G:15:GLN:HB3   | 1:G:17:LEU:CD2   | 2.42                     | 0.50              |
| 1:G:61:LYS:HE2   | 1:G:96:SER:OG    | 2.11                     | 0.50              |
| 1:G:431:THR:CG2  | 1:G:434:GLY:HA2  | 2.41                     | 0.50              |
| 1:G:493:MET:HG2  | 1:G:530:PRO:HD2  | 1.94                     | 0.50              |
| 1:A:267:ILE:HD13 | 1:A:267:ILE:N    | 2.18                     | 0.50              |
| 1:A:411:MET:O    | 1:A:415:SER:OG   | 2.30                     | 0.50              |
| 1:B:167:VAL:HG12 | 1:B:168:ASP:N    | 2.26                     | 0.50              |
| 1:C:238:MET:HE1  | 1:C:464:LEU:CD1  | 2.42                     | 0.50              |
| 1:C:447:ALA:HB1  | 1:C:448:PRO:HD2  | 1.94                     | 0.50              |
| 1:E:75:PHE:CZ    | 1:E:83:HIS:CD2   | 3.00                     | 0.50              |
| 1:E:339:PRO:HG3  | 1:E:376:MET:HG2  | 1.93                     | 0.50              |
| 1:F:122:LEU:HA   | 1:F:204:SER:OG   | 2.11                     | 0.50              |
| 1:G:158:LEU:HD23 | 1:G:163:ILE:HD13 | 1.93                     | 0.50              |
| 1:G:228:LEU:CD1  | 1:G:256:ILE:HG21 | 2.42                     | 0.50              |
| 1:H:80:HIS:HB3   | 1:H:230:PHE:CE1  | 2.47                     | 0.50              |
| 1:H:403:HIS:H    | 1:H:403:HIS:CD2  | 2.29                     | 0.50              |
| 1:A:54:SER:O     | 1:A:60:LEU:HD13  | 2.11                     | 0.50              |
| 1:A:131:VAL:HG22 | 1:A:153:GLU:HB3  | 1.93                     | 0.50              |
| 1:D:504:LYS:O    | 1:D:529:VAL:O    | 2.30                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:102:ILE:HG22 | 1:E:103:LEU:HD11 | 1.93                     | 0.50              |
| 1:E:340:THR:HB   | 1:G:328:GLN:NE2  | 2.26                     | 0.50              |
| 1:F:240:PHE:CD2  | 1:F:290:MET:HE1  | 2.47                     | 0.50              |
| 1:F:293:ARG:O    | 1:H:341:ARG:NE   | 2.43                     | 0.50              |
| 1:H:272:ASN:HD22 | 1:H:272:ASN:N    | 2.09                     | 0.50              |
| 1:B:25:PHE:CE1   | 1:B:392:LYS:HD3  | 2.47                     | 0.49              |
| 1:B:237:ASP:OD1  | 1:B:460:ARG:HD2  | 2.11                     | 0.49              |
| 1:D:271:GLU:HG2  | 1:D:295:ASP:HB2  | 1.94                     | 0.49              |
| 1:E:421:LYS:HE3  | 1:F:404:SER:O    | 2.12                     | 0.49              |
| 1:E:504:LYS:O    | 1:E:529:VAL:O    | 2.30                     | 0.49              |
| 1:G:14:THR:O     | 1:G:15:GLN:HB2   | 2.12                     | 0.49              |
| 1:H:22:ALA:HA    | 1:H:31:ARG:NH1   | 2.27                     | 0.49              |
| 1:H:293:ARG:HH22 | 1:H:346:ASP:CG   | 2.19                     | 0.49              |
| 1:A:124:LYS:C    | 1:A:126:SER:H    | 2.20                     | 0.49              |
| 1:A:209:ASN:C    | 1:A:211:PRO:HD3  | 2.37                     | 0.49              |
| 1:A:417:GLU:OE1  | 1:B:417:GLU:OE1  | 2.30                     | 0.49              |
| 1:B:481:TRP:CZ3  | 1:B:516:PRO:HA   | 2.47                     | 0.49              |
| 1:C:408:MET:HE2  | 1:C:436:SER:C    | 2.37                     | 0.49              |
| 1:C:504:LYS:O    | 1:C:529:VAL:O    | 2.29                     | 0.49              |
| 1:D:113:THR:HG23 | 1:D:115:GLY:N    | 2.27                     | 0.49              |
| 1:E:215:VAL:CG1  | 1:E:217:LEU:HD13 | 2.41                     | 0.49              |
| 1:E:429:VAL:O    | 1:E:451:ALA:HA   | 2.12                     | 0.49              |
| 1:F:376:MET:HA   | 1:F:376:MET:CE   | 2.38                     | 0.49              |
| 1:G:55:ARG:NH1   | 1:G:82:TYR:CE1   | 2.80                     | 0.49              |
| 1:G:215:VAL:HG13 | 1:G:217:LEU:H    | 1.77                     | 0.49              |
| 1:G:527:VAL:CG1  | 1:G:528:PRO:HD2  | 2.42                     | 0.49              |
| 1:H:77:HIS:O     | 1:H:78:GLY:O     | 2.30                     | 0.49              |
| 1:A:43:ASN:CB    | 1:A:467:GLY:HA2  | 2.36                     | 0.49              |
| 1:C:322:PRO:HB3  | 1:C:464:LEU:O    | 2.13                     | 0.49              |
| 1:D:411:MET:HE1  | 1:D:524:MET:HB2  | 1.95                     | 0.49              |
| 1:E:75:PHE:CE2   | 1:E:83:HIS:CD2   | 3.00                     | 0.49              |
| 1:F:63:MET:HG3   | 1:F:371:LEU:HD21 | 1.93                     | 0.49              |
| 1:H:17:LEU:O     | 1:H:20:ALA:HB3   | 2.12                     | 0.49              |
| 1:H:292:ALA:CB   | 4:H:532:PEQ:H21  | 2.41                     | 0.49              |
| 1:H:316:CYS:O    | 1:H:320:GLY:N    | 2.45                     | 0.49              |
| 5:A:6133:HOH:O   | 1:C:345:SER:HB2  | 2.12                     | 0.49              |
| 1:B:221:SER:N    | 1:B:224:ASP:HB2  | 2.24                     | 0.49              |
| 1:C:41:ALA:HB2   | 1:C:501:PHE:CE1  | 2.47                     | 0.49              |
| 1:C:185:LYS:HG2  | 1:C:193:VAL:HG12 | 1.94                     | 0.49              |
| 1:D:228:LEU:HD22 | 1:D:257:LEU:HD11 | 1.93                     | 0.49              |
| 1:D:290:MET:HE3  | 1:D:326:ALA:CB   | 2.40                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:475:ASP:HB3  | 1:E:476:PRO:HD2  | 1.93                     | 0.49              |
| 1:G:327:THR:HG22 | 1:G:328:GLN:HG3  | 1.93                     | 0.49              |
| 1:G:461:GLN:O    | 1:G:464:LEU:HB2  | 2.12                     | 0.49              |
| 1:H:332:SER:OG   | 1:H:343:GLU:OE1  | 2.29                     | 0.49              |
| 1:A:415:SER:CA   | 1:A:524:MET:HE2  | 2.39                     | 0.49              |
| 1:B:221:SER:H    | 1:B:224:ASP:CB   | 2.22                     | 0.49              |
| 1:F:22:ALA:O     | 1:F:389:PHE:HZ   | 1.96                     | 0.49              |
| 1:G:63:MET:CA    | 1:G:371:LEU:HD21 | 2.42                     | 0.49              |
| 1:B:273:HIS:CD2  | 1:B:277:ARG:HH21 | 2.29                     | 0.49              |
| 1:D:497:LYS:HD2  | 1:D:529:VAL:CG1  | 2.42                     | 0.49              |
| 1:F:135:LYS:HA   | 1:F:196:VAL:HG12 | 1.94                     | 0.49              |
| 1:F:242:SER:CA   | 1:F:269:LYS:HE2  | 2.38                     | 0.49              |
| 1:G:182:LEU:HD23 | 1:G:196:VAL:HG22 | 1.94                     | 0.49              |
| 1:H:279:PHE:HE1  | 1:H:289:ILE:HD13 | 1.78                     | 0.49              |
| 1:C:290:MET:HE1  | 1:C:359:MET:CE   | 2.42                     | 0.49              |
| 1:E:74:ASN:OD1   | 1:E:76:SER:OG    | 2.30                     | 0.49              |
| 1:F:152:ASP:O    | 1:F:155:ILE:O    | 2.30                     | 0.49              |
| 1:D:144:ASP:HB3  | 1:D:147:TYR:HD2  | 1.77                     | 0.49              |
| 1:E:73:MET:HE3   | 1:E:87:ILE:HG13  | 1.93                     | 0.49              |
| 1:G:109:VAL:CG1  | 1:G:236:VAL:HG12 | 2.42                     | 0.49              |
| 1:G:333:MET:HE2  | 1:G:372:GLU:C    | 2.38                     | 0.49              |
| 1:A:276:VAL:O    | 1:A:279:PHE:HB2  | 2.13                     | 0.49              |
| 1:A:283:LEU:O    | 1:A:283:LEU:HD22 | 2.13                     | 0.49              |
| 1:B:326:ALA:O    | 1:B:327:THR:HB   | 2.12                     | 0.49              |
| 1:B:333:MET:HE1  | 1:B:339:PRO:HD3  | 1.93                     | 0.49              |
| 1:B:503:LYS:HG2  | 1:B:504:LYS:N    | 2.22                     | 0.49              |
| 1:C:279:PHE:CE1  | 1:C:289:ILE:HD12 | 2.46                     | 0.49              |
| 1:E:419:SER:HB3  | 1:E:509:ILE:HD12 | 1.95                     | 0.49              |
| 1:G:48:CYS:SG    | 1:G:68:MET:HG3   | 2.52                     | 0.49              |
| 1:G:105:ARG:HD3  | 1:G:499:ARG:NH2  | 2.27                     | 0.49              |
| 1:G:503:LYS:O    | 1:G:529:VAL:HB   | 2.12                     | 0.49              |
| 1:A:429:VAL:C    | 1:A:430:LEU:HD12 | 2.38                     | 0.49              |
| 1:B:411:MET:O    | 1:B:415:SER:OG   | 2.31                     | 0.49              |
| 1:C:329:MET:O    | 1:C:330:LEU:HD12 | 2.12                     | 0.49              |
| 1:F:328:GLN:NE2  | 1:H:340:THR:HA   | 2.27                     | 0.49              |
| 1:F:411:MET:O    | 1:F:415:SER:OG   | 2.31                     | 0.49              |
| 1:H:119:ARG:HA   | 1:H:206:LYS:O    | 2.12                     | 0.49              |
| 1:A:16:GLN:HA    | 5:A:6092:HOH:O   | 2.12                     | 0.48              |
| 1:A:329:MET:O    | 1:A:343:GLU:HG2  | 2.13                     | 0.48              |
| 1:B:160:TYR:HE2  | 1:B:166:VAL:HG11 | 1.78                     | 0.48              |
| 1:D:445:PRO:HG2  | 1:D:449:ILE:HD11 | 1.95                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:456:HIS:N    | 1:E:456:HIS:CD2  | 2.80                     | 0.48              |
| 1:G:439:GLN:HE21 | 1:G:439:GLN:CA   | 2.26                     | 0.48              |
| 1:H:103:LEU:HA   | 1:H:499:ARG:NH1  | 2.23                     | 0.48              |
| 1:A:407:LEU:N    | 1:A:407:LEU:HD23 | 2.28                     | 0.48              |
| 1:B:254:ARG:O    | 1:B:258:GLY:N    | 2.39                     | 0.48              |
| 1:D:152:ASP:O    | 1:D:155:ILE:O    | 2.31                     | 0.48              |
| 1:D:197:GLU:O    | 1:D:198:ASN:HB2  | 2.12                     | 0.48              |
| 1:F:167:VAL:HG12 | 1:F:168:ASP:O    | 2.13                     | 0.48              |
| 1:F:179:LEU:HA   | 1:H:338:ARG:HH22 | 1.78                     | 0.48              |
| 1:B:115:GLY:HA2  | 1:B:224:ASP:OD2  | 2.13                     | 0.48              |
| 1:E:220:VAL:HG11 | 1:E:225:ILE:HG12 | 1.96                     | 0.48              |
| 1:F:24:THR:HG23  | 1:F:27:GLU:H     | 1.77                     | 0.48              |
| 1:F:220:VAL:CG2  | 1:F:224:ASP:HB3  | 2.43                     | 0.48              |
| 1:G:61:LYS:HE2   | 1:G:96:SER:CB    | 2.44                     | 0.48              |
| 1:H:515:ARG:HB3  | 1:H:516:PRO:CD   | 2.42                     | 0.48              |
| 1:A:73:MET:HB3   | 1:A:75:PHE:CE1   | 2.47                     | 0.48              |
| 1:B:100:ASP:OD1  | 1:B:102:ILE:HB   | 2.12                     | 0.48              |
| 1:B:192:LEU:HD12 | 1:B:192:LEU:HA   | 1.70                     | 0.48              |
| 1:B:254:ARG:NH2  | 1:B:266:ILE:HD12 | 2.29                     | 0.48              |
| 1:C:102:ILE:CG2  | 1:C:103:LEU:HD12 | 2.40                     | 0.48              |
| 1:D:22:ALA:HB1   | 1:D:27:GLU:HB3   | 1.95                     | 0.48              |
| 1:F:52:PRO:HD2   | 1:F:365:ALA:O    | 2.13                     | 0.48              |
| 1:H:19:ALA:HA    | 1:H:31:ARG:CB    | 2.42                     | 0.48              |
| 1:A:47:ILE:HG12  | 1:A:70:VAL:HB    | 1.95                     | 0.48              |
| 1:C:439:GLN:OE1  | 1:C:439:GLN:HA   | 2.13                     | 0.48              |
| 1:C:462:ALA:HB3  | 1:C:470:PRO:HG3  | 1.96                     | 0.48              |
| 1:D:220:VAL:O    | 1:D:220:VAL:HG13 | 2.12                     | 0.48              |
| 1:F:245:ARG:HB2  | 1:F:249:ASP:OD2  | 2.13                     | 0.48              |
| 1:G:191:PHE:N    | 1:G:191:PHE:CD1  | 2.81                     | 0.48              |
| 1:G:360:LEU:HD22 | 1:G:373:ALA:HB1  | 1.96                     | 0.48              |
| 1:H:108:ALA:HA   | 1:H:237:ASP:OD2  | 2.12                     | 0.48              |
| 1:A:143:LEU:O    | 1:A:145:ASN:ND2  | 2.47                     | 0.48              |
| 1:A:209:ASN:ND2  | 1:A:298:ILE:HD13 | 2.28                     | 0.48              |
| 1:A:271:GLU:HG2  | 1:A:295:ASP:HB2  | 1.96                     | 0.48              |
| 1:C:66:SER:HB3   | 1:C:375:ARG:HG3  | 1.96                     | 0.48              |
| 1:C:102:ILE:HG22 | 1:C:103:LEU:N    | 2.27                     | 0.48              |
| 1:C:503:LYS:O    | 1:C:529:VAL:HG11 | 2.14                     | 0.48              |
| 1:D:220:VAL:CG2  | 1:D:224:ASP:HB2  | 2.43                     | 0.48              |
| 1:F:230:PHE:O    | 1:F:233:GLU:HB2  | 2.14                     | 0.48              |
| 1:F:315:ARG:NH1  | 1:H:30:CYS:O     | 2.39                     | 0.48              |
| 1:B:123:ILE:O    | 1:B:123:ILE:HG22 | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:55:ARG:NH2   | 1:C:85:GLU:HB3   | 2.28                     | 0.48              |
| 1:E:379:LEU:HD13 | 1:E:379:LEU:N    | 2.29                     | 0.48              |
| 1:E:439:GLN:CA   | 1:E:439:GLN:HE21 | 2.25                     | 0.48              |
| 1:F:266:ILE:O    | 1:F:266:ILE:HG22 | 2.11                     | 0.48              |
| 1:G:439:GLN:HA   | 1:G:439:GLN:NE2  | 2.27                     | 0.48              |
| 1:H:16:GLN:HG2   | 1:H:32:LEU:HD23  | 1.96                     | 0.48              |
| 1:H:108:ALA:HB2  | 1:H:460:ARG:O    | 2.13                     | 0.48              |
| 1:H:488:ARG:O    | 1:H:491:LEU:HB3  | 2.14                     | 0.48              |
| 1:B:12:ILE:HG21  | 1:B:33:ASP:OD2   | 2.14                     | 0.48              |
| 1:B:120:THR:HG22 | 1:B:156:LEU:CD1  | 2.43                     | 0.48              |
| 1:B:133:LEU:HB2  | 1:B:200:GLY:O    | 2.14                     | 0.48              |
| 1:B:288:GLY:O    | 1:B:289:ILE:HG12 | 2.14                     | 0.48              |
| 1:D:62:GLU:OE2   | 1:D:65:LYS:NZ    | 2.40                     | 0.48              |
| 1:D:369:TYR:HB3  | 1:D:372:GLU:HB2  | 1.96                     | 0.48              |
| 1:E:269:LYS:HG2  | 1:E:290:MET:HB3  | 1.95                     | 0.48              |
| 1:F:147:TYR:O    | 1:F:157:TRP:HB2  | 2.14                     | 0.48              |
| 1:G:70:VAL:HG11  | 1:G:238:MET:CE   | 2.44                     | 0.48              |
| 1:H:499:ARG:HB3  | 1:H:501:PHE:CD1  | 2.49                     | 0.48              |
| 1:B:80:HIS:N     | 1:B:80:HIS:CD2   | 2.79                     | 0.48              |
| 1:B:131:VAL:HG12 | 1:B:133:LEU:HD23 | 1.95                     | 0.48              |
| 1:B:328:GLN:HG2  | 1:B:331:GLU:CG   | 2.41                     | 0.48              |
| 1:B:375:ARG:O    | 1:B:378:HIS:HB3  | 2.13                     | 0.48              |
| 1:C:145:ASN:H    | 1:C:145:ASN:HD22 | 0.74                     | 0.48              |
| 1:E:111:LEU:HD23 | 1:E:111:LEU:C    | 2.39                     | 0.48              |
| 1:F:332:SER:C    | 1:F:334:ILE:H    | 2.22                     | 0.48              |
| 1:G:63:MET:HA    | 1:G:371:LEU:CD2  | 2.41                     | 0.48              |
| 1:G:237:ASP:OD1  | 1:G:460:ARG:HD2  | 2.14                     | 0.48              |
| 1:A:296:LEU:O    | 1:A:300:ILE:HG12 | 2.13                     | 0.48              |
| 1:A:501:PHE:N    | 1:A:501:PHE:CD1  | 2.79                     | 0.48              |
| 1:B:328:GLN:HA   | 1:B:331:GLU:HG3  | 1.94                     | 0.48              |
| 1:B:431:THR:HG21 | 1:B:434:GLY:HA2  | 1.96                     | 0.48              |
| 1:C:465:TYR:CB   | 1:C:468:ILE:HD12 | 2.40                     | 0.48              |
| 1:D:145:ASN:O    | 1:D:148:MET:HB3  | 2.14                     | 0.48              |
| 1:D:185:LYS:HD3  | 1:D:195:GLU:CB   | 2.42                     | 0.48              |
| 1:D:209:ASN:C    | 1:D:211:PRO:HD3  | 2.38                     | 0.48              |
| 1:E:428:ILE:CD1  | 1:E:508:VAL:HG11 | 2.44                     | 0.48              |
| 1:H:238:MET:HB2  | 1:H:265:LYS:O    | 2.14                     | 0.48              |
| 1:B:240:PHE:N    | 1:B:240:PHE:CD1  | 2.80                     | 0.47              |
| 1:C:272:ASN:HB2  | 1:C:299:GLU:HG2  | 1.96                     | 0.47              |
| 1:C:273:HIS:CB   | 1:C:277:ARG:HH11 | 2.12                     | 0.47              |
| 1:D:77:HIS:O     | 1:D:78:GLY:O     | 2.31                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:271:GLU:OE2  | 1:D:295:ASP:OD2  | 2.30                     | 0.47              |
| 1:D:457:GLN:O    | 1:D:461:GLN:HG3  | 2.14                     | 0.47              |
| 1:G:43:ASN:HB3   | 1:G:467:GLY:N    | 2.29                     | 0.47              |
| 1:H:480:ALA:O    | 1:H:483:GLU:HB2  | 2.14                     | 0.47              |
| 1:A:187:LYS:HA   | 1:A:192:LEU:CD1  | 2.44                     | 0.47              |
| 1:B:266:ILE:O    | 1:B:287:ASP:HB2  | 2.14                     | 0.47              |
| 1:B:337:PRO:HB3  | 1:B:369:TYR:CE2  | 2.50                     | 0.47              |
| 1:B:382:ARG:HH11 | 1:B:382:ARG:CG   | 2.27                     | 0.47              |
| 1:D:472:VAL:HG12 | 1:D:473:CYS:N    | 2.28                     | 0.47              |
| 1:E:43:ASN:HD21  | 1:E:448:PRO:HB3  | 1.79                     | 0.47              |
| 1:E:268:SER:HB2  | 1:E:289:ILE:HD13 | 1.95                     | 0.47              |
| 1:E:330:LEU:O    | 1:E:363:GLU:HG2  | 2.14                     | 0.47              |
| 1:G:62:GLU:CB    | 1:G:371:LEU:HD11 | 2.39                     | 0.47              |
| 1:G:106:PRO:C    | 1:G:107:VAL:HG23 | 2.39                     | 0.47              |
| 1:H:266:ILE:N    | 1:H:287:ASP:OD2  | 2.40                     | 0.47              |
| 1:A:326:ALA:O    | 1:A:327:THR:HB   | 2.13                     | 0.47              |
| 1:A:397:LEU:HD12 | 1:A:397:LEU:HA   | 1.60                     | 0.47              |
| 1:B:84:ALA:HB2   | 1:B:230:PHE:CZ   | 2.47                     | 0.47              |
| 1:C:514:TRP:HA   | 1:C:514:TRP:CE3  | 2.49                     | 0.47              |
| 1:E:293:ARG:HH22 | 1:E:346:ASP:CG   | 2.22                     | 0.47              |
| 1:F:111:LEU:HD23 | 1:F:111:LEU:C    | 2.39                     | 0.47              |
| 1:H:359:MET:C    | 1:H:360:LEU:HD12 | 2.39                     | 0.47              |
| 1:A:57:VAL:O     | 1:A:61:LYS:HG2   | 2.14                     | 0.47              |
| 1:C:185:LYS:CD   | 1:C:195:GLU:HB2  | 2.44                     | 0.47              |
| 1:D:158:LEU:HD23 | 1:D:163:ILE:HD13 | 1.96                     | 0.47              |
| 1:E:112:ASP:OD2  | 1:E:269:LYS:NZ   | 2.30                     | 0.47              |
| 1:G:145:ASN:O    | 1:G:148:MET:HB3  | 2.14                     | 0.47              |
| 1:H:256:ILE:HA   | 1:H:256:ILE:HD13 | 1.72                     | 0.47              |
| 1:A:118:ILE:HG23 | 1:A:160:TYR:HB2  | 1.95                     | 0.47              |
| 1:B:50:ILE:HG23  | 1:B:50:ILE:HD12  | 1.45                     | 0.47              |
| 1:G:69:ASN:HB3   | 1:G:463:HIS:HD2  | 1.73                     | 0.47              |
| 1:G:166:VAL:HG13 | 1:G:213:ALA:HB1  | 1.97                     | 0.47              |
| 1:G:338:ARG:NH2  | 1:G:341:ARG:NH1  | 2.62                     | 0.47              |
| 1:A:453:THR:HG21 | 1:A:459:ALA:HB2  | 1.97                     | 0.47              |
| 1:B:290:MET:HE3  | 1:B:326:ALA:HB2  | 1.97                     | 0.47              |
| 1:C:122:LEU:HD11 | 1:C:205:LYS:HE2  | 1.95                     | 0.47              |
| 1:E:334:ILE:HG23 | 1:E:367:GLY:HA2  | 1.96                     | 0.47              |
| 1:F:171:SER:O    | 1:F:184:VAL:HG23 | 2.14                     | 0.47              |
| 1:F:334:ILE:HG22 | 1:F:335:LYS:HG3  | 1.96                     | 0.47              |
| 1:F:449:ILE:HB   | 1:F:468:ILE:HA   | 1.97                     | 0.47              |
| 1:G:57:VAL:CG1   | 1:G:93:ALA:HB2   | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:166:VAL:O    | 1:H:166:VAL:HG12 | 2.15                     | 0.47              |
| 1:A:302:ALA:CB   | 1:C:376:MET:HE1  | 2.41                     | 0.47              |
| 1:B:252:GLU:O    | 1:B:256:ILE:HG12 | 2.14                     | 0.47              |
| 1:B:290:MET:CE   | 1:B:326:ALA:HB2  | 2.45                     | 0.47              |
| 1:C:322:PRO:HA   | 1:C:356:ASP:OD2  | 2.14                     | 0.47              |
| 1:D:135:LYS:HB2  | 1:D:135:LYS:HE3  | 1.77                     | 0.47              |
| 1:D:181:SER:OG   | 1:D:198:ASN:HB2  | 2.14                     | 0.47              |
| 1:D:424:ALA:HB2  | 1:D:509:ILE:HD12 | 1.97                     | 0.47              |
| 1:G:184:VAL:O    | 1:G:184:VAL:HG12 | 2.14                     | 0.47              |
| 1:H:279:PHE:CE1  | 1:H:289:ILE:CD1  | 2.98                     | 0.47              |
| 1:B:111:LEU:HB3  | 1:B:239:VAL:HG22 | 1.97                     | 0.47              |
| 1:B:342:ALA:HB1  | 1:D:346:ASP:CB   | 2.39                     | 0.47              |
| 1:C:294:GLY:N    | 1:C:327:THR:HG21 | 2.29                     | 0.47              |
| 1:D:122:LEU:HD13 | 1:D:122:LEU:HA   | 1.59                     | 0.47              |
| 1:E:342:ALA:HA   | 1:G:346:ASP:OD2  | 2.15                     | 0.47              |
| 1:E:354:GLY:O    | 1:E:444:ARG:NH2  | 2.48                     | 0.47              |
| 1:E:375:ARG:O    | 1:E:379:LEU:HD22 | 2.15                     | 0.47              |
| 1:F:123:ILE:O    | 1:F:123:ILE:HG22 | 2.14                     | 0.47              |
| 1:G:501:PHE:N    | 1:G:501:PHE:CD1  | 2.81                     | 0.47              |
| 1:A:186:GLN:CB   | 1:A:193:VAL:HB   | 2.45                     | 0.47              |
| 1:A:237:ASP:OD1  | 1:A:237:ASP:N    | 2.48                     | 0.47              |
| 1:B:12:ILE:O     | 1:B:13:GLN:O     | 2.33                     | 0.47              |
| 1:B:425:ALA:O    | 1:B:426:ALA:HB2  | 2.14                     | 0.47              |
| 1:C:182:LEU:HB2  | 1:C:194:THR:HB   | 1.96                     | 0.47              |
| 1:C:501:PHE:N    | 1:C:501:PHE:CD1  | 2.82                     | 0.47              |
| 1:D:183:GLN:O    | 1:D:194:THR:HA   | 2.15                     | 0.47              |
| 1:F:176:ASP:O    | 1:F:179:LEU:HB2  | 2.14                     | 0.47              |
| 1:H:157:TRP:O    | 1:H:158:LEU:HD13 | 2.15                     | 0.47              |
| 1:H:401:SER:O    | 1:H:403:HIS:N    | 2.48                     | 0.47              |
| 1:B:187:LYS:HG3  | 1:B:192:LEU:HD11 | 1.97                     | 0.46              |
| 1:B:306:PHE:O    | 1:B:310:LYS:HG2  | 2.14                     | 0.46              |
| 1:C:493:MET:HE1  | 1:C:529:VAL:HG13 | 1.97                     | 0.46              |
| 1:E:95:GLU:C     | 1:E:97:PHE:H     | 2.23                     | 0.46              |
| 1:E:328:GLN:HE21 | 1:G:341:ARG:N    | 2.02                     | 0.46              |
| 1:F:191:PHE:CD1  | 1:F:193:VAL:HG23 | 2.50                     | 0.46              |
| 1:G:425:ALA:O    | 1:G:426:ALA:HB2  | 2.16                     | 0.46              |
| 1:H:219:ALA:HB2  | 1:H:249:ASP:HA   | 1.97                     | 0.46              |
| 1:H:382:ARG:HH11 | 1:H:382:ARG:HB2  | 1.81                     | 0.46              |
| 1:B:131:VAL:HG12 | 1:B:133:LEU:CD2  | 2.45                     | 0.46              |
| 1:D:14:THR:HG22  | 1:D:37:ALA:O     | 2.15                     | 0.46              |
| 1:D:123:ILE:HD13 | 1:D:131:VAL:HB   | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:390:HIS:HD2  | 1:E:446:ARG:NH1  | 2.12                     | 0.46              |
| 1:F:240:PHE:HA   | 1:F:267:ILE:HB   | 1.97                     | 0.46              |
| 1:H:160:TYR:OH   | 1:H:166:VAL:HG21 | 2.15                     | 0.46              |
| 1:H:184:VAL:HA   | 1:H:194:THR:HG22 | 1.97                     | 0.46              |
| 1:A:413:MET:SD   | 1:B:421:LYS:HE2  | 2.55                     | 0.46              |
| 1:B:14:THR:HG22  | 1:B:15:GLN:HE21  | 1.79                     | 0.46              |
| 1:B:220:VAL:HG13 | 1:B:221:SER:N    | 2.30                     | 0.46              |
| 1:B:328:GLN:HG2  | 1:B:331:GLU:CD   | 2.41                     | 0.46              |
| 1:D:120:THR:HA   | 1:D:157:TRP:O    | 2.16                     | 0.46              |
| 1:D:156:LEU:CD2  | 1:D:157:TRP:H    | 2.29                     | 0.46              |
| 1:D:189:PRO:CD   | 1:D:191:PHE:CE1  | 2.99                     | 0.46              |
| 1:D:369:TYR:N    | 1:D:370:PRO:HD3  | 2.30                     | 0.46              |
| 1:D:453:THR:OG1  | 1:D:454:ARG:N    | 2.48                     | 0.46              |
| 1:E:340:THR:HG23 | 1:E:343:GLU:CD   | 2.40                     | 0.46              |
| 1:B:167:VAL:CG1  | 1:B:168:ASP:N    | 2.78                     | 0.46              |
| 1:E:257:LEU:HD23 | 1:E:261:GLY:HA3  | 1.97                     | 0.46              |
| 1:G:527:VAL:HG13 | 1:G:528:PRO:HD2  | 1.97                     | 0.46              |
| 1:H:333:MET:HA   | 1:H:336:LYS:O    | 2.14                     | 0.46              |
| 1:A:55:ARG:HG3   | 1:A:86:THR:CG2   | 2.45                     | 0.46              |
| 1:A:120:THR:HA   | 1:A:157:TRP:O    | 2.16                     | 0.46              |
| 1:A:244:ILE:HG22 | 1:A:282:ILE:HD13 | 1.97                     | 0.46              |
| 1:B:122:LEU:HA   | 1:B:122:LEU:HD12 | 1.51                     | 0.46              |
| 1:D:113:THR:HG23 | 1:D:115:GLY:H    | 1.81                     | 0.46              |
| 1:D:252:GLU:OE2  | 1:D:255:LYS:NZ   | 2.45                     | 0.46              |
| 1:D:276:VAL:O    | 1:D:279:PHE:HB2  | 2.15                     | 0.46              |
| 1:D:454:ARG:NH2  | 1:D:484:ASP:OD1  | 2.46                     | 0.46              |
| 1:F:63:MET:HG2   | 1:F:371:LEU:HD23 | 1.98                     | 0.46              |
| 1:F:140:LYS:HA   | 1:F:192:LEU:O    | 2.15                     | 0.46              |
| 1:F:224:ASP:O    | 1:F:228:LEU:HG   | 2.15                     | 0.46              |
| 1:F:465:TYR:N    | 1:F:465:TYR:CD1  | 2.84                     | 0.46              |
| 1:G:409:GLU:O    | 1:G:412:ALA:HB3  | 2.15                     | 0.46              |
| 1:H:63:MET:CG    | 1:H:371:LEU:HD23 | 2.38                     | 0.46              |
| 1:H:123:ILE:CD1  | 1:H:131:VAL:HG23 | 2.36                     | 0.46              |
| 1:H:363:GLU:OE1  | 1:H:363:GLU:N    | 2.39                     | 0.46              |
| 1:H:371:LEU:O    | 1:H:374:VAL:N    | 2.49                     | 0.46              |
| 1:B:141:ILE:HD13 | 1:B:141:ILE:O    | 2.16                     | 0.46              |
| 1:B:514:TRP:O    | 1:B:515:ARG:HG2  | 2.16                     | 0.46              |
| 1:E:47:ILE:CD1   | 1:E:324:ILE:HG23 | 2.46                     | 0.46              |
| 1:G:158:LEU:CD2  | 1:G:163:ILE:HD13 | 2.45                     | 0.46              |
| 1:H:209:ASN:C    | 1:H:210:LEU:HD13 | 2.40                     | 0.46              |
| 1:H:228:LEU:O    | 1:H:231:GLY:N    | 2.48                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:411:MET:O    | 1:H:415:SER:OG   | 2.33                     | 0.46              |
| 1:H:477:VAL:HG12 | 1:H:478:GLN:N    | 2.30                     | 0.46              |
| 1:A:267:ILE:HG21 | 1:A:324:ILE:HD12 | 1.98                     | 0.46              |
| 1:C:311:MET:HG2  | 1:C:315:ARG:HD3  | 1.96                     | 0.46              |
| 1:C:487:LEU:HD23 | 1:C:488:ARG:N    | 2.31                     | 0.46              |
| 1:D:43:ASN:ND2   | 1:D:467:GLY:HA2  | 2.31                     | 0.46              |
| 1:D:148:MET:HB3  | 1:D:148:MET:HE2  | 1.90                     | 0.46              |
| 1:D:355:ALA:O    | 1:D:466:ARG:NH1  | 2.49                     | 0.46              |
| 1:D:436:SER:HB3  | 1:D:521:THR:HG23 | 1.96                     | 0.46              |
| 1:E:63:MET:HG3   | 1:E:371:LEU:HD21 | 1.98                     | 0.46              |
| 1:G:176:ASP:O    | 1:G:177:ASP:HB2  | 2.15                     | 0.46              |
| 1:G:333:MET:HE2  | 1:G:373:ALA:N    | 2.30                     | 0.46              |
| 1:H:223:LYS:O    | 1:H:226:GLN:HB2  | 2.15                     | 0.46              |
| 1:H:491:LEU:O    | 1:H:494:ASN:N    | 2.49                     | 0.46              |
| 1:A:56:SER:O     | 1:A:60:LEU:HD22  | 2.16                     | 0.46              |
| 1:B:43:ASN:CG    | 1:B:467:GLY:HA2  | 2.40                     | 0.46              |
| 1:B:182:LEU:HD13 | 1:B:194:THR:HG21 | 1.97                     | 0.46              |
| 1:C:515:ARG:HB3  | 1:C:516:PRO:CD   | 2.40                     | 0.46              |
| 1:D:189:PRO:HD3  | 1:D:191:PHE:CE1  | 2.50                     | 0.46              |
| 1:D:368:ASP:C    | 1:D:370:PRO:HD3  | 2.41                     | 0.46              |
| 1:D:503:LYS:O    | 1:D:529:VAL:HB   | 2.16                     | 0.46              |
| 1:F:328:GLN:NE2  | 1:H:340:THR:CA   | 2.79                     | 0.46              |
| 1:F:425:ALA:HB1  | 1:F:502:PHE:HB3  | 1.98                     | 0.46              |
| 1:G:330:LEU:HD12 | 1:G:330:LEU:HA   | 1.75                     | 0.46              |
| 1:G:333:MET:CE   | 1:G:373:ALA:HA   | 2.45                     | 0.46              |
| 1:H:113:THR:HG23 | 1:H:114:LYS:N    | 2.31                     | 0.46              |
| 1:H:300:ILE:HB   | 1:H:301:PRO:HD2  | 1.97                     | 0.46              |
| 1:H:327:THR:HG22 | 1:H:328:GLN:HG3  | 1.97                     | 0.46              |
| 1:A:160:TYR:CE1  | 1:A:217:LEU:CD1  | 2.99                     | 0.46              |
| 1:B:317:ASN:N    | 1:B:317:ASN:HD22 | 2.11                     | 0.46              |
| 1:E:221:SER:H    | 1:E:224:ASP:HB2  | 1.81                     | 0.46              |
| 1:F:501:PHE:N    | 1:F:501:PHE:CD1  | 2.82                     | 0.46              |
| 1:G:33:ASP:HB3   | 1:G:36:SER:HB2   | 1.98                     | 0.46              |
| 1:A:118:ILE:HB   | 1:A:208:VAL:HB   | 1.98                     | 0.46              |
| 1:B:392:LYS:O    | 1:B:396:GLU:HG3  | 2.15                     | 0.46              |
| 1:B:416:VAL:HG21 | 1:B:443:TYR:HB2  | 1.98                     | 0.46              |
| 1:B:512:THR:CA   | 1:B:521:THR:HG22 | 2.46                     | 0.46              |
| 1:B:512:THR:C    | 1:B:521:THR:HG22 | 2.40                     | 0.46              |
| 1:C:156:LEU:HD23 | 1:C:156:LEU:HA   | 1.71                     | 0.46              |
| 1:E:105:ARG:HD3  | 1:E:499:ARG:NH1  | 2.31                     | 0.46              |
| 1:E:269:LYS:HG2  | 1:E:290:MET:SD   | 2.56                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:240:PHE:CD2  | 1:F:290:MET:CE   | 2.99                     | 0.46              |
| 1:F:256:ILE:HD13 | 1:F:256:ILE:N    | 2.31                     | 0.46              |
| 1:F:462:ALA:HB1  | 1:F:468:ILE:HG21 | 1.97                     | 0.46              |
| 1:G:50:ILE:HB    | 1:G:73:MET:CE    | 2.46                     | 0.46              |
| 1:G:311:MET:HG2  | 1:G:315:ARG:HD3  | 1.98                     | 0.46              |
| 1:G:416:VAL:HG13 | 1:G:445:PRO:CB   | 2.43                     | 0.46              |
| 1:H:51:GLY:O     | 1:H:55:ARG:HB2   | 2.16                     | 0.46              |
| 1:H:158:LEU:HD12 | 1:H:158:LEU:HA   | 1.62                     | 0.46              |
| 1:A:454:ARG:HG3  | 1:A:473:CYS:HB3  | 1.99                     | 0.45              |
| 1:D:162:ASN:O    | 1:D:165:LYS:HB2  | 2.16                     | 0.45              |
| 1:D:450:ILE:HG21 | 1:D:492:ALA:HB1  | 1.98                     | 0.45              |
| 1:D:475:ASP:HB3  | 1:D:476:PRO:HD2  | 1.97                     | 0.45              |
| 1:D:477:VAL:HG12 | 1:D:478:GLN:O    | 2.15                     | 0.45              |
| 1:F:139:LEU:HD23 | 1:F:141:ILE:HG22 | 1.98                     | 0.45              |
| 1:F:167:VAL:HG13 | 1:F:171:SER:HB2  | 1.98                     | 0.45              |
| 1:F:330:LEU:HD12 | 1:F:343:GLU:HB2  | 1.99                     | 0.45              |
| 1:G:84:ALA:HB2   | 1:G:230:PHE:HZ   | 1.81                     | 0.45              |
| 1:H:170:GLY:HA2  | 1:H:183:GLN:HE21 | 1.79                     | 0.45              |
| 1:A:340:THR:CA   | 1:C:328:GLN:NE2  | 2.79                     | 0.45              |
| 1:G:156:LEU:CD2  | 1:G:157:TRP:N    | 2.79                     | 0.45              |
| 1:G:352:LEU:HD12 | 1:G:352:LEU:HA   | 1.84                     | 0.45              |
| 1:G:439:GLN:CA   | 1:G:439:GLN:NE2  | 2.80                     | 0.45              |
| 1:A:525:ARG:HD3  | 1:B:514:TRP:CE3  | 2.52                     | 0.45              |
| 1:B:189:PRO:HD2  | 1:B:191:PHE:CE1  | 2.51                     | 0.45              |
| 1:B:340:THR:OG1  | 1:B:343:GLU:HG3  | 2.16                     | 0.45              |
| 1:B:515:ARG:HB3  | 1:B:516:PRO:CD   | 2.46                     | 0.45              |
| 1:D:125:GLY:HA2  | 1:D:149:GLU:O    | 2.15                     | 0.45              |
| 1:D:247:ALA:C    | 1:D:250:VAL:HG23 | 2.42                     | 0.45              |
| 1:E:282:ILE:O    | 1:E:286:SER:OG   | 2.29                     | 0.45              |
| 1:E:388:MET:HE3  | 1:E:466:ARG:NH2  | 2.30                     | 0.45              |
| 1:E:428:ILE:HD13 | 1:E:508:VAL:HG11 | 1.98                     | 0.45              |
| 1:F:247:ALA:HB2  | 1:F:281:GLU:CG   | 2.38                     | 0.45              |
| 1:F:488:ARG:O    | 1:F:491:LEU:HB3  | 2.16                     | 0.45              |
| 1:G:174:TYR:CD2  | 1:G:298:ILE:CG2  | 2.99                     | 0.45              |
| 1:G:333:MET:O    | 1:G:336:LYS:O    | 2.34                     | 0.45              |
| 1:H:172:LYS:NZ   | 1:H:197:GLU:OE2  | 2.46                     | 0.45              |
| 1:H:431:THR:CG2  | 1:H:434:GLY:HA2  | 2.46                     | 0.45              |
| 1:H:441:ALA:O    | 1:H:444:ARG:N    | 2.37                     | 0.45              |
| 1:A:60:LEU:HD23  | 1:A:89:ASN:C     | 2.42                     | 0.45              |
| 1:A:281:GLU:CG   | 1:A:282:ILE:N    | 2.79                     | 0.45              |
| 1:B:185:LYS:HA   | 1:B:185:LYS:HD3  | 1.58                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:57:VAL:O     | 1:D:61:LYS:HG3   | 2.17                     | 0.45              |
| 1:D:493:MET:CE   | 1:D:529:VAL:HG22 | 2.43                     | 0.45              |
| 1:F:147:TYR:CD2  | 1:F:155:ILE:HG21 | 2.52                     | 0.45              |
| 1:H:102:ILE:HG12 | 1:H:103:LEU:HD12 | 1.98                     | 0.45              |
| 1:H:328:GLN:CG   | 1:H:331:GLU:HG3  | 2.44                     | 0.45              |
| 1:H:464:LEU:HD12 | 1:H:464:LEU:HA   | 1.79                     | 0.45              |
| 1:H:493:MET:HE2  | 1:H:530:PRO:CD   | 2.46                     | 0.45              |
| 1:H:507:VAL:CG1  | 1:H:508:VAL:N    | 2.79                     | 0.45              |
| 1:A:460:ARG:NH2  | 5:A:6091:HOH:O   | 2.49                     | 0.45              |
| 1:B:515:ARG:CB   | 1:B:516:PRO:HD2  | 2.44                     | 0.45              |
| 1:C:318:ARG:HD2  | 5:C:6031:HOH:O   | 2.16                     | 0.45              |
| 1:D:192:LEU:HD13 | 1:D:192:LEU:HA   | 1.74                     | 0.45              |
| 1:F:139:LEU:HD21 | 1:F:156:LEU:HB2  | 1.98                     | 0.45              |
| 1:H:106:PRO:C    | 1:H:107:VAL:HG23 | 2.42                     | 0.45              |
| 1:H:477:VAL:CG1  | 1:H:478:GLN:N    | 2.80                     | 0.45              |
| 1:A:22:ALA:HA    | 1:A:31:ARG:NH1   | 2.32                     | 0.45              |
| 1:B:64:ILE:HD12  | 1:B:94:THR:HA    | 1.99                     | 0.45              |
| 1:C:137:ALA:O    | 1:C:196:VAL:N    | 2.37                     | 0.45              |
| 1:D:186:GLN:O    | 1:D:186:GLN:HG2  | 2.15                     | 0.45              |
| 1:E:379:LEU:N    | 1:E:379:LEU:CD1  | 2.79                     | 0.45              |
| 1:E:407:LEU:N    | 1:E:407:LEU:CD1  | 2.80                     | 0.45              |
| 1:F:220:VAL:HG22 | 1:F:224:ASP:CB   | 2.46                     | 0.45              |
| 1:F:369:TYR:N    | 1:F:370:PRO:CD   | 2.80                     | 0.45              |
| 1:G:339:PRO:CD   | 1:G:376:MET:HE2  | 2.47                     | 0.45              |
| 1:G:407:LEU:N    | 1:G:407:LEU:CD1  | 2.79                     | 0.45              |
| 1:A:47:ILE:CG2   | 1:A:359:MET:HG3  | 2.47                     | 0.45              |
| 1:A:325:CYS:SG   | 1:A:329:MET:HE3  | 2.57                     | 0.45              |
| 1:A:520:PHE:HD1  | 1:A:521:THR:O    | 2.00                     | 0.45              |
| 1:B:269:LYS:HD2  | 1:B:290:MET:SD   | 2.57                     | 0.45              |
| 1:B:524:MET:HE3  | 1:B:524:MET:HB3  | 1.45                     | 0.45              |
| 1:C:487:LEU:HD23 | 1:C:487:LEU:C    | 2.42                     | 0.45              |
| 1:D:289:ILE:CG2  | 1:D:290:MET:N    | 2.80                     | 0.45              |
| 1:E:88:LYS:O     | 1:E:88:LYS:HG2   | 2.11                     | 0.45              |
| 1:F:202:LEU:CD2  | 1:F:203:GLY:N    | 2.80                     | 0.45              |
| 1:G:256:ILE:HD13 | 1:G:256:ILE:N    | 2.31                     | 0.45              |
| 1:G:351:VAL:O    | 1:G:351:VAL:HG12 | 2.17                     | 0.45              |
| 1:G:410:ALA:CB   | 1:H:422:CYS:HB3  | 2.46                     | 0.45              |
| 1:H:141:ILE:O    | 1:H:191:PHE:HA   | 2.16                     | 0.45              |
| 1:H:209:ASN:C    | 1:H:211:PRO:HD3  | 2.42                     | 0.45              |
| 1:H:430:LEU:HD21 | 1:H:488:ARG:HB2  | 1.99                     | 0.45              |
| 1:A:399:ARG:NH1  | 1:B:23:ASP:HB3   | 2.31                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:421:LYS:HE2  | 1:B:413:MET:SD   | 2.57                     | 0.45              |
| 1:A:525:ARG:HB3  | 1:A:527:VAL:HG23 | 1.98                     | 0.45              |
| 1:B:480:ALA:HB3  | 1:B:483:GLU:CG   | 2.44                     | 0.45              |
| 1:C:62:GLU:O     | 1:C:65:LYS:HB2   | 2.16                     | 0.45              |
| 1:C:407:LEU:N    | 1:C:407:LEU:CD1  | 2.80                     | 0.45              |
| 1:D:123:ILE:HG22 | 1:D:123:ILE:O    | 2.15                     | 0.45              |
| 1:D:154:ASN:CB   | 1:D:155:ILE:HD12 | 2.41                     | 0.45              |
| 1:E:511:LEU:C    | 1:E:512:THR:HG23 | 2.42                     | 0.45              |
| 1:F:48:CYS:SG    | 1:F:68:MET:HG3   | 2.57                     | 0.45              |
| 1:F:57:VAL:HG12  | 1:F:61:LYS:HE2   | 1.98                     | 0.45              |
| 1:F:447:ALA:HB1  | 1:F:448:PRO:HD2  | 1.99                     | 0.45              |
| 1:G:55:ARG:CZ    | 1:G:82:TYR:CE1   | 2.99                     | 0.45              |
| 1:H:202:LEU:CD2  | 1:H:203:GLY:H    | 2.30                     | 0.45              |
| 1:H:381:ALA:O    | 1:H:385:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:462:ALA:HB3  | 1:A:470:PRO:HG3  | 1.99                     | 0.45              |
| 1:B:247:ALA:HA   | 1:B:250:VAL:HG23 | 1.99                     | 0.45              |
| 1:B:430:LEU:N    | 1:B:430:LEU:CD1  | 2.80                     | 0.45              |
| 1:C:303:GLU:H    | 1:C:303:GLU:HG3  | 1.24                     | 0.45              |
| 1:D:47:ILE:HD13  | 1:D:324:ILE:HD13 | 1.99                     | 0.45              |
| 1:F:133:LEU:HD11 | 1:F:202:LEU:HD12 | 1.98                     | 0.45              |
| 1:F:296:LEU:O    | 1:F:300:ILE:HG12 | 2.17                     | 0.45              |
| 1:F:355:ALA:O    | 1:F:466:ARG:NH1  | 2.46                     | 0.45              |
| 1:H:100:ASP:OD1  | 1:H:102:ILE:HG23 | 2.17                     | 0.45              |
| 1:H:141:ILE:HA   | 1:H:156:LEU:O    | 2.17                     | 0.45              |
| 1:H:491:LEU:HA   | 1:H:491:LEU:HD12 | 1.54                     | 0.45              |
| 1:A:162:ASN:H    | 1:A:162:ASN:ND2  | 2.14                     | 0.45              |
| 1:B:138:THR:CG2  | 1:B:139:LEU:N    | 2.80                     | 0.45              |
| 1:B:376:MET:O    | 1:B:380:ILE:HG13 | 2.17                     | 0.45              |
| 1:C:57:VAL:O     | 1:C:60:LEU:HB2   | 2.16                     | 0.45              |
| 1:C:145:ASN:O    | 1:C:148:MET:HE3  | 2.17                     | 0.45              |
| 1:C:244:ILE:HG21 | 1:C:268:SER:OG   | 2.17                     | 0.45              |
| 1:C:262:LYS:H    | 1:C:262:LYS:HG3  | 1.46                     | 0.45              |
| 1:C:330:LEU:HD12 | 1:C:330:LEU:HA   | 1.66                     | 0.45              |
| 1:C:493:MET:HE2  | 1:C:493:MET:HB3  | 1.54                     | 0.45              |
| 1:D:123:ILE:HD11 | 1:D:131:VAL:HG12 | 1.99                     | 0.45              |
| 1:D:371:LEU:O    | 1:D:375:ARG:HD2  | 2.17                     | 0.45              |
| 1:E:422:CYS:O    | 1:E:423:LEU:HB2  | 2.17                     | 0.45              |
| 1:F:131:VAL:HG11 | 1:F:153:GLU:HA   | 1.99                     | 0.45              |
| 1:F:183:GLN:HG3  | 1:F:184:VAL:N    | 2.31                     | 0.45              |
| 1:F:322:PRO:HA   | 1:F:356:ASP:OD2  | 2.17                     | 0.45              |
| 1:F:358:ILE:HD13 | 1:F:358:ILE:HG21 | 1.74                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:423:LEU:HD12 | 1:F:423:LEU:HA   | 1.53                     | 0.45              |
| 1:G:46:ILE:HG23  | 1:G:377:GLN:HE22 | 1.78                     | 0.45              |
| 1:G:327:THR:CG2  | 1:G:328:GLN:HG3  | 2.47                     | 0.45              |
| 1:H:407:LEU:N    | 1:H:407:LEU:CD1  | 2.80                     | 0.45              |
| 1:H:465:TYR:N    | 1:H:465:TYR:CD1  | 2.85                     | 0.45              |
| 1:A:368:ASP:C    | 1:A:370:PRO:HD3  | 2.42                     | 0.44              |
| 1:B:415:SER:O    | 1:B:419:SER:HB3  | 2.17                     | 0.44              |
| 1:F:385:GLU:HA   | 1:F:388:MET:HE2  | 1.99                     | 0.44              |
| 1:G:283:LEU:HD22 | 1:G:321:LYS:HD2  | 1.98                     | 0.44              |
| 1:H:160:TYR:CD1  | 1:H:217:LEU:HD21 | 2.53                     | 0.44              |
| 1:H:314:GLY:O    | 1:H:318:ARG:HB2  | 2.17                     | 0.44              |
| 1:A:73:MET:HE3   | 1:A:86:THR:HB    | 1.99                     | 0.44              |
| 1:B:491:LEU:O    | 1:B:495:VAL:HG23 | 2.16                     | 0.44              |
| 1:C:173:VAL:HB   | 1:C:182:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:514:TRP:C    | 1:C:515:ARG:HG2  | 2.42                     | 0.44              |
| 1:D:208:VAL:CG1  | 1:D:209:ASN:N    | 2.79                     | 0.44              |
| 1:D:237:ASP:OD1  | 1:D:460:ARG:NH1  | 2.47                     | 0.44              |
| 1:D:279:PHE:CE1  | 1:D:312:ILE:HD13 | 2.52                     | 0.44              |
| 1:D:425:ALA:O    | 1:D:426:ALA:HB2  | 2.17                     | 0.44              |
| 1:F:329:MET:HE2  | 1:F:329:MET:HB3  | 1.85                     | 0.44              |
| 1:G:238:MET:O    | 1:G:238:MET:HG2  | 2.14                     | 0.44              |
| 1:G:300:ILE:HB   | 1:G:301:PRO:CD   | 2.47                     | 0.44              |
| 1:G:408:MET:O    | 1:G:408:MET:HG3  | 2.17                     | 0.44              |
| 1:H:131:VAL:O    | 1:H:202:LEU:N    | 2.48                     | 0.44              |
| 1:H:192:LEU:HD12 | 1:H:192:LEU:HA   | 1.82                     | 0.44              |
| 1:H:493:MET:HG2  | 1:H:530:PRO:HD2  | 1.97                     | 0.44              |
| 1:H:514:TRP:HA   | 1:H:514:TRP:HE3  | 1.82                     | 0.44              |
| 1:A:310:LYS:HD3  | 1:A:353:ASP:OD2  | 2.17                     | 0.44              |
| 1:A:508:VAL:CG1  | 1:A:509:ILE:N    | 2.80                     | 0.44              |
| 1:B:148:MET:HE3  | 1:B:148:MET:HB3  | 1.46                     | 0.44              |
| 1:C:221:SER:O    | 1:C:225:ILE:HG13 | 2.18                     | 0.44              |
| 1:C:299:GLU:OE1  | 5:C:6192:HOH:O   | 2.21                     | 0.44              |
| 1:D:134:LYS:O    | 1:D:196:VAL:HG11 | 2.17                     | 0.44              |
| 1:E:26:LEU:HD12  | 1:E:26:LEU:HA    | 1.78                     | 0.44              |
| 1:F:50:ILE:HD12  | 1:F:50:ILE:HA    | 1.65                     | 0.44              |
| 1:F:507:VAL:HG13 | 1:F:527:VAL:O    | 2.17                     | 0.44              |
| 1:G:488:ARG:O    | 1:G:491:LEU:HB3  | 2.16                     | 0.44              |
| 1:H:232:VAL:HG11 | 1:H:260:LYS:HB3  | 2.00                     | 0.44              |
| 1:H:397:LEU:O    | 1:H:400:SER:OG   | 2.35                     | 0.44              |
| 1:H:453:THR:HG21 | 1:H:459:ALA:HB2  | 1.99                     | 0.44              |
| 1:A:152:ASP:OD1  | 1:A:154:ASN:N    | 2.46                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:LEU:HA   | 1:A:202:LEU:HD23 | 1.76                     | 0.44              |
| 1:A:274:GLU:OE2  | 1:A:278:ARG:NH1  | 2.42                     | 0.44              |
| 1:A:338:ARG:HA   | 1:A:339:PRO:HD3  | 1.85                     | 0.44              |
| 1:A:399:ARG:HH12 | 1:B:23:ASP:HB3   | 1.82                     | 0.44              |
| 1:B:120:THR:CG2  | 1:B:156:LEU:HD11 | 2.47                     | 0.44              |
| 1:B:436:SER:HB3  | 1:B:521:THR:OG1  | 2.18                     | 0.44              |
| 1:C:289:ILE:CG2  | 1:C:290:MET:N    | 2.79                     | 0.44              |
| 1:D:160:TYR:O    | 1:D:163:ILE:HG22 | 2.18                     | 0.44              |
| 1:D:324:ILE:HD13 | 1:D:324:ILE:HG21 | 1.58                     | 0.44              |
| 1:D:388:MET:SD   | 1:D:466:ARG:NH2  | 2.90                     | 0.44              |
| 1:F:272:ASN:O    | 1:F:276:VAL:HG23 | 2.17                     | 0.44              |
| 1:F:507:VAL:CG1  | 1:F:508:VAL:N    | 2.80                     | 0.44              |
| 1:F:527:VAL:HA   | 1:F:528:PRO:HD3  | 1.74                     | 0.44              |
| 1:G:17:LEU:N     | 1:G:17:LEU:CD2   | 2.79                     | 0.44              |
| 1:G:174:TYR:CD2  | 1:G:178:GLY:HA2  | 2.52                     | 0.44              |
| 1:G:210:LEU:HA   | 1:G:210:LEU:HD12 | 1.76                     | 0.44              |
| 1:G:477:VAL:CG1  | 1:G:478:GLN:N    | 2.79                     | 0.44              |
| 1:B:158:LEU:HD22 | 1:B:158:LEU:N    | 2.31                     | 0.44              |
| 1:B:499:ARG:HD3  | 1:B:499:ARG:HA   | 1.85                     | 0.44              |
| 1:E:415:SER:CA   | 1:E:524:MET:HE2  | 2.48                     | 0.44              |
| 1:G:232:VAL:HG12 | 1:G:260:LYS:HD2  | 1.99                     | 0.44              |
| 1:H:19:ALA:CA    | 1:H:31:ARG:HB3   | 2.46                     | 0.44              |
| 1:H:133:LEU:N    | 1:H:133:LEU:CD2  | 2.80                     | 0.44              |
| 1:H:428:ILE:HD12 | 1:H:508:VAL:CG1  | 2.47                     | 0.44              |
| 1:A:222:GLU:HA   | 1:A:225:ILE:HG13 | 1.99                     | 0.44              |
| 1:A:245:ARG:O    | 1:A:278:ARG:HD3  | 2.17                     | 0.44              |
| 1:A:371:LEU:O    | 1:A:375:ARG:HD2  | 2.17                     | 0.44              |
| 1:C:422:CYS:O    | 1:C:423:LEU:HB2  | 2.16                     | 0.44              |
| 1:C:423:LEU:HD22 | 1:D:405:THR:HG21 | 2.00                     | 0.44              |
| 1:D:50:ILE:HB    | 1:D:73:MET:HE3   | 1.99                     | 0.44              |
| 1:D:105:ARG:CZ   | 1:D:499:ARG:NH2  | 2.81                     | 0.44              |
| 1:D:231:GLY:O    | 1:D:236:VAL:HG22 | 2.18                     | 0.44              |
| 1:F:155:ILE:CG2  | 1:F:156:LEU:N    | 2.80                     | 0.44              |
| 1:F:156:LEU:HD23 | 1:F:156:LEU:HA   | 1.76                     | 0.44              |
| 1:G:156:LEU:HD23 | 1:G:157:TRP:N    | 2.32                     | 0.44              |
| 1:G:524:MET:HE3  | 1:G:524:MET:HB3  | 1.77                     | 0.44              |
| 1:H:246:LYS:H    | 1:H:246:LYS:HG2  | 1.63                     | 0.44              |
| 1:A:416:VAL:HG21 | 1:A:443:TYR:HB2  | 2.00                     | 0.44              |
| 1:B:267:ILE:N    | 1:B:267:ILE:CD1  | 2.80                     | 0.44              |
| 1:C:43:ASN:CG    | 1:C:467:GLY:HA2  | 2.43                     | 0.44              |
| 1:C:55:ARG:CZ    | 1:C:82:TYR:CE1   | 3.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:354:GLY:CA   | 1:C:466:ARG:HH12 | 2.31                     | 0.44              |
| 1:D:210:LEU:HD13 | 1:D:210:LEU:N    | 2.33                     | 0.44              |
| 1:F:120:THR:O    | 1:F:205:LYS:HA   | 2.17                     | 0.44              |
| 1:F:243:PHE:N    | 1:F:271:GLU:OE1  | 2.37                     | 0.44              |
| 1:F:336:LYS:HB3  | 1:F:337:PRO:CD   | 2.46                     | 0.44              |
| 1:F:430:LEU:N    | 1:F:430:LEU:CD1  | 2.80                     | 0.44              |
| 1:H:17:LEU:HA    | 1:H:17:LEU:HD22  | 1.74                     | 0.44              |
| 1:B:73:MET:CE    | 1:B:86:THR:HG21  | 2.48                     | 0.44              |
| 1:B:133:LEU:HD11 | 1:B:139:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:44:THR:OG1   | 1:C:385:GLU:OE2  | 2.34                     | 0.44              |
| 1:C:145:ASN:ND2  | 1:C:145:ASN:N    | 2.30                     | 0.44              |
| 1:C:454:ARG:NE   | 1:C:475:ASP:O    | 2.41                     | 0.44              |
| 1:E:334:ILE:CD1  | 1:E:363:GLU:N    | 2.79                     | 0.44              |
| 1:F:69:ASN:C     | 1:F:70:VAL:HG23  | 2.42                     | 0.44              |
| 1:F:315:ARG:CG   | 1:H:30:CYS:HB3   | 2.47                     | 0.44              |
| 1:F:379:LEU:HD12 | 1:F:379:LEU:HA   | 1.76                     | 0.44              |
| 1:G:253:VAL:O    | 1:G:257:LEU:HD13 | 2.18                     | 0.44              |
| 1:H:89:ASN:C     | 1:H:92:THR:HB    | 2.43                     | 0.44              |
| 1:H:279:PHE:CE1  | 1:H:289:ILE:HD13 | 2.53                     | 0.44              |
| 1:H:292:ALA:HB1  | 4:H:532:PEQ:C2   | 2.47                     | 0.44              |
| 1:H:508:VAL:O    | 1:H:509:ILE:HD13 | 2.18                     | 0.44              |
| 1:A:246:LYS:HE2  | 1:A:249:ASP:OD1  | 2.18                     | 0.44              |
| 1:C:47:ILE:O     | 1:C:359:MET:HG3  | 2.17                     | 0.44              |
| 1:D:122:LEU:HD12 | 1:D:123:ILE:N    | 2.29                     | 0.44              |
| 1:D:294:GLY:CA   | 1:D:327:THR:HG21 | 2.47                     | 0.44              |
| 1:A:225:ILE:O    | 1:A:229:LYS:HG3  | 2.18                     | 0.43              |
| 1:B:64:ILE:HD13  | 1:B:107:VAL:HG21 | 1.99                     | 0.43              |
| 1:B:435:ARG:O    | 1:B:438:HIS:HB2  | 2.18                     | 0.43              |
| 1:B:501:PHE:N    | 1:B:501:PHE:CD1  | 2.85                     | 0.43              |
| 1:C:354:GLY:HA2  | 1:C:466:ARG:HH12 | 1.83                     | 0.43              |
| 1:D:123:ILE:H    | 1:D:204:SER:HG   | 1.61                     | 0.43              |
| 1:D:493:MET:HG2  | 1:D:530:PRO:HD2  | 1.99                     | 0.43              |
| 1:E:98:ALA:HA    | 1:E:104:TYR:CD1  | 2.53                     | 0.43              |
| 1:E:105:ARG:CD   | 1:E:499:ARG:NH1  | 2.81                     | 0.43              |
| 1:E:245:ARG:C    | 1:E:282:ILE:HD11 | 2.42                     | 0.43              |
| 1:E:371:LEU:O    | 1:E:375:ARG:HD2  | 2.18                     | 0.43              |
| 1:F:141:ILE:H    | 1:F:141:ILE:HD13 | 1.83                     | 0.43              |
| 1:F:328:GLN:NE2  | 1:H:340:THR:HB   | 2.33                     | 0.43              |
| 1:G:174:TYR:CE2  | 1:G:298:ILE:HG23 | 2.53                     | 0.43              |
| 1:G:226:GLN:H    | 1:G:226:GLN:HG3  | 1.63                     | 0.43              |
| 1:G:520:PHE:CE1  | 1:G:522:ASN:HB3  | 2.53                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:42:ARG:HG2   | 1:H:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:H:202:LEU:CD2  | 1:H:203:GLY:N    | 2.79                     | 0.43              |
| 1:A:183:GLN:O    | 1:A:194:THR:HA   | 2.18                     | 0.43              |
| 1:A:528:PRO:O    | 1:A:530:PRO:HD3  | 2.18                     | 0.43              |
| 1:B:160:TYR:OH   | 1:B:216:ASP:HB2  | 2.18                     | 0.43              |
| 1:C:232:VAL:O    | 1:C:232:VAL:HG12 | 2.17                     | 0.43              |
| 1:C:296:LEU:HD12 | 1:C:296:LEU:C    | 2.42                     | 0.43              |
| 1:E:240:PHE:CD2  | 1:E:290:MET:CE   | 2.99                     | 0.43              |
| 1:E:262:LYS:HE2  | 1:E:262:LYS:HB2  | 1.63                     | 0.43              |
| 1:F:111:LEU:HD23 | 1:F:112:ASP:N    | 2.33                     | 0.43              |
| 1:F:139:LEU:HD23 | 1:F:141:ILE:CG2  | 2.48                     | 0.43              |
| 1:G:174:TYR:CD2  | 1:G:298:ILE:HG23 | 2.53                     | 0.43              |
| 1:H:238:MET:HA   | 1:H:264:ILE:HG22 | 2.01                     | 0.43              |
| 1:H:268:SER:HB2  | 1:H:286:SER:CB   | 2.48                     | 0.43              |
| 1:B:375:ARG:O    | 1:B:379:LEU:HD13 | 2.19                     | 0.43              |
| 1:B:503:LYS:O    | 1:B:529:VAL:HG11 | 2.18                     | 0.43              |
| 1:C:338:ARG:HD3  | 5:C:6018:HOH:O   | 2.17                     | 0.43              |
| 1:C:408:MET:HE2  | 1:C:436:SER:CA   | 2.48                     | 0.43              |
| 1:D:131:VAL:CG1  | 1:D:202:LEU:HB3  | 2.48                     | 0.43              |
| 1:F:463:HIS:CE1  | 1:F:470:PRO:HG2  | 2.53                     | 0.43              |
| 1:G:141:ILE:CG2  | 1:G:158:LEU:HD22 | 2.49                     | 0.43              |
| 1:H:440:VAL:HG12 | 1:H:449:ILE:HD13 | 1.99                     | 0.43              |
| 1:B:202:LEU:HA   | 1:B:202:LEU:HD23 | 1.77                     | 0.43              |
| 1:B:225:ILE:O    | 1:B:229:LYS:HG3  | 2.18                     | 0.43              |
| 1:B:484:ASP:O    | 1:B:487:LEU:HB3  | 2.17                     | 0.43              |
| 1:C:141:ILE:O    | 1:C:191:PHE:HA   | 2.18                     | 0.43              |
| 1:D:189:PRO:HD2  | 1:D:191:PHE:HD1  | 1.84                     | 0.43              |
| 1:E:401:SER:O    | 1:F:421:LYS:NZ   | 2.51                     | 0.43              |
| 1:F:50:ILE:N     | 1:F:50:ILE:CD1   | 2.79                     | 0.43              |
| 1:F:145:ASN:HB3  | 1:F:148:MET:HE2  | 1.98                     | 0.43              |
| 1:F:328:GLN:O    | 1:H:342:ALA:HB2  | 2.18                     | 0.43              |
| 1:G:57:VAL:O     | 1:G:57:VAL:HG12  | 2.17                     | 0.43              |
| 1:G:334:ILE:HG12 | 1:G:363:GLU:HA   | 1.99                     | 0.43              |
| 1:A:330:LEU:HD12 | 1:A:330:LEU:HA   | 1.77                     | 0.43              |
| 1:A:340:THR:CB   | 1:C:328:GLN:NE2  | 2.81                     | 0.43              |
| 1:B:496:GLY:HA3  | 1:B:502:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:123:ILE:HG23 | 1:C:131:VAL:CG2  | 2.48                     | 0.43              |
| 1:D:190:ASP:OD1  | 1:D:190:ASP:N    | 2.51                     | 0.43              |
| 1:E:60:LEU:O     | 1:E:63:MET:N     | 2.51                     | 0.43              |
| 1:E:447:ALA:HB1  | 1:E:448:PRO:HD2  | 1.99                     | 0.43              |
| 1:E:525:ARG:HB3  | 1:F:522:ASN:O    | 2.17                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:44:THR:CG2   | 1:F:358:ILE:HG12 | 2.49                     | 0.43              |
| 1:F:50:ILE:N     | 1:F:50:ILE:HD13  | 2.33                     | 0.43              |
| 1:F:145:ASN:HB3  | 1:F:148:MET:HE1  | 2.00                     | 0.43              |
| 1:G:202:LEU:HD23 | 1:G:202:LEU:HA   | 1.65                     | 0.43              |
| 1:G:515:ARG:HB2  | 1:G:516:PRO:CD   | 2.47                     | 0.43              |
| 1:H:156:LEU:HA   | 1:H:156:LEU:HD23 | 1.67                     | 0.43              |
| 1:A:47:ILE:HG22  | 1:A:359:MET:HG3  | 2.00                     | 0.43              |
| 1:A:122:LEU:HB2  | 1:A:149:GLU:HA   | 1.99                     | 0.43              |
| 1:B:345:SER:O    | 1:B:349:ASN:HB2  | 2.18                     | 0.43              |
| 1:D:322:PRO:HA   | 1:D:356:ASP:OD2  | 2.18                     | 0.43              |
| 1:E:455:ASN:OD1  | 1:E:458:THR:N    | 2.47                     | 0.43              |
| 1:F:24:THR:CG2   | 1:F:27:GLU:H     | 2.31                     | 0.43              |
| 1:A:76:SER:HA    | 1:A:114:LYS:HB2  | 2.00                     | 0.43              |
| 1:B:44:THR:HG22  | 1:B:357:CYS:HA   | 2.00                     | 0.43              |
| 1:B:102:ILE:HD12 | 1:B:102:ILE:HA   | 1.76                     | 0.43              |
| 1:C:17:LEU:HA    | 1:C:17:LEU:HD23  | 1.77                     | 0.43              |
| 1:C:296:LEU:HD11 | 1:C:300:ILE:HG23 | 2.01                     | 0.43              |
| 1:G:15:GLN:CB    | 1:G:17:LEU:HD21  | 2.47                     | 0.43              |
| 1:H:16:GLN:HG2   | 1:H:32:LEU:HD22  | 2.00                     | 0.43              |
| 1:A:145:ASN:H    | 1:A:145:ASN:ND2  | 2.00                     | 0.43              |
| 1:A:228:LEU:O    | 1:A:232:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:417:GLU:O    | 1:A:417:GLU:HG3  | 2.19                     | 0.43              |
| 1:B:106:PRO:C    | 1:B:107:VAL:HG23 | 2.44                     | 0.43              |
| 1:C:296:LEU:CD1  | 1:C:300:ILE:HG23 | 2.49                     | 0.43              |
| 1:F:122:LEU:HB2  | 1:F:149:GLU:HG2  | 1.99                     | 0.43              |
| 1:F:240:PHE:N    | 1:F:240:PHE:CD1  | 2.84                     | 0.43              |
| 1:F:246:LYS:O    | 1:F:249:ASP:HB2  | 2.19                     | 0.43              |
| 1:G:131:VAL:HG12 | 1:G:202:LEU:HB3  | 2.00                     | 0.43              |
| 1:G:175:VAL:CG1  | 1:G:176:ASP:N    | 2.81                     | 0.43              |
| 1:G:440:VAL:O    | 1:G:445:PRO:HD3  | 2.19                     | 0.43              |
| 1:G:464:LEU:HD12 | 1:G:464:LEU:HA   | 1.76                     | 0.43              |
| 1:H:411:MET:HE1  | 1:H:524:MET:HB2  | 2.00                     | 0.43              |
| 1:H:432:GLU:HA   | 1:H:432:GLU:OE1  | 2.18                     | 0.43              |
| 1:H:503:LYS:H    | 1:H:506:ASP:CG   | 2.21                     | 0.43              |
| 1:A:245:ARG:HG2  | 1:A:272:ASN:HD21 | 1.83                     | 0.43              |
| 1:B:328:GLN:CB   | 1:B:331:GLU:HG3  | 2.49                     | 0.43              |
| 1:E:326:ALA:HB2  | 1:E:359:MET:HE2  | 2.00                     | 0.43              |
| 1:E:404:SER:OG   | 1:E:409:GLU:OE2  | 2.31                     | 0.43              |
| 1:F:138:THR:CG2  | 1:F:193:VAL:HG13 | 2.49                     | 0.43              |
| 1:F:276:VAL:HG11 | 1:H:34:ILE:HD13  | 2.00                     | 0.43              |
| 1:G:45:GLY:O     | 1:G:357:CYS:HB3  | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:95:GLU:C     | 1:G:97:PHE:H     | 2.27                     | 0.43              |
| 1:G:317:ASN:N    | 1:G:317:ASN:HD22 | 2.16                     | 0.43              |
| 1:G:329:MET:HE2  | 1:G:329:MET:HB3  | 1.95                     | 0.43              |
| 1:H:16:GLN:CG    | 1:H:32:LEU:HD23  | 2.49                     | 0.43              |
| 1:H:50:ILE:HD12  | 1:H:60:LEU:CD1   | 2.48                     | 0.43              |
| 1:A:124:LYS:O    | 1:A:126:SER:N    | 2.51                     | 0.43              |
| 1:C:60:LEU:O     | 1:C:64:ILE:N     | 2.47                     | 0.43              |
| 1:C:411:MET:HE1  | 1:C:524:MET:HB2  | 2.01                     | 0.43              |
| 1:C:427:LEU:N    | 1:C:427:LEU:CD1  | 2.82                     | 0.43              |
| 1:D:210:LEU:N    | 1:D:210:LEU:CD1  | 2.82                     | 0.43              |
| 1:E:39:ILE:O     | 1:E:382:ARG:HD3  | 2.19                     | 0.43              |
| 1:G:333:MET:HE2  | 1:G:373:ALA:CA   | 2.48                     | 0.43              |
| 1:G:506:ASP:O    | 1:G:529:VAL:HG23 | 2.19                     | 0.43              |
| 1:H:79:THR:HG22  | 1:H:80:HIS:N     | 2.34                     | 0.43              |
| 1:H:328:GLN:CB   | 1:H:331:GLU:HG3  | 2.48                     | 0.43              |
| 1:B:118:ILE:CG2  | 1:B:208:VAL:HB   | 2.49                     | 0.42              |
| 1:B:237:ASP:OD2  | 1:B:460:ARG:HD2  | 2.19                     | 0.42              |
| 1:C:122:LEU:HD12 | 1:C:204:SER:CB   | 2.49                     | 0.42              |
| 1:C:238:MET:HE1  | 1:C:464:LEU:HD11 | 2.00                     | 0.42              |
| 1:D:300:ILE:HB   | 1:D:301:PRO:HD2  | 2.00                     | 0.42              |
| 1:E:436:SER:HB3  | 1:E:521:THR:HG1  | 1.84                     | 0.42              |
| 1:F:148:MET:HE2  | 1:F:148:MET:HB2  | 1.61                     | 0.42              |
| 1:G:60:LEU:HD12  | 1:G:60:LEU:HA    | 1.49                     | 0.42              |
| 1:G:132:GLU:HB2  | 1:G:201:PHE:HE1  | 1.84                     | 0.42              |
| 1:G:184:VAL:HG13 | 1:G:186:GLN:O    | 2.19                     | 0.42              |
| 1:H:40:THR:HG22  | 1:H:40:THR:O     | 2.17                     | 0.42              |
| 1:H:109:VAL:N    | 1:H:237:ASP:OD2  | 2.49                     | 0.42              |
| 1:H:261:GLY:HA3  | 1:H:264:ILE:HD12 | 2.00                     | 0.42              |
| 1:A:55:ARG:NH2   | 1:A:85:GLU:HB3   | 2.34                     | 0.42              |
| 1:A:303:GLU:H    | 1:A:303:GLU:HG3  | 1.09                     | 0.42              |
| 1:C:408:MET:HE2  | 1:C:436:SER:HA   | 2.00                     | 0.42              |
| 1:C:504:LYS:O    | 1:C:504:LYS:HG2  | 2.18                     | 0.42              |
| 1:D:301:PRO:HB3  | 1:D:303:GLU:OE2  | 2.19                     | 0.42              |
| 1:D:468:ILE:HG21 | 1:D:468:ILE:HD13 | 1.73                     | 0.42              |
| 1:E:47:ILE:HG21  | 1:E:359:MET:SD   | 2.59                     | 0.42              |
| 1:F:158:LEU:HD12 | 1:F:158:LEU:HA   | 1.42                     | 0.42              |
| 1:F:291:VAL:HG12 | 1:F:293:ARG:HG3  | 2.01                     | 0.42              |
| 1:H:120:THR:HA   | 1:H:158:LEU:HD12 | 2.01                     | 0.42              |
| 1:H:444:ARG:HA   | 1:H:445:PRO:HD2  | 1.81                     | 0.42              |
| 1:A:42:ARG:NH1   | 1:A:44:THR:O     | 2.50                     | 0.42              |
| 1:A:122:LEU:HA   | 1:A:122:LEU:HD13 | 1.63                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:488:ARG:O    | 1:B:491:LEU:HB3  | 2.19                     | 0.42              |
| 1:D:152:ASP:C    | 1:D:154:ASN:H    | 2.27                     | 0.42              |
| 1:E:75:PHE:CE2   | 1:E:83:HIS:HD2   | 2.37                     | 0.42              |
| 1:E:529:VAL:HA   | 1:E:530:PRO:HD3  | 1.91                     | 0.42              |
| 1:F:57:VAL:HG13  | 1:F:93:ALA:HB2   | 2.01                     | 0.42              |
| 1:F:328:GLN:NE2  | 1:H:341:ARG:HG2  | 2.33                     | 0.42              |
| 1:G:60:LEU:N     | 1:G:60:LEU:CD1   | 2.79                     | 0.42              |
| 1:G:75:PHE:C     | 1:G:77:HIS:H     | 2.27                     | 0.42              |
| 1:H:514:TRP:HA   | 1:H:514:TRP:CE3  | 2.54                     | 0.42              |
| 1:B:300:ILE:HB   | 1:B:301:PRO:HD2  | 2.02                     | 0.42              |
| 1:B:491:LEU:HA   | 1:B:491:LEU:HD12 | 1.76                     | 0.42              |
| 1:C:123:ILE:HG21 | 1:C:131:VAL:HG23 | 2.00                     | 0.42              |
| 1:C:202:LEU:HD23 | 1:C:202:LEU:HA   | 1.78                     | 0.42              |
| 1:C:202:LEU:CD2  | 1:C:203:GLY:N    | 2.80                     | 0.42              |
| 1:C:411:MET:HB3  | 1:C:411:MET:HE3  | 1.58                     | 0.42              |
| 1:C:515:ARG:CB   | 1:C:516:PRO:HD2  | 2.41                     | 0.42              |
| 1:D:390:HIS:CD2  | 1:D:390:HIS:H    | 2.36                     | 0.42              |
| 1:E:17:LEU:N     | 1:E:17:LEU:HD23  | 2.34                     | 0.42              |
| 1:E:86:THR:O     | 1:E:90:VAL:HG23  | 2.20                     | 0.42              |
| 1:F:376:MET:HE2  | 1:F:380:ILE:CD1  | 2.44                     | 0.42              |
| 1:F:430:LEU:N    | 1:F:430:LEU:HD12 | 2.35                     | 0.42              |
| 1:F:438:HIS:O    | 1:F:441:ALA:HB3  | 2.19                     | 0.42              |
| 1:G:433:SER:HB2  | 1:G:435:ARG:HD2  | 2.01                     | 0.42              |
| 1:H:278:ARG:O    | 1:H:281:GLU:HG2  | 2.18                     | 0.42              |
| 1:C:229:LYS:HE3  | 5:C:6127:HOH:O   | 2.19                     | 0.42              |
| 1:E:509:ILE:O    | 1:E:509:ILE:HG22 | 2.19                     | 0.42              |
| 1:F:21:MET:HE1   | 1:F:391:ARG:HH12 | 1.84                     | 0.42              |
| 1:F:122:LEU:HA   | 1:F:204:SER:HG   | 1.85                     | 0.42              |
| 1:F:238:MET:HE2  | 1:F:238:MET:HB3  | 1.94                     | 0.42              |
| 1:F:271:GLU:HG2  | 1:F:295:ASP:HB2  | 2.01                     | 0.42              |
| 1:F:329:MET:O    | 1:F:330:LEU:HD13 | 2.19                     | 0.42              |
| 1:G:293:ARG:HH22 | 1:G:346:ASP:CG   | 2.26                     | 0.42              |
| 1:G:421:LYS:HE2  | 1:H:413:MET:SD   | 2.60                     | 0.42              |
| 1:A:242:SER:HA   | 1:A:269:LYS:HE2  | 2.01                     | 0.42              |
| 1:B:370:PRO:HD2  | 1:B:371:LEU:H    | 1.83                     | 0.42              |
| 1:B:407:LEU:HD12 | 1:B:407:LEU:HA   | 1.64                     | 0.42              |
| 1:C:267:ILE:N    | 1:C:267:ILE:CD1  | 2.83                     | 0.42              |
| 1:D:412:ALA:O    | 1:D:416:VAL:HG23 | 2.19                     | 0.42              |
| 1:D:496:GLY:HA3  | 1:D:502:PHE:CZ   | 2.54                     | 0.42              |
| 1:E:30:CYS:HB3   | 1:G:315:ARG:HD2  | 2.01                     | 0.42              |
| 1:E:511:LEU:C    | 1:E:521:THR:HG22 | 2.45                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:375:ARG:HH11 | 1:F:375:ARG:HD2  | 1.60                     | 0.42              |
| 1:G:100:ASP:HB3  | 1:G:103:LEU:H    | 1.85                     | 0.42              |
| 1:G:300:ILE:HG13 | 1:G:301:PRO:O    | 2.19                     | 0.42              |
| 1:G:388:MET:HE2  | 1:G:388:MET:HB3  | 1.79                     | 0.42              |
| 1:G:506:ASP:HB2  | 1:G:529:VAL:HG21 | 2.01                     | 0.42              |
| 1:H:220:VAL:CG1  | 1:H:225:ILE:HG13 | 2.49                     | 0.42              |
| 1:A:133:LEU:HD13 | 1:A:196:VAL:CG2  | 2.50                     | 0.42              |
| 1:A:390:HIS:CD2  | 1:A:446:ARG:NH1  | 2.88                     | 0.42              |
| 1:A:476:PRO:O    | 1:A:478:GLN:NE2  | 2.50                     | 0.42              |
| 1:B:334:ILE:HG23 | 1:B:367:GLY:HA2  | 2.02                     | 0.42              |
| 1:C:453:THR:CG2  | 1:C:459:ALA:HB2  | 2.49                     | 0.42              |
| 1:C:465:TYR:HB2  | 1:C:468:ILE:CD1  | 2.42                     | 0.42              |
| 1:D:123:ILE:HG12 | 1:D:151:CYS:O    | 2.20                     | 0.42              |
| 1:D:270:ILE:O    | 1:D:270:ILE:HG22 | 2.18                     | 0.42              |
| 1:D:289:ILE:HG22 | 1:D:290:MET:N    | 2.34                     | 0.42              |
| 1:D:408:MET:O    | 1:D:408:MET:HG3  | 2.19                     | 0.42              |
| 1:E:103:LEU:CD1  | 1:E:103:LEU:N    | 2.82                     | 0.42              |
| 1:E:296:LEU:C    | 1:E:298:ILE:H    | 2.28                     | 0.42              |
| 1:F:493:MET:HG2  | 1:F:530:PRO:CD   | 2.43                     | 0.42              |
| 1:G:60:LEU:HD23  | 1:G:90:VAL:CA    | 2.48                     | 0.42              |
| 1:G:142:THR:C    | 1:G:143:LEU:HG   | 2.40                     | 0.42              |
| 1:G:180:ILE:HD13 | 1:G:180:ILE:N    | 2.34                     | 0.42              |
| 1:H:120:THR:O    | 1:H:205:LYS:HA   | 2.20                     | 0.42              |
| 1:H:137:ALA:O    | 1:H:195:GLU:HA   | 2.20                     | 0.42              |
| 1:H:345:SER:O    | 1:H:349:ASN:HB2  | 2.20                     | 0.42              |
| 1:A:247:ALA:O    | 1:A:250:VAL:HB   | 2.20                     | 0.42              |
| 1:B:288:GLY:C    | 1:B:289:ILE:HG12 | 2.44                     | 0.42              |
| 1:C:45:GLY:N     | 1:C:357:CYS:HB3  | 2.35                     | 0.42              |
| 1:D:119:ARG:NH1  | 1:D:207:GLY:N    | 2.64                     | 0.42              |
| 1:E:439:GLN:CA   | 1:E:439:GLN:NE2  | 2.83                     | 0.42              |
| 1:F:217:LEU:HB3  | 1:F:218:PRO:CD   | 2.48                     | 0.42              |
| 1:F:283:LEU:HD22 | 1:F:321:LYS:HD2  | 2.01                     | 0.42              |
| 1:F:428:ILE:CD1  | 1:F:508:VAL:HG11 | 2.49                     | 0.42              |
| 1:G:202:LEU:HD22 | 1:G:202:LEU:C    | 2.42                     | 0.42              |
| 1:G:296:LEU:O    | 1:G:300:ILE:HG12 | 2.20                     | 0.42              |
| 1:G:382:ARG:CG   | 1:G:382:ARG:NH1  | 2.80                     | 0.42              |
| 1:H:407:LEU:N    | 1:H:407:LEU:HD13 | 2.35                     | 0.42              |
| 1:B:14:THR:CG2   | 1:B:15:GLN:N     | 2.83                     | 0.42              |
| 1:B:139:LEU:HD23 | 1:B:140:LYS:N    | 2.35                     | 0.42              |
| 1:B:311:MET:SD   | 1:B:315:ARG:HD3  | 2.59                     | 0.42              |
| 1:B:397:LEU:HD12 | 1:B:397:LEU:HA   | 1.96                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:472:VAL:CG1  | 1:D:473:CYS:N    | 2.80                     | 0.42              |
| 1:E:94:THR:OG1   | 1:E:107:VAL:HB   | 2.19                     | 0.42              |
| 1:E:398:ALA:HA   | 1:E:413:MET:HE1  | 2.02                     | 0.42              |
| 1:E:456:HIS:CD2  | 1:E:456:HIS:H    | 2.36                     | 0.42              |
| 1:F:118:ILE:HG22 | 1:F:208:VAL:HG21 | 2.01                     | 0.42              |
| 1:G:93:ALA:O     | 1:G:96:SER:HB3   | 2.19                     | 0.42              |
| 1:G:279:PHE:HE1  | 1:G:289:ILE:HG21 | 1.84                     | 0.42              |
| 1:H:75:PHE:CZ    | 1:H:83:HIS:CB    | 3.03                     | 0.42              |
| 1:H:95:GLU:C     | 1:H:97:PHE:H     | 2.28                     | 0.42              |
| 1:H:104:TYR:O    | 1:H:106:PRO:HD3  | 2.19                     | 0.42              |
| 1:H:413:MET:HE2  | 1:H:413:MET:HB3  | 1.74                     | 0.42              |
| 1:A:131:VAL:CG2  | 1:A:153:GLU:HB3  | 2.50                     | 0.42              |
| 1:A:283:LEU:HA   | 1:A:283:LEU:HD23 | 1.83                     | 0.42              |
| 1:C:272:ASN:N    | 1:C:272:ASN:HD22 | 2.17                     | 0.42              |
| 1:D:73:MET:HB3   | 1:D:75:PHE:HE1   | 1.83                     | 0.42              |
| 1:E:23:ASP:OD1   | 1:E:23:ASP:N     | 2.43                     | 0.42              |
| 1:F:25:PHE:CZ    | 1:F:29:MET:HE3   | 2.55                     | 0.42              |
| 1:F:162:ASN:HB3  | 1:F:165:LYS:HB3  | 2.02                     | 0.42              |
| 1:G:84:ALA:HB2   | 1:G:230:PHE:CZ   | 2.55                     | 0.42              |
| 1:G:276:VAL:O    | 1:G:279:PHE:HB2  | 2.19                     | 0.42              |
| 1:H:33:ASP:C     | 1:H:35:ASP:H     | 2.28                     | 0.42              |
| 1:H:189:PRO:HD2  | 1:H:191:PHE:CE2  | 2.55                     | 0.42              |
| 1:H:499:ARG:HB3  | 1:H:501:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:163:ILE:HG23 | 1:A:164:CYS:N    | 2.35                     | 0.41              |
| 1:A:237:ASP:O    | 1:A:461:GLN:NE2  | 2.52                     | 0.41              |
| 1:B:340:THR:O    | 1:B:343:GLU:HB2  | 2.20                     | 0.41              |
| 1:C:14:THR:H     | 1:C:14:THR:HG22  | 1.58                     | 0.41              |
| 1:C:55:ARG:NH2   | 1:C:82:TYR:CD1   | 2.88                     | 0.41              |
| 1:D:228:LEU:CD2  | 1:D:257:LEU:HD11 | 2.49                     | 0.41              |
| 1:D:303:GLU:H    | 1:D:303:GLU:HG3  | 1.40                     | 0.41              |
| 1:E:225:ILE:O    | 1:E:229:LYS:HG3  | 2.19                     | 0.41              |
| 1:F:16:GLN:HE21  | 1:F:16:GLN:HB2   | 1.54                     | 0.41              |
| 1:F:123:ILE:HD13 | 1:F:151:CYS:O    | 2.20                     | 0.41              |
| 1:F:162:ASN:OD1  | 1:F:165:LYS:HE3  | 2.20                     | 0.41              |
| 1:G:348:ALA:O    | 1:G:352:LEU:HD22 | 2.20                     | 0.41              |
| 1:A:17:LEU:O     | 1:A:20:ALA:HB3   | 2.20                     | 0.41              |
| 1:A:493:MET:CE   | 1:A:529:VAL:HG13 | 2.42                     | 0.41              |
| 1:A:506:ASP:C    | 1:A:529:VAL:HG23 | 2.45                     | 0.41              |
| 1:B:156:LEU:HD22 | 1:B:157:TRP:N    | 2.32                     | 0.41              |
| 1:B:182:LEU:H    | 1:B:182:LEU:HG   | 1.68                     | 0.41              |
| 1:B:330:LEU:CD2  | 1:B:377:GLN:HG3  | 2.50                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:257:LEU:HD23 | 1:C:257:LEU:HA   | 1.89                     | 0.41              |
| 1:C:468:ILE:HG22 | 1:C:470:PRO:HD3  | 2.02                     | 0.41              |
| 1:D:51:GLY:O     | 1:D:55:ARG:HB2   | 2.20                     | 0.41              |
| 1:E:324:ILE:HD12 | 1:E:324:ILE:HG21 | 1.82                     | 0.41              |
| 1:F:54:SER:O     | 1:F:60:LEU:HD13  | 2.20                     | 0.41              |
| 1:F:123:ILE:HA   | 1:F:151:CYS:HB2  | 2.01                     | 0.41              |
| 1:F:244:ILE:HD13 | 1:F:244:ILE:HA   | 1.86                     | 0.41              |
| 1:F:507:VAL:CG1  | 1:F:508:VAL:H    | 2.30                     | 0.41              |
| 1:G:421:LYS:HA   | 1:G:421:LYS:HD3  | 1.86                     | 0.41              |
| 1:G:423:LEU:N    | 1:G:423:LEU:CD1  | 2.80                     | 0.41              |
| 1:G:503:LYS:N    | 1:G:506:ASP:OD2  | 2.50                     | 0.41              |
| 1:H:17:LEU:C     | 1:H:20:ALA:HB3   | 2.45                     | 0.41              |
| 1:H:24:THR:O     | 1:H:27:GLU:N     | 2.53                     | 0.41              |
| 1:H:352:LEU:HD12 | 1:H:352:LEU:HA   | 1.67                     | 0.41              |
| 1:A:369:TYR:HB3  | 1:A:372:GLU:HB2  | 2.01                     | 0.41              |
| 1:B:290:MET:HE2  | 1:B:326:ALA:CB   | 2.50                     | 0.41              |
| 1:B:464:LEU:HA   | 1:B:464:LEU:HD12 | 1.79                     | 0.41              |
| 1:B:486:ASP:O    | 1:B:490:ASN:ND2  | 2.54                     | 0.41              |
| 1:C:133:LEU:HD11 | 1:C:202:LEU:HB2  | 2.02                     | 0.41              |
| 1:E:55:ARG:NH2   | 1:E:82:TYR:CD1   | 2.89                     | 0.41              |
| 1:E:79:THR:OG1   | 1:E:80:HIS:N     | 2.48                     | 0.41              |
| 1:G:57:VAL:HG11  | 1:G:92:THR:HG21  | 2.02                     | 0.41              |
| 1:H:168:ASP:O    | 1:H:171:SER:HB2  | 2.21                     | 0.41              |
| 1:A:124:LYS:C    | 1:A:126:SER:N    | 2.78                     | 0.41              |
| 1:A:231:GLY:O    | 1:A:236:VAL:HG22 | 2.20                     | 0.41              |
| 1:A:255:LYS:O    | 1:A:258:GLY:N    | 2.52                     | 0.41              |
| 1:A:440:VAL:HG12 | 1:A:449:ILE:CD1  | 2.51                     | 0.41              |
| 1:B:24:THR:HG22  | 1:B:27:GLU:HB2   | 2.02                     | 0.41              |
| 1:B:424:ALA:HB2  | 1:B:509:ILE:CD1  | 2.50                     | 0.41              |
| 1:C:191:PHE:C    | 1:C:192:LEU:HD13 | 2.46                     | 0.41              |
| 1:D:155:ILE:CG2  | 1:D:156:LEU:N    | 2.83                     | 0.41              |
| 1:E:388:MET:CE   | 1:E:466:ARG:NH2  | 2.83                     | 0.41              |
| 1:H:55:ARG:HD2   | 1:H:86:THR:HG23  | 2.01                     | 0.41              |
| 1:H:113:THR:CG2  | 1:H:114:LYS:N    | 2.80                     | 0.41              |
| 1:H:253:VAL:O    | 1:H:253:VAL:HG12 | 2.18                     | 0.41              |
| 1:H:382:ARG:HH11 | 1:H:382:ARG:CB   | 2.34                     | 0.41              |
| 1:H:504:LYS:HA   | 1:H:530:PRO:OXT  | 2.20                     | 0.41              |
| 1:B:380:ILE:HG13 | 1:B:380:ILE:H    | 1.53                     | 0.41              |
| 1:C:56:SER:O     | 1:C:60:LEU:HD22  | 2.20                     | 0.41              |
| 1:C:293:ARG:HD3  | 1:C:326:ALA:O    | 2.19                     | 0.41              |
| 1:C:477:VAL:HG23 | 5:C:6139:HOH:O   | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:60:LEU:HD12  | 1:D:60:LEU:HA    | 1.78                     | 0.41              |
| 1:E:390:HIS:CD2  | 1:E:446:ARG:HH11 | 2.39                     | 0.41              |
| 1:F:341:ARG:HG2  | 1:H:328:GLN:NE2  | 2.35                     | 0.41              |
| 1:G:168:ASP:O    | 1:G:171:SER:OG   | 2.38                     | 0.41              |
| 1:G:316:CYS:HB3  | 1:G:321:LYS:O    | 2.21                     | 0.41              |
| 1:G:504:LYS:O    | 1:G:529:VAL:HB   | 2.21                     | 0.41              |
| 1:H:300:ILE:HG13 | 1:H:301:PRO:O    | 2.20                     | 0.41              |
| 1:A:72:ARG:HH11  | 1:A:72:ARG:HD3   | 1.62                     | 0.41              |
| 1:B:72:ARG:NH2   | 1:B:112:ASP:OD2  | 2.48                     | 0.41              |
| 1:C:493:MET:HE1  | 1:C:529:VAL:CG2  | 2.43                     | 0.41              |
| 1:D:119:ARG:HH11 | 1:D:206:LYS:C    | 2.27                     | 0.41              |
| 1:E:72:ARG:HG2   | 1:E:73:MET:N     | 2.26                     | 0.41              |
| 1:G:50:ILE:N     | 1:G:50:ILE:HD13  | 2.34                     | 0.41              |
| 1:G:244:ILE:HG13 | 1:G:268:SER:OG   | 2.20                     | 0.41              |
| 1:G:279:PHE:HE2  | 1:G:315:ARG:HB3  | 1.86                     | 0.41              |
| 1:G:438:HIS:O    | 1:G:441:ALA:HB3  | 2.20                     | 0.41              |
| 1:H:49:THR:OG1   | 1:H:72:ARG:HD3   | 2.20                     | 0.41              |
| 1:H:352:LEU:HD12 | 1:H:388:MET:HG2  | 2.02                     | 0.41              |
| 1:H:430:LEU:HD12 | 1:H:430:LEU:HA   | 1.84                     | 0.41              |
| 1:A:62:GLU:HG3   | 1:A:371:LEU:CD1  | 2.50                     | 0.41              |
| 1:A:123:ILE:HB   | 1:A:204:SER:OG   | 2.20                     | 0.41              |
| 1:A:294:GLY:CA   | 1:A:327:THR:HG21 | 2.51                     | 0.41              |
| 1:B:160:TYR:HD2  | 1:B:163:ILE:HB   | 1.81                     | 0.41              |
| 1:C:413:MET:HE3  | 1:C:413:MET:HB3  | 1.94                     | 0.41              |
| 1:C:493:MET:O    | 1:C:497:LYS:HG3  | 2.21                     | 0.41              |
| 1:D:142:THR:HG21 | 1:D:147:TYR:CD2  | 2.56                     | 0.41              |
| 1:D:424:ALA:CB   | 1:D:509:ILE:HD12 | 2.50                     | 0.41              |
| 1:G:481:TRP:O    | 1:G:483:GLU:N    | 2.53                     | 0.41              |
| 1:H:50:ILE:HD12  | 1:H:60:LEU:HD11  | 2.02                     | 0.41              |
| 1:H:112:ASP:HA   | 1:H:240:PHE:HB2  | 2.03                     | 0.41              |
| 1:H:244:ILE:HD13 | 1:H:244:ILE:HA   | 1.93                     | 0.41              |
| 1:H:449:ILE:HD13 | 1:H:449:ILE:HG21 | 1.76                     | 0.41              |
| 1:A:39:ILE:HD12  | 1:A:41:ALA:HB3   | 2.02                     | 0.41              |
| 1:A:72:ARG:NE    | 1:A:112:ASP:OD2  | 2.48                     | 0.41              |
| 1:A:113:THR:CG2  | 1:A:114:LYS:N    | 2.83                     | 0.41              |
| 1:B:48:CYS:SG    | 1:B:68:MET:HG3   | 2.61                     | 0.41              |
| 1:B:133:LEU:CD2  | 1:B:133:LEU:N    | 2.83                     | 0.41              |
| 1:B:283:LEU:HA   | 1:B:283:LEU:HD23 | 1.73                     | 0.41              |
| 1:D:294:GLY:N    | 1:D:327:THR:HG21 | 2.36                     | 0.41              |
| 1:D:453:THR:HG1  | 1:D:455:ASN:H    | 1.64                     | 0.41              |
| 1:E:17:LEU:HD22  | 1:E:17:LEU:HA    | 1.76                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:64:ILE:HG13  | 1:E:68:MET:CE    | 2.51                     | 0.41              |
| 1:E:326:ALA:HB1  | 1:E:359:MET:CE   | 2.51                     | 0.41              |
| 1:E:413:MET:CE   | 1:E:443:TYR:CE1  | 3.00                     | 0.41              |
| 1:F:119:ARG:HA   | 1:F:119:ARG:HD2  | 1.84                     | 0.41              |
| 1:F:327:THR:O    | 1:F:328:GLN:HB2  | 2.21                     | 0.41              |
| 1:F:340:THR:OG1  | 1:F:343:GLU:HG2  | 2.20                     | 0.41              |
| 5:F:6172:HOH:O   | 1:H:342:ALA:HB3  | 2.21                     | 0.41              |
| 1:G:41:ALA:CB    | 1:G:448:PRO:HG3  | 2.51                     | 0.41              |
| 1:G:529:VAL:O    | 1:G:530:PRO:OXT  | 2.39                     | 0.41              |
| 1:H:122:LEU:O    | 1:H:151:CYS:HB2  | 2.21                     | 0.41              |
| 1:H:148:MET:HE3  | 1:H:148:MET:HB3  | 1.83                     | 0.41              |
| 1:A:60:LEU:HD12  | 1:A:60:LEU:HA    | 1.52                     | 0.41              |
| 1:A:60:LEU:HB3   | 1:A:93:ALA:CB    | 2.51                     | 0.41              |
| 1:A:196:VAL:O    | 1:A:196:VAL:HG12 | 2.21                     | 0.41              |
| 1:A:238:MET:HB2  | 1:A:265:LYS:O    | 2.20                     | 0.41              |
| 1:B:46:ILE:HG23  | 1:B:377:GLN:NE2  | 2.35                     | 0.41              |
| 1:B:72:ARG:HH21  | 1:B:112:ASP:CG   | 2.28                     | 0.41              |
| 1:B:111:LEU:HD23 | 1:B:112:ASP:N    | 2.36                     | 0.41              |
| 1:B:147:TYR:CD1  | 1:B:147:TYR:N    | 2.89                     | 0.41              |
| 1:B:342:ALA:CB   | 1:D:346:ASP:CB   | 2.99                     | 0.41              |
| 1:C:51:GLY:O     | 1:C:55:ARG:N     | 2.54                     | 0.41              |
| 1:C:63:MET:HG3   | 1:C:371:LEU:HD23 | 2.03                     | 0.41              |
| 1:C:273:HIS:CB   | 1:C:277:ARG:NH1  | 2.80                     | 0.41              |
| 1:D:162:ASN:OD1  | 1:D:162:ASN:N    | 2.54                     | 0.41              |
| 1:D:189:PRO:CD   | 1:D:190:ASP:N    | 2.80                     | 0.41              |
| 1:D:245:ARG:O    | 1:D:278:ARG:HD3  | 2.20                     | 0.41              |
| 1:E:95:GLU:C     | 1:E:97:PHE:N     | 2.79                     | 0.41              |
| 1:E:102:ILE:CG2  | 1:E:103:LEU:HD12 | 2.49                     | 0.41              |
| 1:E:104:TYR:CD2  | 1:E:106:PRO:HD3  | 2.56                     | 0.41              |
| 1:E:270:ILE:N    | 1:E:270:ILE:CD1  | 2.79                     | 0.41              |
| 1:F:133:LEU:CD1  | 1:F:139:LEU:HD13 | 2.41                     | 0.41              |
| 1:F:145:ASN:HD22 | 1:F:157:TRP:HE1  | 1.69                     | 0.41              |
| 1:F:192:LEU:HD13 | 1:F:192:LEU:HA   | 1.63                     | 0.41              |
| 1:F:503:LYS:HB3  | 1:F:504:LYS:H    | 1.55                     | 0.41              |
| 1:F:504:LYS:HG3  | 1:F:530:PRO:OXT  | 2.21                     | 0.41              |
| 1:G:22:ALA:HB2   | 1:G:31:ARG:HD2   | 2.02                     | 0.41              |
| 1:G:56:SER:C     | 1:G:58:GLU:N     | 2.78                     | 0.41              |
| 1:G:123:ILE:HA   | 1:G:151:CYS:O    | 2.20                     | 0.41              |
| 1:G:316:CYS:CB   | 1:G:323:VAL:CG2  | 2.99                     | 0.41              |
| 1:H:16:GLN:OE1   | 1:H:33:ASP:N     | 2.48                     | 0.41              |
| 1:H:37:ALA:HA    | 1:H:38:PRO:HD3   | 1.97                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:100:ASP:C    | 1:H:102:ILE:N    | 2.78                     | 0.41              |
| 1:H:210:LEU:N    | 1:H:210:LEU:CD1  | 2.80                     | 0.41              |
| 1:H:507:VAL:HG12 | 1:H:508:VAL:H    | 1.84                     | 0.41              |
| 1:A:68:MET:HB3   | 1:A:68:MET:HE2   | 1.69                     | 0.41              |
| 1:A:100:ASP:OD2  | 1:A:103:LEU:HD13 | 2.20                     | 0.41              |
| 1:A:169:VAL:CG1  | 1:A:170:GLY:N    | 2.84                     | 0.41              |
| 1:A:461:GLN:O    | 1:A:464:LEU:HB2  | 2.21                     | 0.41              |
| 1:B:336:LYS:CG   | 1:B:337:PRO:HD2  | 2.50                     | 0.41              |
| 1:B:431:THR:CG2  | 1:B:434:GLY:HA2  | 2.51                     | 0.41              |
| 1:D:267:ILE:N    | 1:D:267:ILE:CD1  | 2.80                     | 0.41              |
| 1:D:352:LEU:HD12 | 1:D:352:LEU:HA   | 1.91                     | 0.41              |
| 1:E:242:SER:HB3  | 1:E:271:GLU:OE2  | 2.21                     | 0.41              |
| 1:F:480:ALA:HB3  | 1:F:483:GLU:HB2  | 2.02                     | 0.41              |
| 1:G:90:VAL:HG23  | 1:G:90:VAL:H     | 1.63                     | 0.41              |
| 1:G:329:MET:CE   | 1:G:347:VAL:HA   | 2.50                     | 0.41              |
| 1:H:368:ASP:C    | 1:H:369:TYR:CG   | 2.99                     | 0.41              |
| 1:A:45:GLY:CA    | 1:A:357:CYS:HB3  | 2.51                     | 0.40              |
| 1:A:429:VAL:O    | 1:A:430:LEU:HD12 | 2.21                     | 0.40              |
| 1:A:503:LYS:HB2  | 1:A:506:ASP:OD2  | 2.22                     | 0.40              |
| 1:B:50:ILE:HA    | 1:B:50:ILE:HD13  | 1.75                     | 0.40              |
| 1:B:514:TRP:CD1  | 1:B:515:ARG:HG3  | 2.56                     | 0.40              |
| 1:C:114:LYS:N    | 5:C:6126:HOH:O   | 2.49                     | 0.40              |
| 1:C:382:ARG:HH11 | 1:C:382:ARG:HB2  | 1.86                     | 0.40              |
| 1:C:491:LEU:HD12 | 1:C:491:LEU:HA   | 1.79                     | 0.40              |
| 1:E:232:VAL:HG12 | 1:E:233:GLU:N    | 2.36                     | 0.40              |
| 1:E:296:LEU:C    | 1:E:298:ILE:N    | 2.80                     | 0.40              |
| 1:E:328:GLN:NE2  | 1:G:341:ARG:N    | 2.65                     | 0.40              |
| 1:F:115:GLY:HA2  | 1:F:116:PRO:HD3  | 1.64                     | 0.40              |
| 1:F:289:ILE:HA   | 1:F:289:ILE:HD13 | 1.80                     | 0.40              |
| 1:H:133:LEU:HD13 | 1:H:139:LEU:HD13 | 2.02                     | 0.40              |
| 1:C:496:GLY:HA3  | 1:C:502:PHE:CZ   | 2.57                     | 0.40              |
| 1:D:322:PRO:HG3  | 1:D:465:TYR:CZ   | 2.57                     | 0.40              |
| 1:E:50:ILE:HD13  | 1:E:50:ILE:HA    | 1.83                     | 0.40              |
| 1:E:64:ILE:HG13  | 1:E:68:MET:HE3   | 2.03                     | 0.40              |
| 1:E:221:SER:HB3  | 1:E:224:ASP:OD2  | 2.20                     | 0.40              |
| 1:E:396:GLU:CD   | 1:G:24:THR:HB    | 2.46                     | 0.40              |
| 1:E:515:ARG:HB3  | 1:E:516:PRO:CD   | 2.49                     | 0.40              |
| 1:F:204:SER:O    | 1:F:206:LYS:HG2  | 2.21                     | 0.40              |
| 1:F:332:SER:C    | 1:F:334:ILE:N    | 2.79                     | 0.40              |
| 1:G:247:ALA:O    | 1:G:250:VAL:N    | 2.54                     | 0.40              |
| 1:G:330:LEU:HD23 | 1:G:360:LEU:HD21 | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:60:LEU:HG    | 1:H:90:VAL:HG22  | 2.03                     | 0.40              |
| 1:H:113:THR:HG22 | 1:H:242:SER:HB2  | 2.02                     | 0.40              |
| 1:H:244:ILE:HG23 | 1:H:244:ILE:HD12 | 1.79                     | 0.40              |
| 1:H:436:SER:HB3  | 1:H:521:THR:OG1  | 2.20                     | 0.40              |
| 1:A:70:VAL:HG22  | 1:A:108:ALA:HB3  | 2.03                     | 0.40              |
| 1:A:336:LYS:HB3  | 1:A:337:PRO:HD2  | 2.04                     | 0.40              |
| 1:B:51:GLY:HA3   | 1:B:52:PRO:HD2   | 1.92                     | 0.40              |
| 1:B:133:LEU:HD11 | 1:B:139:LEU:HD12 | 2.03                     | 0.40              |
| 1:B:174:TYR:CE2  | 1:B:211:PRO:HG3  | 2.57                     | 0.40              |
| 1:C:185:LYS:HG2  | 1:C:193:VAL:O    | 2.21                     | 0.40              |
| 1:C:215:VAL:HG12 | 1:C:217:LEU:HB2  | 2.02                     | 0.40              |
| 1:C:309:GLN:O    | 1:C:313:ILE:HG13 | 2.21                     | 0.40              |
| 1:C:332:SER:HB3  | 1:C:343:GLU:OE1  | 2.22                     | 0.40              |
| 1:C:497:LYS:NZ   | 1:C:530:PRO:C    | 2.79                     | 0.40              |
| 1:D:43:ASN:H     | 1:D:385:GLU:CD   | 2.29                     | 0.40              |
| 1:E:43:ASN:ND2   | 1:E:467:GLY:HA2  | 2.36                     | 0.40              |
| 1:E:100:ASP:C    | 1:E:102:ILE:N    | 2.78                     | 0.40              |
| 1:E:219:ALA:HB2  | 1:E:252:GLU:OE2  | 2.22                     | 0.40              |
| 1:F:50:ILE:HB    | 1:F:73:MET:HE3   | 2.02                     | 0.40              |
| 1:G:100:ASP:C    | 1:G:102:ILE:N    | 2.80                     | 0.40              |
| 1:G:316:CYS:CB   | 1:G:323:VAL:HG22 | 2.51                     | 0.40              |
| 1:H:328:GLN:HG2  | 1:H:331:GLU:CD   | 2.47                     | 0.40              |
| 1:A:239:VAL:CG1  | 1:A:240:PHE:N    | 2.77                     | 0.40              |
| 1:B:56:SER:O     | 1:B:60:LEU:HD22  | 2.21                     | 0.40              |
| 1:B:64:ILE:CD1   | 1:B:94:THR:HA    | 2.51                     | 0.40              |
| 1:B:80:HIS:CD2   | 1:B:80:HIS:H     | 2.39                     | 0.40              |
| 1:B:195:GLU:HG3  | 1:B:196:VAL:N    | 2.36                     | 0.40              |
| 1:B:342:ALA:HB2  | 1:D:346:ASP:OD2  | 2.22                     | 0.40              |
| 1:C:463:HIS:C    | 1:C:465:TYR:N    | 2.79                     | 0.40              |
| 1:D:134:LYS:HB3  | 1:D:134:LYS:HE3  | 1.58                     | 0.40              |
| 1:D:185:LYS:NZ   | 1:D:195:GLU:HB2  | 2.36                     | 0.40              |
| 1:D:428:ILE:HD12 | 1:D:508:VAL:CG1  | 2.51                     | 0.40              |
| 1:E:105:ARG:HA   | 1:E:106:PRO:HD2  | 1.85                     | 0.40              |
| 1:F:95:GLU:C     | 1:F:97:PHE:H     | 2.29                     | 0.40              |
| 1:G:15:GLN:CB    | 1:G:17:LEU:CD2   | 2.99                     | 0.40              |
| 1:G:79:THR:HG23  | 1:G:82:TYR:HB2   | 2.03                     | 0.40              |
| 1:H:61:LYS:HE2   | 1:H:96:SER:OG    | 2.21                     | 0.40              |
| 1:H:425:ALA:HB1  | 1:H:502:PHE:HB3  | 2.02                     | 0.40              |
| 1:A:105:ARG:HG3  | 1:A:499:ARG:HH21 | 1.87                     | 0.40              |
| 1:A:123:ILE:HG13 | 1:A:203:GLY:O    | 2.21                     | 0.40              |
| 1:A:396:GLU:CD   | 1:C:24:THR:HB    | 2.47                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:158:LEU:HD12 | 1:C:158:LEU:HA   | 1.62                     | 0.40              |
| 1:C:289:ILE:HG22 | 1:C:290:MET:N    | 2.36                     | 0.40              |
| 1:C:327:THR:OG1  | 4:C:532:PEQ:O2'  | 2.30                     | 0.40              |
| 1:D:407:LEU:O    | 1:D:410:ALA:HB3  | 2.20                     | 0.40              |
| 1:F:177:ASP:HB3  | 1:F:298:ILE:CD1  | 2.51                     | 0.40              |
| 1:F:330:LEU:O    | 1:F:363:GLU:HG2  | 2.22                     | 0.40              |
| 1:G:221:SER:O    | 1:G:224:ASP:N    | 2.54                     | 0.40              |
| 1:G:332:SER:OG   | 1:G:339:PRO:HA   | 2.21                     | 0.40              |
| 1:H:267:ILE:HD12 | 1:H:267:ILE:HA   | 1.90                     | 0.40              |
| 1:H:306:PHE:CD1  | 1:H:306:PHE:C    | 2.99                     | 0.40              |
| 1:H:450:ILE:H    | 1:H:450:ILE:HG12 | 1.42                     | 0.40              |
| 1:H:511:LEU:HA   | 1:H:523:THR:O    | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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 |
| 4   | PEQ  | F     | 532 | 2    | 8,9,9        | 1.16 | 1 (12%)  | 11,13,13    | 0.87 | 0        |
| 4   | PEQ  | A     | 532 | 2,3  | 8,9,9        | 1.13 | 1 (12%)  | 11,13,13    | 0.85 | 0        |
| 4   | PEQ  | H     | 532 | 2    | 8,9,9        | 1.14 | 0        | 11,13,13    | 0.86 | 0        |
| 4   | PEQ  | D     | 532 | 2    | 8,9,9        | 1.14 | 1 (12%)  | 11,13,13    | 0.86 | 0        |
| 4   | PEQ  | E     | 532 | 2,3  | 8,9,9        | 1.12 | 0        | 11,13,13    | 0.86 | 0        |
| 4   | PEQ  | C     | 532 | 2    | 8,9,9        | 1.12 | 1 (12%)  | 11,13,13    | 0.86 | 0        |
| 4   | PEQ  | B     | 532 | 2    | 8,9,9        | 1.14 | 1 (12%)  | 11,13,13    | 0.86 | 0        |
| 4   | PEQ  | G     | 532 | 2    | 8,9,9        | 1.13 | 0        | 11,13,13    | 0.85 | 0        |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 4   | PEQ  | F     | 532 | 2    | -       | 5/9/9/9  | -     |
| 4   | PEQ  | A     | 532 | 2,3  | -       | 5/9/9/9  | -     |
| 4   | PEQ  | H     | 532 | 2    | -       | 4/9/9/9  | -     |
| 4   | PEQ  | D     | 532 | 2    | -       | 5/9/9/9  | -     |
| 4   | PEQ  | E     | 532 | 2,3  | -       | 5/9/9/9  | -     |
| 4   | PEQ  | C     | 532 | 2    | -       | 6/9/9/9  | -     |
| 4   | PEQ  | B     | 532 | 2    | -       | 5/9/9/9  | -     |
| 4   | PEQ  | G     | 532 | 2    | -       | 4/9/9/9  | -     |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | F     | 532 | PEQ  | P-O2  | 2.12 | 1.63        | 1.59     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | D     | 532 | PEQ  | P-O2  | 2.07 | 1.63        | 1.59     |
| 4   | B     | 532 | PEQ  | P-O2  | 2.03 | 1.63        | 1.59     |
| 4   | A     | 532 | PEQ  | P-O2  | 2.02 | 1.63        | 1.59     |
| 4   | C     | 532 | PEQ  | P-O2  | 2.00 | 1.63        | 1.59     |

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 4   | A     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | A     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | A     | 532 | PEQ  | C1-C2-O2-P   |
| 4   | B     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | B     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | B     | 532 | PEQ  | C1-C2-O2-P   |
| 4   | C     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | C     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | C     | 532 | PEQ  | C1-C2-O2-P   |
| 4   | D     | 532 | PEQ  | O1-C1-C2-O2  |
| 4   | D     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | E     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | E     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | E     | 532 | PEQ  | C1-C2-O2-P   |
| 4   | F     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | F     | 532 | PEQ  | C1-C2-O2-P   |
| 4   | G     | 532 | PEQ  | O1-C1-C2-O2  |
| 4   | G     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | H     | 532 | PEQ  | C3-C2-O2-P   |
| 4   | A     | 532 | PEQ  | O1-C1-C2-O2  |
| 4   | A     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | B     | 532 | PEQ  | O1-C1-C2-O2  |
| 4   | B     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | C     | 532 | PEQ  | O1-C1-C2-O2  |
| 4   | C     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | D     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | D     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | E     | 532 | PEQ  | O1-C1-C2-O2  |
| 4   | E     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | F     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | F     | 532 | PEQ  | O1-C1-C2-O2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 4   | F     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | G     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | G     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | H     | 532 | PEQ  | O1-C1-C2-C3  |
| 4   | H     | 532 | PEQ  | O2'-C1-C2-O2 |
| 4   | D     | 532 | PEQ  | C3-C2-O2-P   |
| 4   | H     | 532 | PEQ  | O2'-C1-C2-C3 |
| 4   | C     | 532 | PEQ  | C2-O2-P-O3P  |

There are no ring outliers.

6 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | F     | 532 | PEQ  | 3       | 0            |
| 4   | A     | 532 | PEQ  | 1       | 0            |
| 4   | H     | 532 | PEQ  | 5       | 0            |
| 4   | D     | 532 | PEQ  | 1       | 0            |
| 4   | C     | 532 | PEQ  | 1       | 0            |
| 4   | B     | 532 | PEQ  | 3       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.