



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:13 AM UTC

PDB ID : 2R7E / pdb\_00002r7e  
Title : Crystal Structure Analysis of Coagulation Factor VIII  
Authors : Stoddard, B.L.; Shen, B.W.  
Deposited on : 2007-09-07  
Resolution : 3.70 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)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

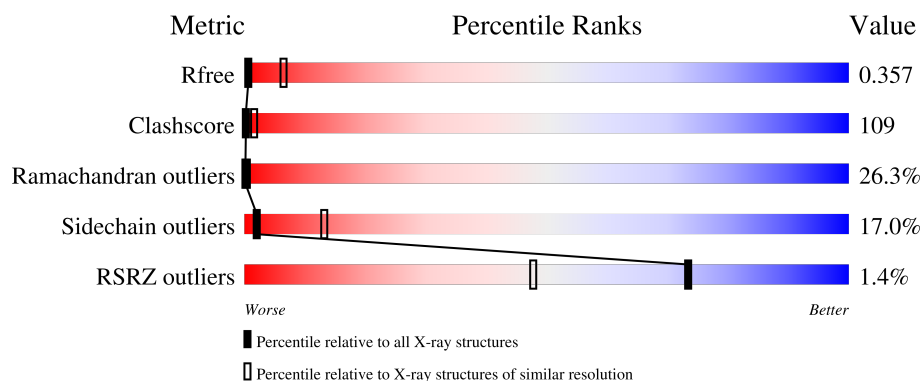
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

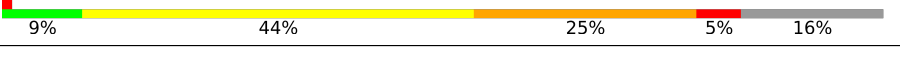
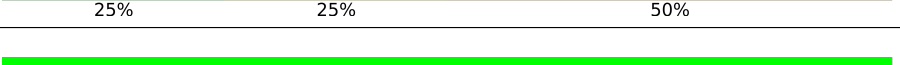
The reported resolution of this entry is 3.70 Å.

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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1131 (3.80-3.60)                                      |
| Clashscore            | 190562                      | 1171 (3.80-3.60)                                      |
| Ramachandran outliers | 187476                      | 1129 (3.80-3.60)                                      |
| Sidechain outliers    | 187428                      | 1126 (3.80-3.60)                                      |
| RSRZ outliers         | 180081                      | 1130 (3.80-3.60)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 742    |  |
| 2   | B     | 770    |  |
| 3   | C     | 4      |  |
| 4   | D     | 2      |  |
| 5   | E     | 7      |  |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10985 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 Coagulation factor VIII.

| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 1   | A     | 693      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5590  | 3592 | 937 | 1035 | 26 |         |         |       |

- Molecule 2 is a protein called Coagulation factor VIII.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 644      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5229  | 3346 | 907 | 944 | 32 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 1838    | SER      | PHE    | engineered mutation | UNP P00451 |

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



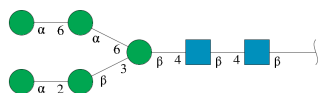
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 3   | C     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4   | D     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranos e-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5   | E     | 7        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |         |       |

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

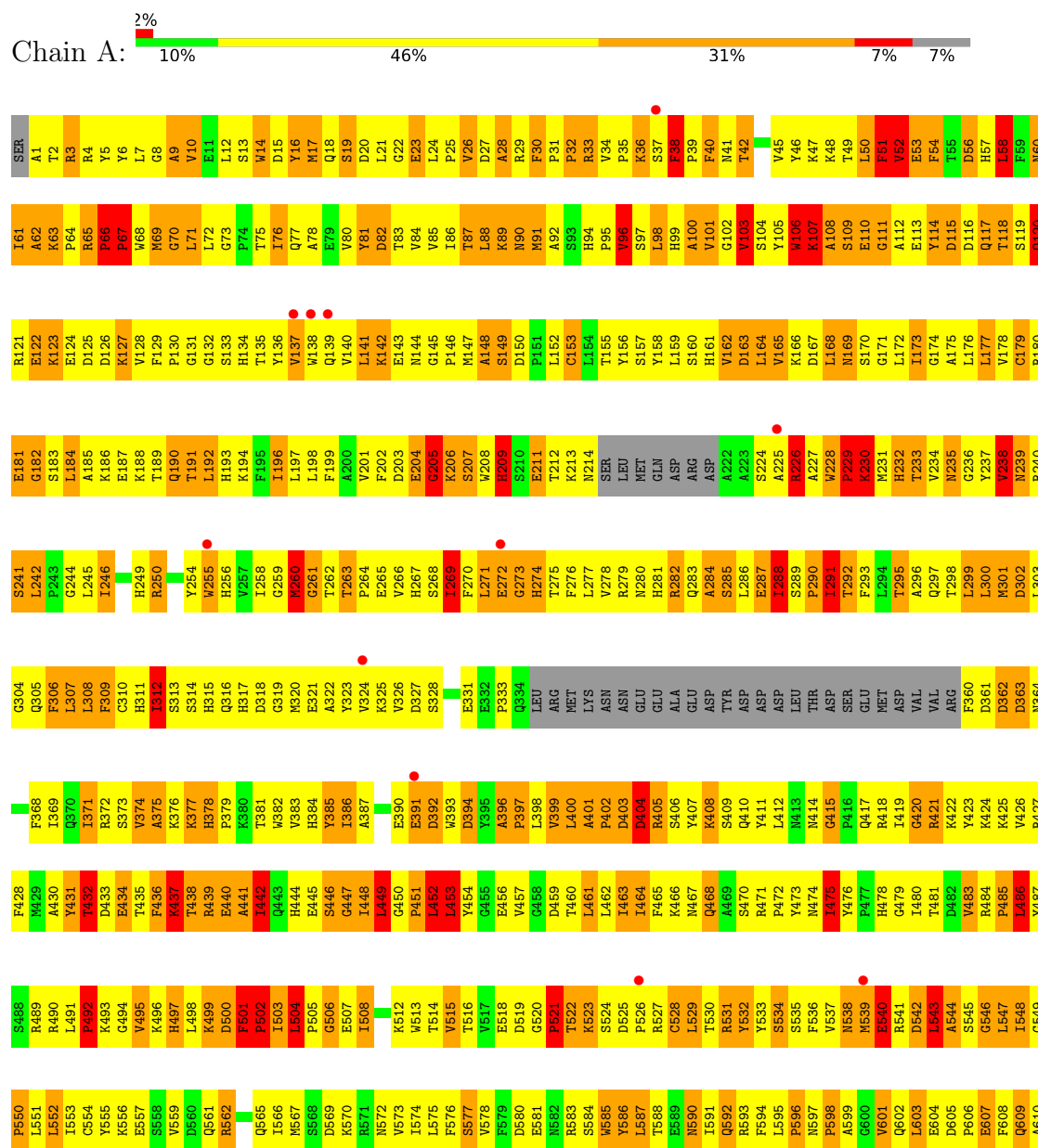
- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

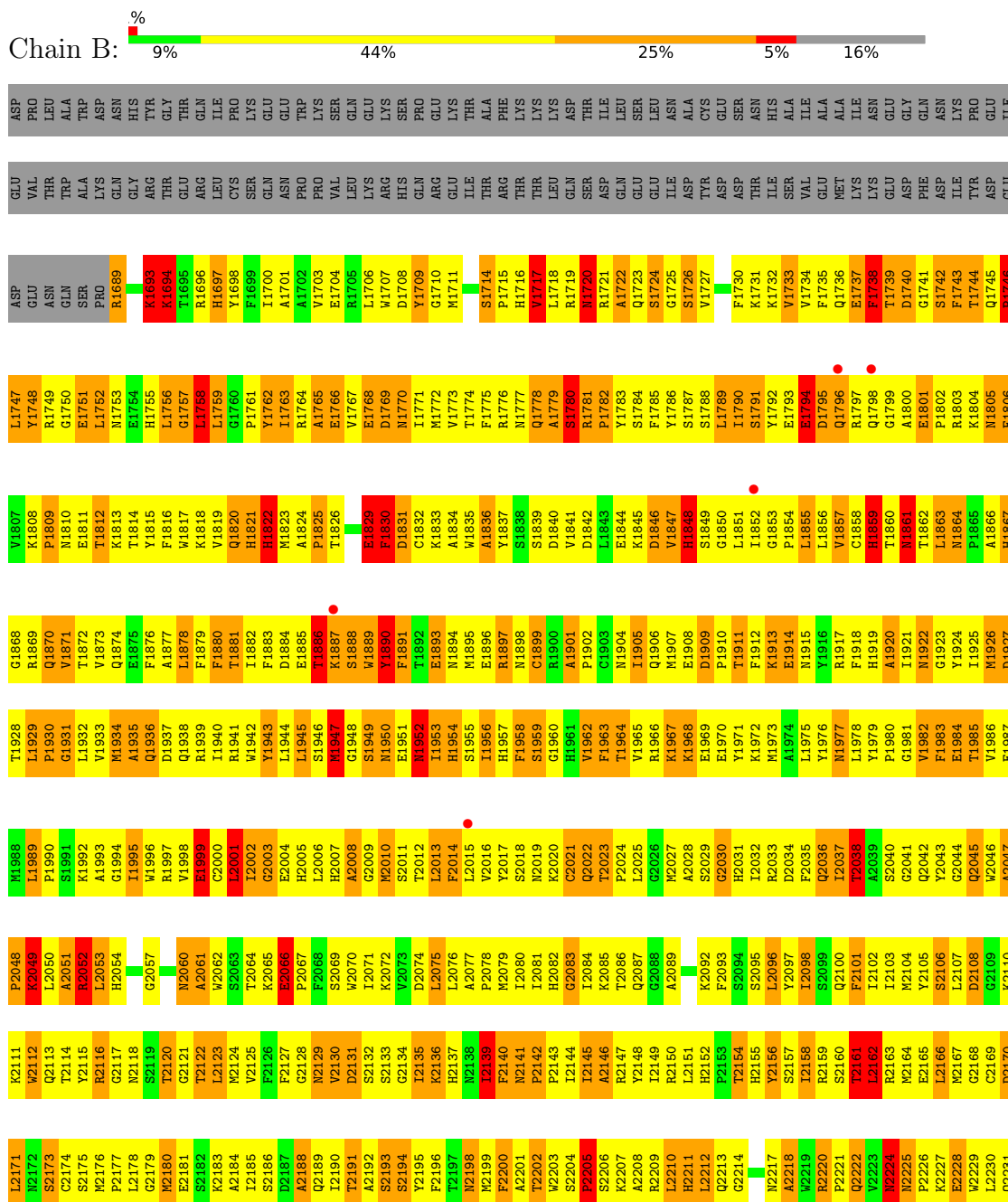
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | A     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | B     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

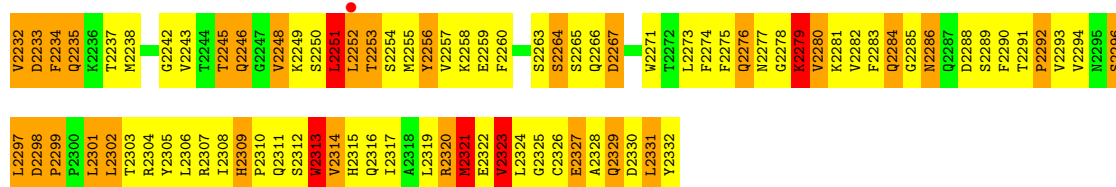
### 3 Residue-property plots

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

#### • Molecule 1: Coagulation factor VIII







- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 25% 25% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%



- Molecule 5: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 29% 71%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 134.57Å 134.57Å 359.50Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 57.37 – 3.70<br>57.37 – 3.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 85.0 (57.37-3.70)<br>85.0 (57.37-3.70)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.79 (at 3.57Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.279 , 0.347<br>0.293 , 0.357                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1924 reflections (4.95%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 125.7                                                       | Xtriage          |
| Anisotropy                                                              | 0.320                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 147.4                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 10985                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 168.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG, CA, CU

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.71         | 9/5749 (0.2%)  | 1.25        | 73/7806 (0.9%)   |
| 2   | B     | 0.55         | 0/5377         | 1.12        | 52/7280 (0.7%)   |
| All | All   | 0.64         | 9/11126 (0.1%) | 1.19        | 125/15086 (0.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 437 | LYS  | N-CA   | 8.30 | 1.56        | 1.46     |
| 1   | A     | 226 | ARG  | CZ-NH1 | 8.05 | 1.44        | 1.32     |
| 1   | A     | 226 | ARG  | N-CA   | 8.01 | 1.56        | 1.45     |
| 1   | A     | 226 | ARG  | CA-C   | 7.32 | 1.62        | 1.52     |
| 1   | A     | 226 | ARG  | CZ-NH2 | 6.68 | 1.42        | 1.33     |
| 1   | A     | 226 | ARG  | NE-CZ  | 6.34 | 1.40        | 1.33     |
| 1   | A     | 226 | ARG  | CA-CB  | 6.12 | 1.63        | 1.53     |
| 1   | A     | 437 | LYS  | CA-C   | 5.92 | 1.60        | 1.52     |
| 1   | A     | 437 | LYS  | CD-CE  | 5.53 | 1.69        | 1.52     |

All (125) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 694 | ASN  | N-CA-C | -14.11 | 96.53       | 113.88   |
| 1   | A     | 274 | HIS  | N-CA-C | 12.75  | 125.07      | 108.24   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | B     | 1929 | LEU  | CA-C-N | 12.11 | 134.98      | 119.84   |
| 2   | B     | 1929 | LEU  | C-N-CA | 12.11 | 134.98      | 119.84   |
| 1   | A     | 228  | TRP  | CA-C-N | 11.80 | 134.59      | 119.84   |
| 1   | A     | 228  | TRP  | C-N-CA | 11.80 | 134.59      | 119.84   |
| 1   | A     | 226  | ARG  | N-CA-C | 10.32 | 125.75      | 110.48   |
| 1   | A     | 504  | LEU  | CA-C-N | 9.70  | 131.96      | 119.84   |
| 1   | A     | 504  | LEU  | C-N-CA | 9.70  | 131.96      | 119.84   |
| 1   | A     | 442  | ILE  | N-CA-C | 9.63  | 121.17      | 107.88   |
| 1   | A     | 520  | GLY  | CA-C-N | 8.57  | 130.56      | 119.84   |
| 1   | A     | 520  | GLY  | C-N-CA | 8.57  | 130.56      | 119.84   |
| 1   | A     | 677  | THR  | N-CA-C | 8.37  | 120.86      | 108.14   |
| 1   | A     | 664  | TYR  | N-CA-C | -8.10 | 98.84       | 110.59   |
| 2   | B     | 1920 | ALA  | N-CA-C | 7.93  | 120.92      | 108.79   |
| 1   | A     | 515  | VAL  | N-CA-C | 7.71  | 118.98      | 106.72   |
| 1   | A     | 184  | LEU  | N-CA-C | -7.54 | 102.97      | 113.37   |
| 2   | B     | 1859 | HIS  | N-CA-C | 7.54  | 121.43      | 108.02   |
| 1   | A     | 31   | PRO  | CA-C-N | 7.49  | 129.21      | 119.84   |
| 1   | A     | 31   | PRO  | C-N-CA | 7.49  | 129.21      | 119.84   |
| 1   | A     | 66   | PRO  | CA-C-N | 7.48  | 129.19      | 119.84   |
| 1   | A     | 66   | PRO  | C-N-CA | 7.48  | 129.19      | 119.84   |
| 1   | A     | 229  | PRO  | N-CA-C | 7.41  | 127.74      | 112.47   |
| 1   | A     | 432  | THR  | N-CA-C | 7.34  | 120.86      | 112.57   |
| 2   | B     | 2188 | ALA  | N-CA-C | -7.25 | 104.04      | 114.12   |
| 1   | A     | 192  | LEU  | N-CA-C | -7.11 | 105.03      | 113.21   |
| 1   | A     | 108  | ALA  | N-CA-C | -7.04 | 105.51      | 112.97   |
| 2   | B     | 1999 | GLU  | N-CA-C | 7.02  | 119.19      | 108.52   |
| 2   | B     | 1922 | ASN  | N-CA-C | -6.99 | 104.33      | 112.86   |
| 1   | A     | 648  | PHE  | N-CA-C | 6.97  | 121.03      | 108.48   |
| 1   | A     | 702  | MET  | N-CA-C | -6.92 | 104.96      | 113.41   |
| 1   | A     | 300  | LEU  | N-CA-C | 6.80  | 120.40      | 108.56   |
| 2   | B     | 2320 | ARG  | N-CA-C | -6.70 | 98.92       | 109.50   |
| 2   | B     | 2029 | SER  | N-CA-C | -6.69 | 101.70      | 110.53   |
| 1   | A     | 548  | ILE  | N-CA-C | 6.65  | 115.81      | 107.70   |
| 2   | B     | 2083 | GLY  | N-CA-C | 6.56  | 118.76      | 110.96   |
| 1   | A     | 547  | LEU  | N-CA-C | 6.54  | 118.57      | 109.15   |
| 1   | A     | 453  | LEU  | N-CA-C | 6.53  | 118.13      | 107.23   |
| 2   | B     | 1848 | HIS  | N-CA-C | 6.52  | 118.18      | 111.14   |
| 1   | A     | 16   | TYR  | N-CA-C | -6.49 | 100.07      | 113.31   |
| 2   | B     | 2162 | LEU  | N-CA-C | 6.44  | 118.11      | 107.73   |
| 1   | A     | 205  | GLY  | N-CA-C | -6.36 | 98.11       | 113.18   |
| 1   | A     | 693  | HIS  | N-CA-C | 6.36  | 120.05      | 110.64   |
| 2   | B     | 1956 | ILE  | N-CA-C | 6.35  | 118.25      | 109.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 2049 | LYS  | N-CA-C  | -6.33 | 97.31       | 110.80   |
| 1   | A     | 668  | LEU  | N-CA-C  | -6.30 | 97.38       | 110.80   |
| 2   | B     | 1707 | TRP  | N-CA-C  | 6.25  | 119.76      | 108.69   |
| 1   | A     | 523  | LYS  | N-CA-C  | -6.22 | 103.79      | 112.12   |
| 1   | A     | 364  | ASN  | N-CA-C  | 6.19  | 118.48      | 108.32   |
| 1   | A     | 662  | MET  | N-CA-C  | -6.19 | 103.83      | 112.25   |
| 1   | A     | 298  | THR  | N-CA-C  | 6.17  | 118.23      | 107.49   |
| 1   | A     | 288  | ILE  | N-CA-C  | 6.15  | 117.33      | 108.48   |
| 1   | A     | 137  | VAL  | N-CA-C  | 6.14  | 116.45      | 108.35   |
| 1   | A     | 107  | LYS  | N-CA-C  | -6.11 | 103.69      | 113.28   |
| 2   | B     | 2321 | MET  | N-CA-C  | 6.10  | 116.48      | 107.88   |
| 2   | B     | 1758 | LEU  | N-CA-C  | -6.09 | 104.64      | 111.28   |
| 2   | B     | 1748 | TYR  | N-CA-C  | 6.08  | 118.31      | 109.07   |
| 1   | A     | 25   | PRO  | N-CA-C  | 6.08  | 120.19      | 111.13   |
| 1   | A     | 437  | LYS  | N-CA-C  | 6.06  | 123.71      | 110.80   |
| 2   | B     | 1714 | SER  | CA-C-N  | 6.04  | 127.39      | 119.84   |
| 2   | B     | 1714 | SER  | C-N-CA  | 6.04  | 127.39      | 119.84   |
| 2   | B     | 2096 | LEU  | N-CA-C  | 6.04  | 118.97      | 108.76   |
| 2   | B     | 1836 | ALA  | N-CA-C  | 6.02  | 118.44      | 108.99   |
| 1   | A     | 691  | GLY  | N-CA-C  | -5.99 | 98.99       | 113.18   |
| 2   | B     | 2028 | ALA  | N-CA-C  | -5.97 | 103.55      | 111.96   |
| 2   | B     | 1752 | LEU  | N-CA-C  | -5.96 | 106.01      | 113.28   |
| 1   | A     | 196  | ILE  | CB-CA-C | -5.95 | 104.48      | 111.09   |
| 1   | A     | 232  | HIS  | N-CA-C  | -5.95 | 98.13       | 110.80   |
| 1   | A     | 149  | SER  | N-CA-C  | -5.94 | 105.77      | 114.39   |
| 2   | B     | 1829 | GLU  | N-CA-C  | 5.88  | 123.31      | 110.80   |
| 2   | B     | 1954 | HIS  | N-CA-C  | 5.86  | 117.58      | 109.15   |
| 2   | B     | 2198 | ASN  | N-CA-C  | 5.85  | 116.01      | 108.34   |
| 2   | B     | 1798 | GLN  | CB-CA-C | -5.83 | 107.96      | 116.53   |
| 1   | A     | 230  | LYS  | N-CA-C  | 5.82  | 123.20      | 110.80   |
| 1   | A     | 52   | VAL  | N-CA-C  | 5.78  | 121.36      | 109.34   |
| 1   | A     | 666  | ASP  | N-CA-C  | 5.77  | 118.87      | 109.06   |
| 2   | B     | 1831 | ASP  | N-CA-C  | 5.76  | 123.08      | 110.80   |
| 2   | B     | 1842 | ASP  | N-CA-C  | -5.76 | 106.30      | 113.38   |
| 2   | B     | 1887 | LYS  | N-CA-C  | -5.73 | 98.59       | 110.80   |
| 2   | B     | 2092 | LYS  | CB-CA-C | -5.70 | 109.98      | 116.54   |
| 1   | A     | 78   | ALA  | N-CA-C  | 5.70  | 117.76      | 108.76   |
| 1   | A     | 228  | TRP  | N-CA-C  | 5.67  | 122.34      | 109.81   |
| 1   | A     | 37   | SER  | N-CA-C  | 5.61  | 118.97      | 109.76   |
| 1   | A     | 301  | MET  | N-CA-C  | -5.58 | 102.65      | 110.35   |
| 1   | A     | 587  | LEU  | N-CA-C  | -5.57 | 106.15      | 113.12   |
| 2   | B     | 1798 | GLN  | N-CA-C  | 5.54  | 114.07      | 108.75   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 142  | LYS  | N-CA-C  | -5.52 | 105.26      | 111.28   |
| 2   | B     | 1798 | GLN  | CA-C-O  | 5.51  | 121.80      | 118.33   |
| 1   | A     | 53   | GLU  | CA-C-O  | 5.50  | 121.13      | 117.94   |
| 2   | B     | 2023 | THR  | CA-C-N  | 5.49  | 125.42      | 119.76   |
| 2   | B     | 2023 | THR  | C-N-CA  | 5.49  | 125.42      | 119.76   |
| 2   | B     | 1794 | GLU  | N-CA-C  | 5.45  | 122.40      | 110.80   |
| 2   | B     | 1770 | ASN  | N-CA-C  | 5.42  | 118.28      | 108.69   |
| 1   | A     | 415  | GLY  | CA-C-N  | 5.42  | 125.24      | 119.28   |
| 1   | A     | 415  | GLY  | C-N-CA  | 5.42  | 125.24      | 119.28   |
| 1   | A     | 196  | ILE  | N-CA-C  | 5.42  | 116.25      | 106.61   |
| 2   | B     | 2140 | PHE  | N-CA-C  | -5.41 | 102.28      | 110.28   |
| 1   | A     | 501  | PHE  | N-CA-C  | 5.39  | 121.73      | 109.81   |
| 2   | B     | 2047 | ALA  | N-CA-C  | 5.38  | 121.70      | 109.81   |
| 1   | A     | 721  | ASP  | N-CA-C  | 5.38  | 115.49      | 108.07   |
| 2   | B     | 2222 | GLN  | N-CA-C  | -5.38 | 104.46      | 111.02   |
| 1   | A     | 123  | LYS  | N-CA-C  | -5.36 | 105.38      | 112.94   |
| 2   | B     | 2301 | LEU  | N-CA-C  | -5.35 | 103.83      | 110.41   |
| 1   | A     | 501  | PHE  | CA-C-N  | 5.32  | 126.49      | 119.84   |
| 1   | A     | 501  | PHE  | C-N-CA  | 5.32  | 126.49      | 119.84   |
| 2   | B     | 1724 | SER  | CB-CA-C | -5.31 | 110.43      | 116.54   |
| 1   | A     | 277  | LEU  | N-CA-C  | 5.31  | 118.36      | 107.69   |
| 1   | A     | 377  | LYS  | N-CA-C  | 5.30  | 122.08      | 110.80   |
| 2   | B     | 2122 | THR  | N-CA-C  | -5.25 | 106.85      | 113.20   |
| 2   | B     | 1694 | LYS  | N-CA-C  | 5.23  | 121.93      | 110.80   |
| 1   | A     | 282  | ARG  | N-CA-C  | -5.22 | 102.12      | 109.96   |
| 1   | A     | 506  | GLY  | N-CA-C  | -5.22 | 100.81      | 113.18   |
| 2   | B     | 1693 | LYS  | N-CA-C  | 5.21  | 117.12      | 110.61   |
| 1   | A     | 76   | ILE  | N-CA-C  | 5.20  | 113.86      | 106.53   |
| 1   | A     | 719  | TYR  | N-CA-C  | 5.17  | 116.69      | 108.67   |
| 2   | B     | 1956 | ILE  | CB-CA-C | -5.16 | 104.16      | 111.28   |
| 1   | A     | 96   | VAL  | N-CA-C  | 5.14  | 120.03      | 109.34   |
| 2   | B     | 2156 | TYR  | N-CA-C  | 5.14  | 116.61      | 108.96   |
| 2   | B     | 1872 | THR  | N-CA-C  | -5.13 | 105.19      | 111.75   |
| 1   | A     | 65   | ARG  | N-CA-C  | -5.11 | 104.26      | 110.13   |
| 2   | B     | 1738 | PHE  | N-CA-C  | 5.09  | 121.65      | 110.80   |
| 1   | A     | 58   | LEU  | N-CA-C  | 5.05  | 121.56      | 110.80   |
| 1   | A     | 577  | SER  | N-CA-C  | 5.04  | 116.73      | 108.76   |
| 2   | B     | 1994 | GLY  | N-CA-C  | -5.04 | 105.61      | 112.52   |
| 2   | B     | 1830 | PHE  | N-CA-C  | -5.00 | 100.14      | 110.80   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 385 | TYR  | Sidechain |
| 1   | A     | 656 | TYR  | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5590  | 0        | 5429     | 1243    | 0            |
| 2   | B     | 5229  | 0        | 5098     | 1159    | 0            |
| 3   | C     | 50    | 0        | 43       | 3       | 0            |
| 4   | D     | 28    | 0        | 25       | 0       | 0            |
| 5   | E     | 83    | 0        | 70       | 5       | 0            |
| 6   | A     | 3     | 0        | 0        | 0       | 0            |
| 7   | A     | 1     | 0        | 0        | 0       | 0            |
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 10985 | 0        | 10665    | 2351    | 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 109.

All (2351) 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:A:114:TYR:HE1  | 2:B:1997:ARG:HB2  | 1.11                     | 1.13              |
| 2:B:2284:GLN:HA  | 2:B:2284:GLN:HE21 | 1.14                     | 1.13              |
| 2:B:1901:ALA:HB1 | 2:B:1902:PRO:HD2  | 1.30                     | 1.12              |
| 1:A:499:LYS:HG3  | 1:A:500:ASP:H     | 1.15                     | 1.12              |
| 1:A:651:VAL:HG12 | 1:A:652:PHE:H     | 1.15                     | 1.11              |
| 1:A:18:GLN:HG2   | 1:A:19:SER:H      | 1.15                     | 1.09              |
| 1:A:228:TRP:HB3  | 1:A:229:PRO:HD2   | 1.22                     | 1.09              |
| 1:A:128:VAL:HG12 | 1:A:129:PHE:H     | 1.17                     | 1.09              |
| 2:B:2013:LEU:H   | 2:B:2013:LEU:HD22 | 1.16                     | 1.08              |
| 2:B:2176:MET:HG2 | 2:B:2177:PRO:HD2  | 1.30                     | 1.08              |
| 1:A:396:ALA:HB1  | 1:A:397:PRO:HA    | 1.19                     | 1.08              |
| 2:B:1934:MET:HB2 | 2:B:2016:VAL:HA   | 1.31                     | 1.08              |
| 1:A:65:ARG:HG3   | 1:A:66:PRO:HD2    | 1.30                     | 1.07              |
| 1:A:574:ILE:HB   | 1:A:639:ILE:HG23  | 1.27                     | 1.06              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:651:VAL:HG11  | 1:A:668:LEU:HA    | 1.37                     | 1.06              |
| 2:B:1929:LEU:HB3  | 2:B:2012:THR:HG21 | 1.36                     | 1.06              |
| 1:A:86:ILE:HG22   | 1:A:87:THR:H      | 1.15                     | 1.05              |
| 1:A:507:GLU:HG3   | 1:A:508:ILE:H     | 1.18                     | 1.03              |
| 2:B:2194:SER:HB3  | 2:B:2222:GLN:H    | 1.24                     | 1.03              |
| 2:B:2248:VAL:HG22 | 2:B:2249:LYS:H    | 1.24                     | 1.03              |
| 1:A:228:TRP:CB    | 1:A:229:PRO:HD2   | 1.88                     | 1.02              |
| 2:B:1820:GLN:NE2  | 2:B:1822:HIS:H    | 1.56                     | 1.02              |
| 1:A:266:VAL:HG12  | 1:A:267:HIS:H     | 1.25                     | 1.02              |
| 1:A:160:SER:HB3   | 1:A:172:LEU:HD23  | 1.39                     | 1.02              |
| 1:A:53:GLU:HG2    | 1:A:54:PHE:H      | 1.24                     | 1.02              |
| 2:B:2052:ARG:H    | 2:B:2163:ARG:HB3  | 1.21                     | 1.02              |
| 1:A:267:HIS:NE2   | 1:A:320:MET:HG3   | 1.75                     | 1.00              |
| 1:A:307:LEU:HD22  | 1:A:309:PHE:HB3   | 1.42                     | 1.00              |
| 2:B:2145:ILE:HD12 | 2:B:2145:ILE:H    | 1.26                     | 1.00              |
| 2:B:2225:ASN:HD22 | 2:B:2228:GLU:HG2  | 1.25                     | 1.00              |
| 2:B:2047:ALA:HA   | 2:B:2062:TRP:HD1  | 1.24                     | 1.00              |
| 1:A:444:HIS:HB2   | 1:A:620:TYR:OH    | 1.61                     | 1.00              |
| 1:A:167:ASP:HB3   | 1:A:172:LEU:HD22  | 1.41                     | 1.00              |
| 1:A:314:SER:HA    | 1:A:316:GLN:HE22  | 1.23                     | 0.99              |
| 1:A:60:ASN:O      | 1:A:61:ILE:HG13   | 1.61                     | 0.99              |
| 2:B:2180:MET:HE1  | 2:B:2190:ILE:HD11 | 1.44                     | 0.99              |
| 2:B:2053:LEU:HA   | 2:B:2163:ARG:HH21 | 1.26                     | 0.99              |
| 2:B:1764:ARG:HG2  | 2:B:1856:LEU:HD21 | 1.46                     | 0.98              |
| 1:A:168:LEU:HD13  | 1:A:260:MET:HE3   | 1.42                     | 0.97              |
| 1:A:275:THR:HA    | 1:A:284:ALA:HB2   | 1.43                     | 0.97              |
| 1:A:427:ARG:HH11  | 1:A:448:ILE:HA    | 1.30                     | 0.97              |
| 1:A:662:MET:HB2   | 1:A:680:MET:HE1   | 1.47                     | 0.97              |
| 2:B:1757:GLY:HA3  | 2:B:1922:ASN:HB3  | 1.46                     | 0.96              |
| 1:A:386:ILE:HD12  | 1:A:387:ALA:N     | 1.80                     | 0.96              |
| 1:A:642:ILE:HG22  | 1:A:643:GLY:H     | 1.30                     | 0.96              |
| 2:B:2081:ILE:HD11 | 2:B:2144:ILE:HB   | 1.47                     | 0.95              |
| 1:A:405:ARG:O     | 1:A:409:SER:HB3   | 1.67                     | 0.95              |
| 1:A:114:TYR:CE1   | 2:B:1997:ARG:HB2  | 2.01                     | 0.94              |
| 2:B:1715:PRO:HB2  | 2:B:1718:LEU:HB2  | 1.45                     | 0.94              |
| 1:A:561:GLN:HG2   | 1:A:562:ARG:H     | 1.32                     | 0.94              |
| 1:A:147:MET:C     | 1:A:149:SER:H     | 1.76                     | 0.93              |
| 1:A:80:VAL:HA     | 1:A:140:VAL:HG11  | 1.51                     | 0.93              |
| 2:B:2052:ARG:HE   | 2:B:2087:GLN:HE22 | 1.15                     | 0.93              |
| 2:B:2038:THR:HG22 | 2:B:2072:LYS:HG2  | 1.48                     | 0.93              |
| 1:A:106:TRP:NE1   | 2:B:2329:GLN:H    | 1.67                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:472:PRO:HB2   | 1:A:503:ILE:HG22  | 1.50                     | 0.93              |
| 1:A:656:TYR:CD1   | 1:A:686:GLY:HA2   | 2.04                     | 0.93              |
| 2:B:1767:VAL:HA   | 2:B:1819:VAL:HG11 | 1.51                     | 0.92              |
| 1:A:467:ASN:HD22  | 1:A:506:GLY:HA2   | 1.31                     | 0.91              |
| 2:B:1898:ASN:O    | 2:B:1899:CYS:HB2  | 1.70                     | 0.91              |
| 2:B:1689:ARG:NH1  | 2:B:1689:ARG:HB2  | 1.86                     | 0.91              |
| 1:A:448:ILE:HD13  | 1:A:448:ILE:H     | 1.32                     | 0.91              |
| 2:B:2194:SER:CB   | 2:B:2222:GLN:H    | 1.82                     | 0.91              |
| 2:B:2238:MET:HE1  | 2:B:2326:CYS:N    | 1.86                     | 0.91              |
| 1:A:474:ASN:ND2   | 1:A:475:ILE:H     | 1.68                     | 0.91              |
| 2:B:2186:SER:OG   | 2:B:2189:GLN:HG3  | 1.71                     | 0.90              |
| 2:B:1995:ILE:HD13 | 2:B:1995:ILE:N    | 1.87                     | 0.90              |
| 1:A:147:MET:HG3   | 2:B:1970:GLU:O    | 1.71                     | 0.90              |
| 1:A:424:LYS:H     | 1:A:590:ASN:HD21  | 1.19                     | 0.90              |
| 1:A:14:TRP:O      | 1:A:45:VAL:HG13   | 1.72                     | 0.90              |
| 2:B:2052:ARG:N    | 2:B:2163:ARG:HB3  | 1.85                     | 0.90              |
| 2:B:2052:ARG:NE   | 2:B:2087:GLN:HE22 | 1.69                     | 0.90              |
| 2:B:1700:ILE:HD11 | 2:B:1735:PHE:HB3  | 1.53                     | 0.90              |
| 2:B:2078:PRO:HB3  | 2:B:2107:LEU:HD21 | 1.54                     | 0.90              |
| 1:A:412:LEU:O     | 1:A:421:ARG:HB2   | 1.72                     | 0.90              |
| 1:A:65:ARG:CG     | 1:A:66:PRO:HD2    | 2.02                     | 0.89              |
| 2:B:2052:ARG:HE   | 2:B:2087:GLN:NE2  | 1.71                     | 0.89              |
| 1:A:529:LEU:CD1   | 1:A:553:ILE:HB    | 2.03                     | 0.89              |
| 1:A:266:VAL:HG12  | 1:A:267:HIS:N     | 1.86                     | 0.89              |
| 1:A:279:ARG:NH2   | 2:B:1971:TYR:HB3  | 1.87                     | 0.89              |
| 2:B:2024:PRO:HA   | 2:B:2167:MET:HB3  | 1.54                     | 0.89              |
| 1:A:411:TYR:O     | 1:A:420:GLY:HA3   | 1.74                     | 0.88              |
| 2:B:2251:LEU:O    | 2:B:2253:THR:HG22 | 1.72                     | 0.88              |
| 1:A:471:ARG:HG2   | 1:A:585:TRP:CE3   | 2.08                     | 0.88              |
| 1:A:35:PRO:HD2    | 1:A:40:PHE:HZ     | 1.36                     | 0.88              |
| 2:B:1715:PRO:HG2  | 2:B:1718:LEU:HD22 | 1.53                     | 0.88              |
| 2:B:1790:ILE:HA   | 2:B:1817:TRP:CE3  | 2.09                     | 0.88              |
| 1:A:617:ILE:HG13  | 1:A:704:ALA:HA    | 1.54                     | 0.88              |
| 2:B:2022:GLN:HG3  | 2:B:2082:HIS:HB2  | 1.55                     | 0.88              |
| 2:B:2116:ARG:HG3  | 2:B:2116:ARG:HH11 | 1.37                     | 0.88              |
| 1:A:392:ASP:HA    | 1:A:424:LYS:HA    | 1.56                     | 0.87              |
| 2:B:1883:PHE:HB2  | 2:B:1918:PHE:HB2  | 1.55                     | 0.87              |
| 2:B:1868:GLY:C    | 2:B:1869:ARG:HD2  | 2.00                     | 0.87              |
| 2:B:1794:GLU:HG3  | 2:B:1795:ASP:H    | 1.38                     | 0.87              |
| 2:B:1847:VAL:HG11 | 2:B:1947:MET:HE1  | 1.54                     | 0.87              |
| 1:A:661:LYS:HG2   | 1:A:665:GLU:HG2   | 1.57                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1736:GLN:HB3  | 2:B:1747:LEU:HD11 | 1.55                     | 0.86              |
| 2:B:1863:LEU:CD2  | 2:B:1863:LEU:H    | 1.88                     | 0.86              |
| 2:B:2209:ARG:H    | 2:B:2212:LEU:HD23 | 1.39                     | 0.86              |
| 1:A:106:TRP:HE1   | 2:B:2329:GLN:H    | 1.21                     | 0.86              |
| 1:A:456:GLU:O     | 1:A:459:ASP:HB2   | 1.76                     | 0.86              |
| 2:B:1863:LEU:H    | 2:B:1863:LEU:HD23 | 1.38                     | 0.86              |
| 1:A:53:GLU:HG2    | 1:A:54:PHE:N      | 1.91                     | 0.86              |
| 1:A:423:TYR:CD2   | 1:A:581:GLU:HG3   | 2.10                     | 0.85              |
| 1:A:267:HIS:O     | 1:A:288:ILE:HG23  | 1.77                     | 0.85              |
| 1:A:51:PHE:CE1    | 1:A:172:LEU:HA    | 2.11                     | 0.85              |
| 2:B:1929:LEU:HB3  | 2:B:2012:THR:CG2  | 2.06                     | 0.85              |
| 2:B:1932:LEU:HD13 | 2:B:2014:PHE:HB3  | 1.56                     | 0.85              |
| 1:A:228:TRP:HB3   | 1:A:229:PRO:CD    | 2.06                     | 0.85              |
| 1:A:249:HIS:HD2   | 1:A:303:LEU:HD12  | 1.39                     | 0.85              |
| 1:A:615:HIS:HB2   | 1:A:703:THR:HG23  | 1.58                     | 0.85              |
| 2:B:2064:THR:HG23 | 2:B:2160:SER:HB2  | 1.56                     | 0.85              |
| 1:A:587:LEU:HD23  | 1:A:588:THR:H     | 1.42                     | 0.84              |
| 1:A:152:LEU:HD23  | 1:A:179:CYS:HB3   | 1.58                     | 0.84              |
| 1:A:86:ILE:HG22   | 1:A:87:THR:N      | 1.90                     | 0.84              |
| 2:B:1784:SER:O    | 2:B:1839:SER:HA   | 1.77                     | 0.84              |
| 2:B:2145:ILE:HD12 | 2:B:2145:ILE:N    | 1.90                     | 0.84              |
| 1:A:396:ALA:HB1   | 1:A:397:PRO:CA    | 2.05                     | 0.84              |
| 1:A:651:VAL:H     | 1:A:693:HIS:CB    | 1.90                     | 0.84              |
| 1:A:663:VAL:HG13  | 2:B:1968:LYS:HG3  | 1.59                     | 0.84              |
| 1:A:658:PHE:CZ    | 1:A:686:GLY:HA3   | 2.12                     | 0.84              |
| 2:B:1996:TRP:O    | 2:B:2013:LEU:HA   | 1.77                     | 0.84              |
| 2:B:2084:ILE:HG12 | 2:B:2085:LYS:N    | 1.91                     | 0.84              |
| 2:B:1689:ARG:HB2  | 2:B:1689:ARG:HH11 | 1.41                     | 0.84              |
| 1:A:452:LEU:C     | 1:A:453:LEU:HD23  | 2.02                     | 0.83              |
| 2:B:1934:MET:HB2  | 2:B:2016:VAL:CA   | 2.08                     | 0.83              |
| 2:B:2084:ILE:HG12 | 2:B:2085:LYS:H    | 1.40                     | 0.83              |
| 2:B:1782:PRO:HB3  | 2:B:1808:LYS:HA   | 1.60                     | 0.83              |
| 1:A:47:LYS:HD3    | 1:A:225:ALA:HB1   | 1.60                     | 0.83              |
| 1:A:303:LEU:HD23  | 1:A:304:GLY:N     | 1.93                     | 0.83              |
| 2:B:2116:ARG:HH21 | 2:B:2120:THR:HA   | 1.42                     | 0.83              |
| 2:B:2313:TRP:CD1  | 2:B:2313:TRP:H    | 1.90                     | 0.83              |
| 1:A:499:LYS:HG3   | 1:A:500:ASP:N     | 1.94                     | 0.82              |
| 1:A:639:ILE:H     | 1:A:639:ILE:HD12  | 1.44                     | 0.82              |
| 2:B:2036:GLN:O    | 2:B:2037:ILE:HG23 | 1.79                     | 0.82              |
| 2:B:2053:LEU:HA   | 2:B:2163:ARG:NH2  | 1.94                     | 0.82              |
| 2:B:1801:GLU:H    | 2:B:1802:PRO:HD2  | 1.44                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2209:ARG:H    | 2:B:2212:LEU:CD2  | 1.92                     | 0.82              |
| 2:B:1745:GLN:HG2  | 2:B:1746:PRO:HB3  | 1.60                     | 0.82              |
| 2:B:1976:TYR:OH   | 2:B:1984:GLU:HG3  | 1.78                     | 0.82              |
| 1:A:655:GLY:HA3   | 1:A:687:LEU:HB3   | 1.61                     | 0.82              |
| 2:B:2284:GLN:HA   | 2:B:2284:GLN:NE2  | 1.93                     | 0.82              |
| 1:A:53:GLU:CG     | 1:A:54:PHE:H      | 1.85                     | 0.82              |
| 1:A:698:ARG:O     | 1:A:702:MET:HB2   | 1.80                     | 0.82              |
| 2:B:1905:ILE:CG2  | 2:B:1910:PRO:HB2  | 2.10                     | 0.82              |
| 2:B:2100:GLN:HG3  | 2:B:2154:THR:HB   | 1.62                     | 0.82              |
| 1:A:121:ARG:HH11  | 2:B:2302:LEU:HD21 | 1.45                     | 0.82              |
| 1:A:249:HIS:CD2   | 1:A:303:LEU:HD12  | 2.15                     | 0.81              |
| 2:B:1697:HIS:HA   | 2:B:1772:MET:HB3  | 1.61                     | 0.81              |
| 2:B:1785:PHE:HB3  | 2:B:1815:TYR:HE2  | 1.45                     | 0.81              |
| 1:A:461:LEU:HB3   | 1:A:463:ILE:HD11  | 1.63                     | 0.81              |
| 1:A:507:GLU:CG    | 1:A:508:ILE:H     | 1.93                     | 0.81              |
| 2:B:1878:LEU:HB2  | 2:B:1880:PHE:HE1  | 1.42                     | 0.81              |
| 1:A:121:ARG:O     | 1:A:122:GLU:HG3   | 1.79                     | 0.81              |
| 2:B:2095:SER:C    | 2:B:2096:LEU:HD22 | 2.05                     | 0.81              |
| 2:B:2301:LEU:HD23 | 2:B:2302:LEU:H    | 1.44                     | 0.81              |
| 1:A:34:VAL:N      | 1:A:35:PRO:HD3    | 1.96                     | 0.81              |
| 2:B:1982:VAL:HG22 | 2:B:1983:PHE:H    | 1.45                     | 0.81              |
| 1:A:51:PHE:HD1    | 1:A:51:PHE:H      | 1.26                     | 0.81              |
| 1:A:540:GLU:HG2   | 1:A:541:ARG:N     | 1.95                     | 0.81              |
| 2:B:1882:ILE:HG22 | 2:B:1952:ASN:ND2  | 1.96                     | 0.81              |
| 2:B:2052:ARG:H    | 2:B:2163:ARG:CB   | 1.93                     | 0.81              |
| 2:B:1731:LYS:H    | 2:B:1893:GLU:CD   | 1.88                     | 0.81              |
| 1:A:18:GLN:HG2    | 1:A:19:SER:N      | 1.94                     | 0.80              |
| 1:A:578:VAL:CG2   | 1:A:644:ALA:H     | 1.95                     | 0.80              |
| 2:B:2264:SER:HB2  | 2:B:2301:LEU:HD11 | 1.64                     | 0.80              |
| 1:A:4:ARG:HD2     | 1:A:6:TYR:HE2     | 1.45                     | 0.80              |
| 1:A:471:ARG:HG2   | 1:A:585:TRP:HE3   | 1.42                     | 0.80              |
| 2:B:1901:ALA:HB1  | 2:B:1902:PRO:CD   | 2.09                     | 0.80              |
| 2:B:2201:ALA:O    | 2:B:2202:THR:HG23 | 1.81                     | 0.80              |
| 1:A:106:TRP:HE1   | 2:B:2329:GLN:N    | 1.79                     | 0.80              |
| 1:A:268:SER:H     | 1:A:312:ILE:HD11  | 1.47                     | 0.80              |
| 2:B:2078:PRO:HG2  | 2:B:2171:LEU:HD21 | 1.62                     | 0.80              |
| 2:B:2023:THR:HG23 | 2:B:2024:PRO:HD2  | 1.64                     | 0.80              |
| 2:B:1776:ARG:HG3  | 2:B:1812:THR:CG2  | 2.12                     | 0.80              |
| 2:B:1968:LYS:O    | 2:B:1969:GLU:HG2  | 1.80                     | 0.80              |
| 1:A:555:TYR:O     | 1:A:556:LYS:HG2   | 1.82                     | 0.80              |
| 2:B:1717:VAL:HG12 | 2:B:1720:ASN:HA   | 1.62                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:266:VAL:CG1   | 1:A:267:HIS:H     | 1.93                     | 0.80              |
| 1:A:461:LEU:HD23  | 1:A:513:TRP:CE3   | 2.17                     | 0.80              |
| 1:A:663:VAL:HG22  | 2:B:1968:LYS:HD2  | 1.62                     | 0.80              |
| 2:B:2298:ASP:HB2  | 2:B:2299:PRO:HD3  | 1.63                     | 0.80              |
| 2:B:1837:TYR:CE1  | 2:B:1853:GLY:HA3  | 2.17                     | 0.79              |
| 1:A:148:ALA:HA    | 1:A:180:ARG:HH21  | 1.45                     | 0.79              |
| 1:A:616:SER:HB2   | 1:A:619:GLY:H     | 1.47                     | 0.79              |
| 2:B:2052:ARG:NH2  | 2:B:2053:LEU:HG   | 1.97                     | 0.79              |
| 5:E:2:NAG:H62     | 5:E:3:BMA:H2      | 1.62                     | 0.79              |
| 1:A:86:ILE:CG2    | 1:A:87:THR:H      | 1.95                     | 0.79              |
| 1:A:473:TYR:HA    | 1:A:537:VAL:CG2   | 2.12                     | 0.79              |
| 1:A:495:VAL:HG22  | 1:A:496:LYS:H     | 1.48                     | 0.79              |
| 1:A:503:ILE:H     | 1:A:503:ILE:HD12  | 1.47                     | 0.79              |
| 1:A:527:ARG:O     | 1:A:528:CYS:HB2   | 1.80                     | 0.79              |
| 2:B:1938:GLN:O    | 2:B:1940:ILE:HG13 | 1.82                     | 0.79              |
| 1:A:424:LYS:H     | 1:A:590:ASN:ND2   | 1.80                     | 0.79              |
| 1:A:507:GLU:HG3   | 1:A:508:ILE:N     | 1.98                     | 0.79              |
| 1:A:575:LEU:HA    | 1:A:640:LEU:O     | 1.81                     | 0.79              |
| 1:A:651:VAL:HG12  | 1:A:652:PHE:N     | 1.96                     | 0.79              |
| 1:A:432:THR:HA    | 1:A:438:THR:OG1   | 1.82                     | 0.79              |
| 1:A:484:ARG:HH11  | 1:A:486:LEU:HA    | 1.46                     | 0.79              |
| 2:B:1992:LYS:HE3  | 2:B:1993:ALA:H    | 1.48                     | 0.79              |
| 1:A:526:PRO:HB2   | 1:A:679:PHE:CE2   | 2.17                     | 0.79              |
| 2:B:2052:ARG:NH1  | 2:B:2053:LEU:HD12 | 1.98                     | 0.79              |
| 2:B:2209:ARG:O    | 2:B:2212:LEU:HB3  | 1.82                     | 0.79              |
| 1:A:497:HIS:ND1   | 1:A:499:LYS:HG2   | 1.97                     | 0.79              |
| 2:B:1758:LEU:HD22 | 2:B:1758:LEU:H    | 1.47                     | 0.79              |
| 2:B:2224:ASN:HD21 | 2:B:2316:GLN:HE21 | 1.29                     | 0.79              |
| 1:A:271:LEU:O     | 1:A:273:GLY:N     | 2.16                     | 0.78              |
| 1:A:639:ILE:HD12  | 1:A:639:ILE:N     | 1.98                     | 0.78              |
| 1:A:654:SER:HB2   | 1:A:690:LEU:HA    | 1.65                     | 0.78              |
| 1:A:662:MET:O     | 1:A:663:VAL:HB    | 1.82                     | 0.78              |
| 1:A:434:GLU:HB2   | 1:A:466:LYS:HE3   | 1.63                     | 0.78              |
| 2:B:1782:PRO:HB3  | 2:B:1809:PRO:HD3  | 1.65                     | 0.78              |
| 2:B:2279:LYS:HD3  | 2:B:2279:LYS:H    | 1.47                     | 0.78              |
| 2:B:1909:ASP:HB3  | 2:B:1910:PRO:HD3  | 1.64                     | 0.78              |
| 1:A:273:GLY:HA3   | 1:A:306:PHE:HD2   | 1.49                     | 0.78              |
| 2:B:2098:ILE:HD13 | 2:B:2098:ILE:N    | 1.99                     | 0.78              |
| 2:B:1719:ARG:HA   | 2:B:1719:ARG:HE   | 1.49                     | 0.78              |
| 2:B:1946:SER:O    | 2:B:1947:MET:HB2  | 1.82                     | 0.78              |
| 2:B:2096:LEU:HD12 | 2:B:2159:ARG:O    | 1.83                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:128:VAL:HG12  | 1:A:129:PHE:N     | 1.94                     | 0.78              |
| 2:B:1772:MET:HE3  | 2:B:1773:VAL:N    | 1.99                     | 0.78              |
| 2:B:2304:ARG:HG3  | 2:B:2305:TYR:HD1  | 1.48                     | 0.78              |
| 1:A:431:TYR:HD2   | 1:A:434:GLU:HB3   | 1.46                     | 0.77              |
| 2:B:2176:MET:CG   | 2:B:2177:PRO:HD2  | 2.13                     | 0.77              |
| 1:A:617:ILE:O     | 1:A:618:ASN:HB2   | 1.84                     | 0.77              |
| 2:B:1905:ILE:HG23 | 2:B:1910:PRO:HB2  | 1.66                     | 0.77              |
| 1:A:498:LEU:H     | 1:A:498:LEU:HD12  | 1.50                     | 0.77              |
| 1:A:521:PRO:HD3   | 1:A:529:LEU:HD11  | 1.66                     | 0.77              |
| 2:B:1821:HIS:C    | 2:B:1823:MET:H    | 1.91                     | 0.77              |
| 2:B:1857:VAL:HG23 | 2:B:1858:CYS:N    | 1.98                     | 0.77              |
| 2:B:2000:CYS:SG   | 2:B:2002:ILE:HD12 | 2.25                     | 0.77              |
| 2:B:2286:ASN:H    | 2:B:2293:VAL:HG11 | 1.47                     | 0.77              |
| 1:A:7:LEU:HD11    | 1:A:51:PHE:HB3    | 1.64                     | 0.77              |
| 2:B:2144:ILE:HG22 | 2:B:2145:ILE:N    | 1.98                     | 0.77              |
| 1:A:51:PHE:HE1    | 1:A:172:LEU:HA    | 1.48                     | 0.77              |
| 1:A:102:GLY:C     | 1:A:103:VAL:HG22  | 2.10                     | 0.77              |
| 1:A:396:ALA:CB    | 1:A:397:PRO:HA    | 2.09                     | 0.77              |
| 1:A:430:ALA:HB3   | 1:A:440:GLU:HB3   | 1.67                     | 0.77              |
| 2:B:1885:GLU:O    | 2:B:1887:LYS:N    | 2.18                     | 0.77              |
| 2:B:2077:ALA:C    | 2:B:2147:ARG:HG3  | 2.10                     | 0.77              |
| 2:B:2192:ALA:HB2  | 2:B:2230:LEU:HD12 | 1.66                     | 0.77              |
| 2:B:2276:GLN:C    | 2:B:2278:GLY:H    | 1.92                     | 0.77              |
| 1:A:17:MET:SD     | 1:A:63:LYS:HE2    | 2.24                     | 0.77              |
| 2:B:1878:LEU:HD11 | 2:B:1942:TRP:CZ3  | 2.20                     | 0.77              |
| 1:A:114:TYR:HE1   | 2:B:1997:ARG:CB   | 1.94                     | 0.77              |
| 1:A:147:MET:O     | 1:A:149:SER:N     | 2.18                     | 0.77              |
| 1:A:378:HIS:HB2   | 1:A:379:PRO:HD2   | 1.67                     | 0.77              |
| 1:A:450:GLY:O     | 1:A:550:PRO:HD2   | 1.85                     | 0.77              |
| 2:B:1856:LEU:HD23 | 2:B:1856:LEU:H    | 1.49                     | 0.77              |
| 1:A:521:PRO:HG3   | 1:A:529:LEU:HG    | 1.67                     | 0.76              |
| 1:A:523:LYS:HD2   | 1:A:523:LYS:N     | 2.00                     | 0.76              |
| 1:A:183:SER:C     | 1:A:185:ALA:H     | 1.91                     | 0.76              |
| 1:A:448:ILE:HD12  | 1:A:619:GLY:HA3   | 1.64                     | 0.76              |
| 1:A:526:PRO:HB2   | 1:A:679:PHE:CZ    | 2.21                     | 0.76              |
| 1:A:624:SER:C     | 1:A:625:LEU:HD12  | 2.11                     | 0.76              |
| 1:A:625:LEU:O     | 1:A:626:GLN:HG2   | 1.85                     | 0.76              |
| 1:A:653:PHE:HA    | 1:A:657:THR:HA    | 1.66                     | 0.76              |
| 1:A:690:LEU:HD13  | 1:A:708:VAL:HG21  | 1.66                     | 0.76              |
| 2:B:1738:PHE:HE1  | 2:B:1742:SER:HA   | 1.51                     | 0.76              |
| 1:A:206:LYS:O     | 1:A:207:SER:HB2   | 1.85                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1738:PHE:HB3  | 2:B:1747:LEU:HA   | 1.65                     | 0.76              |
| 2:B:1785:PHE:HB3  | 2:B:1815:TYR:CE2  | 2.20                     | 0.76              |
| 2:B:2166:LEU:HD12 | 2:B:2166:LEU:O    | 1.85                     | 0.76              |
| 2:B:2237:THR:HG22 | 2:B:2238:MET:H    | 1.50                     | 0.76              |
| 1:A:96:VAL:HA     | 1:A:162:VAL:HG21  | 1.68                     | 0.76              |
| 1:A:692:CYS:HB3   | 1:A:705:LEU:O     | 1.85                     | 0.76              |
| 2:B:1735:PHE:CE1  | 2:B:1851:LEU:HG   | 2.21                     | 0.76              |
| 2:B:2248:VAL:HG22 | 2:B:2249:LYS:N    | 2.01                     | 0.76              |
| 2:B:1770:ASN:HB3  | 2:B:1816:PHE:CE1  | 2.21                     | 0.76              |
| 1:A:461:LEU:HD23  | 1:A:513:TRP:HE3   | 1.48                     | 0.76              |
| 1:A:462:LEU:C     | 1:A:463:ILE:HD13  | 2.11                     | 0.76              |
| 2:B:1770:ASN:HB3  | 2:B:1816:PHE:HE1  | 1.49                     | 0.76              |
| 2:B:2098:ILE:HD12 | 2:B:2161:THR:O    | 1.86                     | 0.76              |
| 1:A:658:PHE:CE1   | 1:A:686:GLY:HA3   | 2.20                     | 0.75              |
| 2:B:2122:THR:HG23 | 2:B:2123:LEU:HG   | 1.66                     | 0.75              |
| 2:B:2210:LEU:HG   | 2:B:2211:HIS:ND1  | 2.00                     | 0.75              |
| 1:A:147:MET:C     | 1:A:149:SER:N     | 2.41                     | 0.75              |
| 1:A:431:TYR:CD2   | 1:A:434:GLU:HB3   | 2.22                     | 0.75              |
| 2:B:1789:LEU:C    | 2:B:1791:SER:H    | 1.93                     | 0.75              |
| 1:A:106:TRP:CD1   | 2:B:2329:GLN:H    | 2.04                     | 0.75              |
| 1:A:192:LEU:O     | 1:A:192:LEU:HD13  | 1.86                     | 0.75              |
| 1:A:232:HIS:HB3   | 1:A:320:MET:HG2   | 1.68                     | 0.75              |
| 2:B:1889:TRP:O    | 2:B:1890:TYR:HB2  | 1.85                     | 0.75              |
| 2:B:1927:ASP:HB3  | 2:B:2013:LEU:HD21 | 1.68                     | 0.75              |
| 2:B:2053:LEU:CA   | 2:B:2163:ARG:HH21 | 1.99                     | 0.75              |
| 2:B:2096:LEU:HB3  | 2:B:2161:THR:HG21 | 1.69                     | 0.75              |
| 1:A:125:ASP:OD1   | 1:A:134:HIS:HB3   | 1.86                     | 0.75              |
| 1:A:450:GLY:H     | 1:A:549:GLY:HA2   | 1.51                     | 0.75              |
| 2:B:1953:ILE:H    | 2:B:1953:ILE:HD12 | 1.50                     | 0.75              |
| 2:B:2271:TRP:HZ3  | 2:B:2307:ARG:HB2  | 1.52                     | 0.75              |
| 1:A:316:GLN:CD    | 1:A:316:GLN:H     | 1.95                     | 0.75              |
| 1:A:373:SER:O     | 1:A:374:VAL:HG22  | 1.86                     | 0.75              |
| 2:B:1982:VAL:HG22 | 2:B:1983:PHE:N    | 2.00                     | 0.75              |
| 2:B:2052:ARG:HH12 | 2:B:2053:LEU:HD12 | 1.52                     | 0.75              |
| 2:B:1799:GLY:HA3  | 2:B:1802:PRO:HG2  | 1.69                     | 0.74              |
| 2:B:2260:PHE:CB   | 2:B:2310:PRO:HA   | 2.17                     | 0.74              |
| 1:A:425:LYS:HE2   | 1:A:581:GLU:CD    | 2.12                     | 0.74              |
| 2:B:1969:GLU:HB2  | 2:B:1971:TYR:CZ   | 2.22                     | 0.74              |
| 2:B:2064:THR:CG2  | 2:B:2160:SER:HB2  | 2.16                     | 0.74              |
| 1:A:461:LEU:HB2   | 1:A:513:TRP:HB2   | 1.67                     | 0.74              |
| 1:A:682:MET:O     | 1:A:683:GLU:C     | 2.30                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1963:PHE:O    | 2:B:1972:LYS:HG3  | 1.86                     | 0.74              |
| 2:B:1796:GLN:O    | 2:B:1797:ARG:HB3  | 1.84                     | 0.74              |
| 2:B:2179:GLY:HA2  | 2:B:2184:ALA:HB3  | 1.70                     | 0.74              |
| 1:A:46:TYR:HE1    | 1:A:227:ALA:HB3   | 1.51                     | 0.74              |
| 1:A:162:VAL:HG23  | 1:A:162:VAL:O     | 1.87                     | 0.74              |
| 1:A:231:MET:HE2   | 1:A:231:MET:HA    | 1.70                     | 0.74              |
| 1:A:657:THR:HG21  | 2:B:1788:SER:HA   | 1.70                     | 0.74              |
| 2:B:1934:MET:HE2  | 2:B:1934:MET:HA   | 1.68                     | 0.74              |
| 1:A:35:PRO:HD2    | 1:A:40:PHE:CZ     | 2.22                     | 0.74              |
| 1:A:688:TRP:HE1   | 2:B:1799:GLY:HA2  | 1.53                     | 0.74              |
| 2:B:2052:ARG:NE   | 2:B:2087:GLN:NE2  | 2.33                     | 0.74              |
| 2:B:2304:ARG:HG3  | 2:B:2305:TYR:CD1  | 2.22                     | 0.74              |
| 1:A:75:THR:HG22   | 1:A:175:ALA:HB3   | 1.70                     | 0.74              |
| 1:A:428:PHE:HE1   | 1:A:547:LEU:HB3   | 1.52                     | 0.74              |
| 1:A:540:GLU:HG2   | 1:A:541:ARG:H     | 1.53                     | 0.74              |
| 2:B:2075:LEU:HB3  | 2:B:2079:MET:HE3  | 1.70                     | 0.74              |
| 2:B:2116:ARG:HG3  | 2:B:2116:ARG:NH1  | 2.02                     | 0.74              |
| 1:A:267:HIS:CE1   | 1:A:315:HIS:HB3   | 2.23                     | 0.73              |
| 2:B:1740:ASP:HA   | 2:B:1776:ARG:HH22 | 1.51                     | 0.73              |
| 1:A:501:PHE:O     | 1:A:503:ILE:N     | 2.20                     | 0.73              |
| 1:A:659:LYS:HD3   | 1:A:659:LYS:N     | 2.03                     | 0.73              |
| 2:B:2107:LEU:HD23 | 2:B:2147:ARG:HB2  | 1.69                     | 0.73              |
| 1:A:88:LEU:HD23   | 1:A:89:LYS:N      | 2.04                     | 0.73              |
| 1:A:574:ILE:HB    | 1:A:639:ILE:CG2   | 2.14                     | 0.73              |
| 1:A:656:TYR:CG    | 1:A:686:GLY:HA2   | 2.23                     | 0.73              |
| 2:B:1945:LEU:HA   | 2:B:1983:PHE:HA   | 1.70                     | 0.73              |
| 1:A:663:VAL:HA    | 2:B:1968:LYS:NZ   | 2.04                     | 0.73              |
| 1:A:661:LYS:C     | 1:A:680:MET:SD    | 2.71                     | 0.73              |
| 2:B:2284:GLN:HE21 | 2:B:2284:GLN:CA   | 1.95                     | 0.73              |
| 1:A:289:SER:HB3   | 1:A:290:PRO:HD2   | 1.69                     | 0.73              |
| 1:A:651:VAL:CG1   | 1:A:668:LEU:HA    | 2.18                     | 0.73              |
| 2:B:1940:ILE:HD12 | 2:B:1990:PRO:HD3  | 1.71                     | 0.73              |
| 2:B:2027:MET:H    | 2:B:2165:GLU:HG3  | 1.52                     | 0.73              |
| 1:A:203:ASP:O     | 1:A:205:GLY:N     | 2.22                     | 0.73              |
| 2:B:2106:SER:OG   | 2:B:2111:LYS:HB3  | 1.87                     | 0.73              |
| 1:A:271:LEU:HD12  | 1:A:274:HIS:N     | 2.03                     | 0.73              |
| 1:A:452:LEU:H     | 1:A:452:LEU:HD13  | 1.53                     | 0.73              |
| 2:B:1998:VAL:O    | 2:B:2011:SER:HA   | 1.88                     | 0.73              |
| 1:A:99:HIS:N      | 1:A:159:LEU:O     | 2.21                     | 0.72              |
| 1:A:169:ASN:HD21  | 1:A:262:THR:HG21  | 1.50                     | 0.72              |
| 1:A:453:LEU:HD21  | 1:A:533:TYR:HE2   | 1.52                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:396:ALA:HB2   | 1:A:421:ARG:HH11  | 1.54                     | 0.72              |
| 1:A:473:TYR:HA    | 1:A:537:VAL:HG21  | 1.70                     | 0.72              |
| 2:B:1763:ILE:HG23 | 2:B:1855:LEU:HG   | 1.69                     | 0.72              |
| 1:A:98:LEU:HB3    | 1:A:136:TYR:CE2   | 2.24                     | 0.72              |
| 1:A:385:TYR:CD2   | 1:A:437:LYS:HB2   | 2.24                     | 0.72              |
| 1:A:528:CYS:HA    | 1:A:553:ILE:O     | 1.89                     | 0.72              |
| 2:B:1920:ALA:HB1  | 2:B:1924:TYR:H    | 1.53                     | 0.72              |
| 2:B:1995:ILE:HD13 | 2:B:1995:ILE:H    | 1.51                     | 0.72              |
| 1:A:21:LEU:HD12   | 1:A:32:PRO:HG2    | 1.70                     | 0.72              |
| 1:A:578:VAL:H     | 1:A:643:GLY:HA3   | 1.55                     | 0.72              |
| 2:B:1771:ILE:HB   | 2:B:1817:TRP:NE1  | 2.04                     | 0.72              |
| 1:A:448:ILE:HD13  | 1:A:448:ILE:N     | 2.02                     | 0.72              |
| 2:B:2210:LEU:O    | 2:B:2212:LEU:N    | 2.21                     | 0.72              |
| 2:B:2259:GLU:H    | 2:B:2312:SER:HB2  | 1.53                     | 0.72              |
| 1:A:128:VAL:CG1   | 1:A:129:PHE:H     | 2.01                     | 0.72              |
| 1:A:498:LEU:HA    | 1:A:502:PRO:HG2   | 1.71                     | 0.72              |
| 2:B:2157:SER:O    | 2:B:2158:ILE:HG22 | 1.89                     | 0.72              |
| 2:B:2313:TRP:CD1  | 2:B:2313:TRP:N    | 2.55                     | 0.72              |
| 1:A:146:PRO:HG3   | 1:A:180:ARG:HG2   | 1.71                     | 0.72              |
| 1:A:241:SER:O     | 1:A:242:LEU:HB3   | 1.88                     | 0.72              |
| 1:A:384:HIS:O     | 1:A:386:ILE:HG23  | 1.89                     | 0.72              |
| 1:A:694:ASN:HD22  | 1:A:699:ASN:HB3   | 1.53                     | 0.72              |
| 2:B:1752:LEU:HD23 | 2:B:1752:LEU:O    | 1.89                     | 0.72              |
| 2:B:2106:SER:O    | 2:B:2146:ALA:HB1  | 1.90                     | 0.72              |
| 1:A:425:LYS:HD3   | 1:A:545:SER:O     | 1.89                     | 0.72              |
| 2:B:1934:MET:O    | 2:B:1935:ALA:HB2  | 1.89                     | 0.72              |
| 2:B:1946:SER:HB2  | 2:B:1978:LEU:HD13 | 1.71                     | 0.72              |
| 2:B:2225:ASN:HD21 | 2:B:2228:GLU:N    | 1.88                     | 0.72              |
| 1:A:86:ILE:O      | 1:A:87:THR:OG1    | 2.06                     | 0.71              |
| 1:A:105:TYR:O     | 1:A:106:TRP:HB2   | 1.90                     | 0.71              |
| 1:A:304:GLY:H     | 1:A:326:VAL:HG13  | 1.54                     | 0.71              |
| 1:A:642:ILE:HG22  | 1:A:643:GLY:N     | 2.04                     | 0.71              |
| 1:A:667:THR:C     | 1:A:669:THR:HG22  | 2.15                     | 0.71              |
| 2:B:1953:ILE:HD12 | 2:B:1953:ILE:N    | 2.05                     | 0.71              |
| 2:B:2237:THR:HG22 | 2:B:2238:MET:N    | 2.04                     | 0.71              |
| 1:A:286:LEU:O     | 1:A:288:ILE:HG22  | 1.90                     | 0.71              |
| 2:B:1946:SER:HB2  | 2:B:1978:LEU:CD1  | 2.19                     | 0.71              |
| 1:A:417:GLN:O     | 1:A:418:ARG:HD3   | 1.91                     | 0.71              |
| 1:A:448:ILE:H     | 1:A:448:ILE:CD1   | 2.01                     | 0.71              |
| 1:A:668:LEU:HD21  | 2:B:1786:TYR:OH   | 1.90                     | 0.71              |
| 2:B:1989:LEU:HD23 | 2:B:1989:LEU:C    | 2.15                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:177:LEU:HD22  | 1:A:256:HIS:CE1   | 2.25                     | 0.71              |
| 1:A:659:LYS:N     | 1:A:659:LYS:CD    | 2.53                     | 0.71              |
| 2:B:2047:ALA:HA   | 2:B:2062:TRP:CD1  | 2.16                     | 0.71              |
| 2:B:2054:HIS:O    | 2:B:2060:ASN:HB2  | 1.89                     | 0.71              |
| 2:B:1820:GLN:HE22 | 2:B:1822:HIS:H    | 1.35                     | 0.71              |
| 1:A:460:THR:HG21  | 1:A:512:LYS:NZ    | 2.05                     | 0.71              |
| 1:A:565:GLN:HG3   | 1:A:566:ILE:H     | 1.55                     | 0.71              |
| 1:A:588:THR:HA    | 1:A:591:ILE:HG22  | 1.73                     | 0.71              |
| 2:B:1764:ARG:HD2  | 2:B:1869:ARG:CB   | 2.21                     | 0.71              |
| 2:B:1878:LEU:HD11 | 2:B:1942:TRP:HZ3  | 1.54                     | 0.71              |
| 1:A:424:LYS:N     | 1:A:590:ASN:HD21  | 1.88                     | 0.71              |
| 1:A:435:THR:O     | 1:A:436:PHE:HD1   | 1.74                     | 0.71              |
| 1:A:640:LEU:N     | 1:A:640:LEU:HD23  | 2.04                     | 0.71              |
| 2:B:1907:MET:HA   | 2:B:1911:THR:HB   | 1.71                     | 0.71              |
| 2:B:2013:LEU:HD22 | 2:B:2013:LEU:N    | 2.00                     | 0.71              |
| 1:A:87:THR:HA     | 1:A:135:THR:HA    | 1.71                     | 0.71              |
| 1:A:480:ILE:HG22  | 1:A:481:THR:H     | 1.56                     | 0.71              |
| 1:A:12:LEU:HD21   | 1:A:61:ILE:HG12   | 1.73                     | 0.71              |
| 1:A:371:ILE:HB    | 1:A:374:VAL:HG12  | 1.73                     | 0.71              |
| 1:A:566:ILE:O     | 1:A:567:MET:HE2   | 1.91                     | 0.71              |
| 2:B:2013:LEU:H    | 2:B:2013:LEU:CD2  | 1.94                     | 0.71              |
| 1:A:102:GLY:O     | 1:A:103:VAL:HG13  | 1.91                     | 0.71              |
| 1:A:275:THR:HA    | 1:A:284:ALA:CB    | 2.18                     | 0.71              |
| 2:B:2225:ASN:ND2  | 2:B:2228:GLU:HG2  | 2.02                     | 0.70              |
| 1:A:246:ILE:HD13  | 1:A:246:ILE:N     | 2.05                     | 0.70              |
| 1:A:713:LYS:NZ    | 1:A:713:LYS:HA    | 2.07                     | 0.70              |
| 2:B:1830:PHE:CZ   | 2:B:1965:VAL:HA   | 2.26                     | 0.70              |
| 2:B:2225:ASN:CG   | 2:B:2227:LYS:H    | 1.98                     | 0.70              |
| 1:A:123:LYS:HA    | 1:A:126:ASP:HB2   | 1.73                     | 0.70              |
| 2:B:2033:ARG:O    | 2:B:2036:GLN:HG2  | 1.90                     | 0.70              |
| 1:A:478:HIS:HB3   | 1:A:532:TYR:CE1   | 2.27                     | 0.70              |
| 1:A:616:SER:HB2   | 1:A:619:GLY:N     | 2.06                     | 0.70              |
| 1:A:625:LEU:C     | 1:A:627:LEU:H     | 1.98                     | 0.70              |
| 2:B:2108:ASP:OD2  | 2:B:2110:LYS:HB2  | 1.90                     | 0.70              |
| 1:A:306:PHE:CD1   | 1:A:306:PHE:N     | 2.59                     | 0.70              |
| 1:A:495:VAL:HG22  | 1:A:496:LYS:N     | 2.05                     | 0.70              |
| 2:B:1741:GLY:O    | 2:B:1745:GLN:O    | 2.09                     | 0.70              |
| 2:B:1773:VAL:HG21 | 2:B:1785:PHE:CE2  | 2.26                     | 0.70              |
| 2:B:1999:GLU:HB2  | 2:B:2006:LEU:HD13 | 1.71                     | 0.70              |
| 2:B:2323:VAL:HG12 | 2:B:2324:LEU:H    | 1.56                     | 0.70              |
| 1:A:427:ARG:HD3   | 1:A:448:ILE:HG22  | 1.74                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:453:LEU:HD21  | 1:A:533:TYR:CE2   | 2.26                     | 0.70              |
| 1:A:529:LEU:HD12  | 1:A:529:LEU:N     | 2.07                     | 0.70              |
| 1:A:530:THR:HG23  | 1:A:679:PHE:HB3   | 1.74                     | 0.70              |
| 2:B:1799:GLY:O    | 2:B:1803:ARG:HB2  | 1.91                     | 0.70              |
| 2:B:1924:TYR:HD2  | 2:B:1928:THR:C    | 2.00                     | 0.70              |
| 1:A:15:ASP:O      | 1:A:16:TYR:HB2    | 1.91                     | 0.70              |
| 1:A:273:GLY:HA3   | 1:A:306:PHE:CD2   | 2.26                     | 0.70              |
| 1:A:651:VAL:N     | 1:A:693:HIS:CB    | 2.53                     | 0.70              |
| 1:A:362:ASP:O     | 1:A:363:ASP:HB2   | 1.91                     | 0.70              |
| 1:A:434:GLU:HG2   | 1:A:435:THR:N     | 2.04                     | 0.70              |
| 2:B:2077:ALA:HB1  | 2:B:2078:PRO:HD2  | 1.74                     | 0.70              |
| 1:A:46:TYR:CE1    | 1:A:227:ALA:HB3   | 2.26                     | 0.70              |
| 1:A:157:SER:HB2   | 1:A:174:GLY:O     | 1.91                     | 0.70              |
| 1:A:649:LEU:HD13  | 1:A:696:ASP:OD1   | 1.91                     | 0.70              |
| 2:B:1701:ALA:HA   | 2:B:1775:PHE:CE1  | 2.27                     | 0.70              |
| 2:B:1794:GLU:HG3  | 2:B:1795:ASP:N    | 2.06                     | 0.70              |
| 2:B:2060:ASN:ND2  | 2:B:2060:ASN:H    | 1.85                     | 0.70              |
| 1:A:65:ARG:O      | 1:A:66:PRO:C      | 2.34                     | 0.70              |
| 1:A:425:LYS:HE2   | 1:A:581:GLU:OE1   | 1.92                     | 0.70              |
| 1:A:444:HIS:HB2   | 1:A:620:TYR:HH    | 1.57                     | 0.70              |
| 1:A:591:ILE:HG23  | 1:A:592:GLN:H     | 1.57                     | 0.70              |
| 1:A:89:LYS:HG3    | 1:A:133:SER:HB2   | 1.74                     | 0.69              |
| 1:A:234:VAL:C     | 1:A:236:GLY:H     | 1.98                     | 0.69              |
| 1:A:625:LEU:C     | 1:A:626:GLN:HG2   | 2.16                     | 0.69              |
| 2:B:1993:ALA:HA   | 2:B:2016:VAL:HG13 | 1.74                     | 0.69              |
| 2:B:2162:LEU:C    | 2:B:2162:LEU:HD12 | 2.16                     | 0.69              |
| 2:B:2274:PHE:HE1  | 2:B:2299:PRO:HG2  | 1.57                     | 0.69              |
| 2:B:1967:LYS:O    | 2:B:1968:LYS:HB2  | 1.92                     | 0.69              |
| 2:B:2209:ARG:HH11 | 2:B:2209:ARG:HG2  | 1.57                     | 0.69              |
| 2:B:2225:ASN:HD21 | 2:B:2228:GLU:H    | 1.40                     | 0.69              |
| 1:A:401:ALA:HB3   | 1:A:405:ARG:NE    | 2.07                     | 0.69              |
| 1:A:598:PRO:HG2   | 1:A:599:ALA:H     | 1.57                     | 0.69              |
| 2:B:2052:ARG:HB2  | 2:B:2164:MET:O    | 1.91                     | 0.69              |
| 1:A:72:LEU:HD23   | 1:A:73:GLY:O      | 1.92                     | 0.69              |
| 1:A:101:VAL:HG13  | 1:A:101:VAL:O     | 1.91                     | 0.69              |
| 2:B:1836:ALA:HB2  | 2:B:1945:LEU:HD23 | 1.75                     | 0.69              |
| 1:A:666:ASP:HB3   | 1:A:669:THR:HG21  | 1.75                     | 0.69              |
| 1:A:704:ALA:O     | 1:A:706:LEU:HD22  | 1.92                     | 0.69              |
| 2:B:2049:LYS:O    | 2:B:2049:LYS:HD3  | 1.93                     | 0.69              |
| 2:B:2084:ILE:HG13 | 2:B:2166:LEU:HB3  | 1.75                     | 0.69              |
| 2:B:2150:ARG:HB3  | 2:B:2152:HIS:HE1  | 1.56                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:5:TYR:CE2     | 1:A:76:ILE:HG23   | 2.27                     | 0.69              |
| 2:B:1737:GLU:H    | 2:B:1737:GLU:CD   | 2.01                     | 0.69              |
| 2:B:2258:LYS:HG3  | 2:B:2259:GLU:HG3  | 1.73                     | 0.69              |
| 1:A:486:LEU:HD12  | 1:A:486:LEU:N     | 2.06                     | 0.69              |
| 1:A:667:THR:O     | 1:A:669:THR:HG22  | 1.93                     | 0.69              |
| 1:A:652:PHE:HE1   | 1:A:682:MET:HG3   | 1.56                     | 0.69              |
| 2:B:2096:LEU:HD11 | 2:B:2158:ILE:HG23 | 1.74                     | 0.69              |
| 2:B:2211:HIS:H    | 2:B:2246:GLN:HE22 | 1.41                     | 0.69              |
| 1:A:186:LYS:HE3   | 1:A:190:GLN:HB2   | 1.73                     | 0.68              |
| 2:B:1756:LEU:O    | 2:B:1759:LEU:HB2  | 1.92                     | 0.68              |
| 1:A:311:HIS:O     | 1:A:312:ILE:HG12  | 1.93                     | 0.68              |
| 2:B:1750:GLY:O    | 2:B:1751:GLU:HB2  | 1.92                     | 0.68              |
| 2:B:2050:LEU:HD22 | 2:B:2054:HIS:HD2  | 1.59                     | 0.68              |
| 1:A:48:LYS:NZ     | 1:A:204:GLU:HB2   | 2.08                     | 0.68              |
| 1:A:570:LYS:HG2   | 1:A:638:TYR:HE2   | 1.58                     | 0.68              |
| 1:A:649:LEU:HD12  | 1:A:649:LEU:N     | 2.09                     | 0.68              |
| 2:B:1878:LEU:HB2  | 2:B:1880:PHE:CE1  | 2.27                     | 0.68              |
| 2:B:2260:PHE:HA   | 2:B:2311:GLN:HG2  | 1.75                     | 0.68              |
| 1:A:141:LEU:H     | 1:A:144:ASN:HD22  | 1.42                     | 0.68              |
| 1:A:407:TYR:HA    | 1:A:410:GLN:HE21  | 1.59                     | 0.68              |
| 1:A:452:LEU:HA    | 1:A:550:PRO:HG2   | 1.76                     | 0.68              |
| 2:B:1771:ILE:HD12 | 2:B:1817:TRP:HE1  | 1.58                     | 0.68              |
| 1:A:475:ILE:HG23  | 1:A:475:ILE:O     | 1.93                     | 0.68              |
| 2:B:1738:PHE:HB2  | 2:B:1746:PRO:HD2  | 1.76                     | 0.68              |
| 1:A:71:LEU:HD13   | 1:A:236:GLY:HA3   | 1.75                     | 0.68              |
| 2:B:2077:ALA:O    | 2:B:2147:ARG:HG3  | 1.94                     | 0.68              |
| 1:A:94:HIS:HB3    | 1:A:96:VAL:HG13   | 1.76                     | 0.68              |
| 1:A:651:VAL:N     | 1:A:693:HIS:HB2   | 2.09                     | 0.68              |
| 2:B:2116:ARG:HH21 | 2:B:2120:THR:CA   | 2.05                     | 0.68              |
| 2:B:1783:TYR:HA   | 2:B:1841:VAL:HG21 | 1.76                     | 0.68              |
| 1:A:314:SER:HA    | 1:A:316:GLN:NE2   | 2.05                     | 0.68              |
| 1:A:663:VAL:HG13  | 2:B:1968:LYS:CG   | 2.24                     | 0.68              |
| 1:A:700:ARG:HH21  | 1:A:705:LEU:HD11  | 1.58                     | 0.68              |
| 2:B:1982:VAL:O    | 2:B:1983:PHE:HB3  | 1.94                     | 0.68              |
| 2:B:2194:SER:HB3  | 2:B:2222:GLN:N    | 2.04                     | 0.68              |
| 2:B:2273:LEU:HD23 | 2:B:2274:PHE:N    | 2.09                     | 0.68              |
| 1:A:432:THR:HA    | 1:A:438:THR:CB    | 2.24                     | 0.67              |
| 2:B:2234:PHE:HB2  | 2:B:2304:ARG:O    | 1.94                     | 0.67              |
| 1:A:4:ARG:HD2     | 1:A:6:TYR:CE2     | 2.29                     | 0.67              |
| 1:A:693:HIS:HD2   | 1:A:695:SER:HB2   | 1.58                     | 0.67              |
| 1:A:80:VAL:HA     | 1:A:140:VAL:CG1   | 2.22                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:116:ASP:O     | 1:A:117:GLN:C     | 2.35                     | 0.67              |
| 1:A:412:LEU:HD22  | 1:A:421:ARG:NH1   | 2.10                     | 0.67              |
| 1:A:414:ASN:HB2   | 1:A:419:ILE:HA    | 1.75                     | 0.67              |
| 1:A:660:HIS:HB2   | 1:A:680:MET:CG    | 2.24                     | 0.67              |
| 2:B:1820:GLN:HE21 | 2:B:1822:HIS:H    | 1.36                     | 0.67              |
| 1:A:13:SER:HB3    | 1:A:47:LYS:HG3    | 1.75                     | 0.67              |
| 1:A:189:THR:O     | 1:A:190:GLN:HB2   | 1.93                     | 0.67              |
| 1:A:527:ARG:H     | 1:A:527:ARG:CD    | 2.07                     | 0.67              |
| 1:A:706:LEU:C     | 1:A:707:LYS:HG3   | 2.18                     | 0.67              |
| 2:B:1789:LEU:HD11 | 2:B:1835:TRP:CD1  | 2.30                     | 0.67              |
| 2:B:2000:CYS:HB2  | 2:B:2010:MET:SD   | 2.34                     | 0.67              |
| 2:B:2047:ALA:HB1  | 2:B:2048:PRO:HD2  | 1.77                     | 0.67              |
| 1:A:202:PHE:O     | 1:A:231:MET:HB2   | 1.94                     | 0.67              |
| 2:B:1738:PHE:CE1  | 2:B:1742:SER:HA   | 2.29                     | 0.67              |
| 1:A:48:LYS:HB3    | 1:A:170:SER:O     | 1.94                     | 0.67              |
| 1:A:155:THR:HG23  | 1:A:295:THR:HG23  | 1.77                     | 0.67              |
| 2:B:1792:TYR:HE1  | 2:B:1820:GLN:HG3  | 1.60                     | 0.67              |
| 1:A:38:PHE:HB3    | 1:A:39:PRO:HD2    | 1.76                     | 0.67              |
| 1:A:164:LEU:H     | 1:A:164:LEU:HD12  | 1.59                     | 0.67              |
| 1:A:591:ILE:HG23  | 1:A:592:GLN:N     | 2.10                     | 0.67              |
| 1:A:69:MET:O      | 1:A:71:LEU:N      | 2.28                     | 0.67              |
| 1:A:273:GLY:O     | 1:A:274:HIS:ND1   | 2.27                     | 0.67              |
| 1:A:467:ASN:HD22  | 1:A:506:GLY:CA    | 2.06                     | 0.67              |
| 1:A:538:ASN:O     | 1:A:539:MET:HB2   | 1.94                     | 0.67              |
| 2:B:2037:ILE:O    | 2:B:2038:THR:HB   | 1.94                     | 0.67              |
| 1:A:424:LYS:HD2   | 1:A:593:ARG:HH22  | 1.60                     | 0.67              |
| 1:A:452:LEU:HD13  | 1:A:452:LEU:N     | 2.10                     | 0.67              |
| 2:B:1763:ILE:HG23 | 2:B:1763:ILE:O    | 1.95                     | 0.67              |
| 2:B:1935:ALA:O    | 2:B:1936:GLN:C    | 2.38                     | 0.67              |
| 1:A:273:GLY:O     | 1:A:274:HIS:CG    | 2.48                     | 0.66              |
| 1:A:107:LYS:HA    | 1:A:107:LYS:HZ2   | 1.59                     | 0.66              |
| 1:A:178:VAL:C     | 1:A:179:CYS:SG    | 2.79                     | 0.66              |
| 1:A:552:LEU:HD12  | 1:A:552:LEU:N     | 2.10                     | 0.66              |
| 2:B:1795:ASP:O    | 2:B:1796:GLN:HG3  | 1.95                     | 0.66              |
| 2:B:1931:GLY:O    | 2:B:1932:LEU:HD23 | 1.95                     | 0.66              |
| 2:B:2052:ARG:CZ   | 2:B:2087:GLN:HE22 | 2.08                     | 0.66              |
| 1:A:63:LYS:CG     | 1:A:64:PRO:HD2    | 2.26                     | 0.66              |
| 1:A:164:LEU:O     | 1:A:167:ASP:HB2   | 1.96                     | 0.66              |
| 1:A:474:ASN:ND2   | 1:A:475:ILE:N     | 2.42                     | 0.66              |
| 1:A:605:ASP:OD2   | 1:A:607:GLU:HB3   | 1.95                     | 0.66              |
| 2:B:1739:THR:O    | 2:B:1740:ASP:HB2  | 1.95                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:651:VAL:H     | 1:A:693:HIS:HB2   | 1.60                     | 0.66              |
| 1:A:664:TYR:CE1   | 2:B:1826:THR:HG23 | 2.31                     | 0.66              |
| 2:B:2313:TRP:HB3  | 2:B:2317:ILE:HG12 | 1.77                     | 0.66              |
| 1:A:156:TYR:HD1   | 1:A:293:PHE:HD1   | 1.42                     | 0.66              |
| 2:B:2065:LYS:C    | 2:B:2067:PRO:HD2  | 2.21                     | 0.66              |
| 1:A:18:GLN:CG     | 1:A:19:SER:H      | 2.03                     | 0.66              |
| 1:A:21:LEU:HD12   | 1:A:32:PRO:CG     | 2.24                     | 0.66              |
| 1:A:267:HIS:NE2   | 1:A:320:MET:CG    | 2.56                     | 0.66              |
| 1:A:621:VAL:HG13  | 1:A:703:THR:OG1   | 1.95                     | 0.66              |
| 2:B:1813:LYS:HE2  | 2:B:1814:THR:O    | 1.96                     | 0.66              |
| 2:B:1993:ALA:HA   | 2:B:2016:VAL:CG1  | 2.26                     | 0.66              |
| 1:A:146:PRO:O     | 1:A:147:MET:HE2   | 1.95                     | 0.66              |
| 2:B:1995:ILE:N    | 2:B:1995:ILE:CD1  | 2.58                     | 0.66              |
| 1:A:299:LEU:H     | 1:A:299:LEU:HD12  | 1.61                     | 0.66              |
| 1:A:446:SER:HB3   | 1:A:449:LEU:HD11  | 1.77                     | 0.66              |
| 1:A:651:VAL:CA    | 1:A:693:HIS:HB2   | 2.26                     | 0.66              |
| 1:A:655:GLY:HA3   | 1:A:687:LEU:CB    | 2.26                     | 0.66              |
| 2:B:2212:LEU:HD12 | 2:B:2213:GLN:O    | 1.96                     | 0.66              |
| 2:B:2234:PHE:O    | 2:B:2235:GLN:HB2  | 1.95                     | 0.66              |
| 2:B:1969:GLU:HB2  | 2:B:1971:TYR:CE2  | 2.30                     | 0.66              |
| 2:B:2105:TYR:CD2  | 2:B:2144:ILE:HG21 | 2.31                     | 0.66              |
| 1:A:96:VAL:HA     | 1:A:162:VAL:CG2   | 2.26                     | 0.65              |
| 1:A:316:GLN:HG2   | 1:A:317:HIS:ND1   | 2.11                     | 0.65              |
| 1:A:504:LEU:HD12  | 1:A:504:LEU:N     | 2.10                     | 0.65              |
| 2:B:1706:LEU:HA   | 2:B:1730:PHE:O    | 1.96                     | 0.65              |
| 1:A:291:ILE:HG23  | 2:B:1955:SER:OG   | 1.95                     | 0.65              |
| 2:B:1731:LYS:HB3  | 2:B:1893:GLU:HG2  | 1.77                     | 0.65              |
| 2:B:2025:LEU:HG   | 2:B:2167:MET:HA   | 1.77                     | 0.65              |
| 2:B:2081:ILE:CD1  | 2:B:2144:ILE:HB   | 2.24                     | 0.65              |
| 2:B:2274:PHE:CE1  | 2:B:2299:PRO:HG2  | 2.32                     | 0.65              |
| 1:A:693:HIS:CD2   | 1:A:695:SER:HB2   | 2.31                     | 0.65              |
| 2:B:1830:PHE:HE2  | 2:B:1985:THR:O    | 1.79                     | 0.65              |
| 2:B:2263:SER:HB2  | 2:B:2307:ARG:HB3  | 1.77                     | 0.65              |
| 1:A:146:PRO:HG3   | 1:A:180:ARG:CG    | 2.26                     | 0.65              |
| 1:A:269:ILE:O     | 1:A:269:ILE:HD13  | 1.95                     | 0.65              |
| 1:A:292:THR:HG23  | 2:B:1977:ASN:ND2  | 2.11                     | 0.65              |
| 1:A:566:ILE:HG13  | 1:A:567:MET:HE2   | 1.78                     | 0.65              |
| 1:A:713:LYS:HE3   | 1:A:714:ASN:H     | 1.62                     | 0.65              |
| 2:B:1726:SER:O    | 2:B:1727:VAL:HG23 | 1.96                     | 0.65              |
| 2:B:1992:LYS:CE   | 2:B:1993:ALA:H    | 2.09                     | 0.65              |
| 1:A:385:TYR:CD1   | 1:A:436:PHE:O     | 2.49                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1997:ARG:HA   | 2:B:2012:THR:O    | 1.95                     | 0.65              |
| 1:A:292:THR:C     | 1:A:293:PHE:HD2   | 2.05                     | 0.65              |
| 1:A:434:GLU:HG3   | 1:A:466:LYS:HZ2   | 1.60                     | 0.65              |
| 2:B:2209:ARG:N    | 2:B:2212:LEU:HD23 | 2.11                     | 0.65              |
| 2:B:1837:TYR:CD1  | 2:B:1853:GLY:HA3  | 2.31                     | 0.65              |
| 2:B:2176:MET:HG2  | 2:B:2177:PRO:CD   | 2.16                     | 0.65              |
| 2:B:2258:LYS:HE3  | 2:B:2284:GLN:NE2  | 2.11                     | 0.65              |
| 1:A:267:HIS:NE2   | 1:A:310:CYS:SG    | 2.69                     | 0.65              |
| 1:A:575:LEU:HG    | 1:A:575:LEU:O     | 1.94                     | 0.65              |
| 1:A:700:ARG:HH21  | 1:A:705:LEU:CD1   | 2.10                     | 0.65              |
| 1:A:183:SER:C     | 1:A:185:ALA:N     | 2.54                     | 0.65              |
| 1:A:548:ILE:HD12  | 1:A:549:GLY:H     | 1.62                     | 0.65              |
| 2:B:1738:PHE:CD2  | 2:B:1738:PHE:N    | 2.65                     | 0.65              |
| 2:B:2301:LEU:CD2  | 2:B:2302:LEU:H    | 2.09                     | 0.65              |
| 1:A:234:VAL:C     | 1:A:236:GLY:N     | 2.54                     | 0.64              |
| 1:A:384:HIS:HB3   | 1:A:386:ILE:CG2   | 2.27                     | 0.64              |
| 2:B:2000:CYS:SG   | 2:B:2002:ILE:HB   | 2.36                     | 0.64              |
| 1:A:15:ASP:OD1    | 1:A:16:TYR:N      | 2.30                     | 0.64              |
| 1:A:272:GLU:O     | 1:A:306:PHE:HB3   | 1.97                     | 0.64              |
| 1:A:437:LYS:O     | 1:A:438:THR:HB    | 1.97                     | 0.64              |
| 1:A:604:GLU:HG2   | 1:A:609:GLN:OE1   | 1.97                     | 0.64              |
| 1:A:654:SER:HB2   | 1:A:690:LEU:CA    | 2.27                     | 0.64              |
| 1:A:673:PHE:O     | 1:A:674:SER:O     | 2.15                     | 0.64              |
| 2:B:1933:VAL:HG23 | 2:B:1933:VAL:O    | 1.96                     | 0.64              |
| 1:A:34:VAL:H      | 1:A:35:PRO:HD3    | 1.60                     | 0.64              |
| 1:A:83:THR:HG23   | 1:A:139:GLN:HA    | 1.79                     | 0.64              |
| 1:A:655:GLY:O     | 1:A:687:LEU:HB2   | 1.97                     | 0.64              |
| 1:A:226:ARG:HE    | 1:A:226:ARG:N     | 1.94                     | 0.64              |
| 1:A:385:TYR:CE2   | 1:A:437:LYS:HD2   | 2.33                     | 0.64              |
| 1:A:435:THR:O     | 1:A:436:PHE:CD1   | 2.50                     | 0.64              |
| 2:B:1857:VAL:CG2  | 2:B:1858:CYS:N    | 2.60                     | 0.64              |
| 2:B:1869:ARG:HD2  | 2:B:1869:ARG:N    | 2.11                     | 0.64              |
| 2:B:1926:MET:O    | 2:B:1928:THR:N    | 2.29                     | 0.64              |
| 2:B:2074:ASP:OD2  | 2:B:2148:TYR:CE1  | 2.50                     | 0.64              |
| 2:B:2248:VAL:CG2  | 2:B:2249:LYS:H    | 2.06                     | 0.64              |
| 1:A:470:SER:HB2   | 1:A:471:ARG:HD2   | 1.80                     | 0.64              |
| 1:A:575:LEU:HD23  | 1:A:618:ASN:OD1   | 1.96                     | 0.64              |
| 1:A:578:VAL:HB    | 1:A:644:ALA:H     | 1.62                     | 0.64              |
| 1:A:660:HIS:O     | 1:A:665:GLU:HA    | 1.98                     | 0.64              |
| 2:B:1864:ASN:HD22 | 2:B:1868:GLY:HA3  | 1.62                     | 0.64              |
| 2:B:1871:VAL:HG13 | 5:E:1:NAG:H61     | 1.78                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:71:LEU:HD23   | 1:A:71:LEU:C      | 2.22                     | 0.64              |
| 1:A:278:VAL:O     | 1:A:280:ASN:N     | 2.30                     | 0.64              |
| 1:A:651:VAL:H     | 1:A:693:HIS:HB3   | 1.61                     | 0.64              |
| 1:A:656:TYR:CE1   | 1:A:686:GLY:HA2   | 2.31                     | 0.64              |
| 1:A:118:THR:HG22  | 1:A:123:LYS:HE3   | 1.80                     | 0.64              |
| 1:A:465:PHE:CD1   | 1:A:466:LYS:N     | 2.66                     | 0.64              |
| 2:B:1703:VAL:HG22 | 2:B:1704:GLU:N    | 2.12                     | 0.64              |
| 2:B:2084:ILE:CG1  | 2:B:2085:LYS:H    | 2.11                     | 0.64              |
| 2:B:2160:SER:C    | 2:B:2161:THR:HG22 | 2.23                     | 0.64              |
| 2:B:2213:GLN:HG2  | 2:B:2214:GLY:H    | 1.62                     | 0.64              |
| 2:B:1863:LEU:CD2  | 2:B:1863:LEU:N    | 2.56                     | 0.64              |
| 2:B:2271:TRP:CZ3  | 2:B:2307:ARG:HB2  | 2.31                     | 0.64              |
| 1:A:130:PRO:O     | 1:A:132:GLY:N     | 2.27                     | 0.64              |
| 1:A:690:LEU:O     | 1:A:707:LYS:HA    | 1.98                     | 0.64              |
| 2:B:1870:GLN:O    | 2:B:1871:VAL:HB   | 1.97                     | 0.64              |
| 2:B:2140:PHE:O    | 2:B:2141:ASN:HB2  | 1.96                     | 0.64              |
| 2:B:2229:TRP:HA   | 2:B:2308:ILE:O    | 1.97                     | 0.64              |
| 2:B:2263:SER:O    | 2:B:2264:SER:HB2  | 1.98                     | 0.64              |
| 1:A:80:VAL:O      | 1:A:81:TYR:HB2    | 1.97                     | 0.64              |
| 1:A:489:ARG:HB2   | 1:A:489:ARG:HH11  | 1.63                     | 0.64              |
| 2:B:1755:HIS:O    | 2:B:1757:GLY:N    | 2.31                     | 0.64              |
| 2:B:1764:ARG:O    | 2:B:1765:ALA:HB2  | 1.98                     | 0.64              |
| 2:B:2135:ILE:HG22 | 2:B:2135:ILE:O    | 1.96                     | 0.64              |
| 1:A:109:SER:O     | 1:A:111:GLY:N     | 2.31                     | 0.63              |
| 1:A:648:PHE:O     | 1:A:672:PRO:HD2   | 1.98                     | 0.63              |
| 2:B:1882:ILE:HG23 | 2:B:1882:ILE:O    | 1.97                     | 0.63              |
| 1:A:407:TYR:C     | 1:A:409:SER:H     | 2.05                     | 0.63              |
| 1:A:428:PHE:CE1   | 1:A:547:LEU:HB3   | 2.32                     | 0.63              |
| 2:B:2047:ALA:HB1  | 2:B:2048:PRO:CD   | 2.27                     | 0.63              |
| 2:B:2159:ARG:O    | 2:B:2161:THR:HG22 | 1.97                     | 0.63              |
| 1:A:99:HIS:O      | 1:A:138:TRP:HZ3   | 1.80                     | 0.63              |
| 1:A:240:ARG:HD2   | 1:A:323:TYR:HE1   | 1.63                     | 0.63              |
| 1:A:303:LEU:HD23  | 1:A:304:GLY:H     | 1.59                     | 0.63              |
| 1:A:535:SER:C     | 1:A:536:PHE:HD1   | 2.05                     | 0.63              |
| 2:B:1989:LEU:HD23 | 2:B:1989:LEU:O    | 1.97                     | 0.63              |
| 2:B:2260:PHE:HB2  | 2:B:2310:PRO:HA   | 1.80                     | 0.63              |
| 2:B:1861:ASN:N    | 2:B:1861:ASN:HD22 | 1.96                     | 0.63              |
| 2:B:2144:ILE:CG2  | 2:B:2145:ILE:N    | 2.61                     | 0.63              |
| 1:A:99:HIS:O      | 1:A:138:TRP:CZ3   | 2.52                     | 0.63              |
| 1:A:100:ALA:HB2   | 1:A:138:TRP:CZ3   | 2.34                     | 0.63              |
| 1:A:141:LEU:CD2   | 1:A:142:LYS:HG2   | 2.27                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:399:VAL:HG13  | 1:A:405:ARG:HH12  | 1.64                     | 0.63              |
| 2:B:2064:THR:OG1  | 2:B:2065:LYS:N    | 2.29                     | 0.63              |
| 2:B:2193:SER:HB3  | 2:B:2229:TRP:NE1  | 2.14                     | 0.63              |
| 2:B:2246:GLN:OE1  | 2:B:2320:ARG:NE   | 2.31                     | 0.63              |
| 2:B:2178:LEU:HD11 | 2:B:2325:GLY:N    | 2.13                     | 0.63              |
| 1:A:39:PRO:C      | 1:A:41:ASN:H      | 2.07                     | 0.63              |
| 1:A:141:LEU:HD23  | 1:A:142:LYS:H     | 1.63                     | 0.63              |
| 1:A:316:GLN:HG2   | 1:A:317:HIS:H     | 1.62                     | 0.63              |
| 1:A:657:THR:O     | 1:A:658:PHE:HB2   | 1.98                     | 0.63              |
| 2:B:1790:ILE:HA   | 2:B:1817:TRP:HE3  | 1.63                     | 0.63              |
| 2:B:1906:GLN:HG3  | 2:B:1907:MET:H    | 1.64                     | 0.63              |
| 2:B:1924:TYR:CD2  | 2:B:1928:THR:HG22 | 2.34                     | 0.63              |
| 1:A:386:ILE:HD12  | 1:A:386:ILE:C     | 2.22                     | 0.63              |
| 1:A:538:ASN:ND2   | 1:A:541:ARG:HB3   | 2.14                     | 0.63              |
| 2:B:1799:GLY:HA3  | 2:B:1803:ARG:HD3  | 1.80                     | 0.63              |
| 2:B:2044:GLY:C    | 2:B:2046:TRP:H    | 2.06                     | 0.63              |
| 2:B:2260:PHE:CE1  | 2:B:2283:PHE:HB3  | 2.33                     | 0.63              |
| 2:B:2275:PHE:HD1  | 2:B:2280:VAL:N    | 1.95                     | 0.63              |
| 2:B:2313:TRP:O    | 2:B:2314:VAL:HG23 | 1.99                     | 0.63              |
| 1:A:460:THR:HG21  | 1:A:512:LYS:HZ2   | 1.63                     | 0.63              |
| 1:A:561:GLN:CG    | 1:A:562:ARG:H     | 2.08                     | 0.63              |
| 1:A:651:VAL:N     | 1:A:693:HIS:HB3   | 2.13                     | 0.63              |
| 2:B:1758:LEU:HD22 | 2:B:1758:LEU:N    | 2.13                     | 0.63              |
| 2:B:1909:ASP:HB3  | 2:B:1910:PRO:CD   | 2.28                     | 0.63              |
| 2:B:2086:THR:HG21 | 2:B:2101:PHE:HE2  | 1.63                     | 0.63              |
| 2:B:2190:ILE:HG22 | 2:B:2190:ILE:O    | 1.98                     | 0.63              |
| 2:B:2296:SER:O    | 2:B:2297:LEU:HG   | 1.99                     | 0.63              |
| 1:A:172:LEU:HD12  | 1:A:172:LEU:N     | 2.14                     | 0.62              |
| 1:A:390:GLU:OE2   | 1:A:586:TYR:HE2   | 1.82                     | 0.62              |
| 1:A:631:LEU:HG    | 1:A:632:HIS:ND1   | 2.15                     | 0.62              |
| 2:B:1738:PHE:N    | 2:B:1738:PHE:HD2  | 1.97                     | 0.62              |
| 2:B:1949:SER:OG   | 2:B:1951:GLU:HG2  | 1.99                     | 0.62              |
| 5:E:3:BMA:O4      | 5:E:4:BMA:H2      | 1.98                     | 0.62              |
| 1:A:587:LEU:HD23  | 1:A:588:THR:N     | 2.11                     | 0.62              |
| 1:A:656:TYR:CE2   | 1:A:685:PRO:HG2   | 2.34                     | 0.62              |
| 2:B:2212:LEU:HD12 | 2:B:2213:GLN:N    | 2.14                     | 0.62              |
| 1:A:156:TYR:HA    | 1:A:293:PHE:CD1   | 2.34                     | 0.62              |
| 1:A:690:LEU:HD13  | 1:A:708:VAL:CG2   | 2.30                     | 0.62              |
| 2:B:1719:ARG:HG2  | 2:B:1723:GLN:NE2  | 2.14                     | 0.62              |
| 2:B:1737:GLU:CD   | 2:B:1737:GLU:N    | 2.56                     | 0.62              |
| 2:B:1999:GLU:HB3  | 2:B:2011:SER:HB3  | 1.82                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:158:TYR:CD1   | 1:A:158:TYR:C     | 2.75                     | 0.62              |
| 2:B:2180:MET:CE   | 2:B:2190:ILE:HD11 | 2.27                     | 0.62              |
| 2:B:2193:SER:HG   | 2:B:2229:TRP:CD1  | 2.17                     | 0.62              |
| 1:A:110:GLU:HG3   | 1:A:110:GLU:O     | 1.98                     | 0.62              |
| 1:A:472:PRO:HB3   | 1:A:505:PRO:HA    | 1.81                     | 0.62              |
| 1:A:527:ARG:H     | 1:A:527:ARG:HD2   | 1.65                     | 0.62              |
| 2:B:1859:HIS:O    | 2:B:1862:THR:HG23 | 1.99                     | 0.62              |
| 2:B:1905:ILE:HG21 | 2:B:1910:PRO:HB2  | 1.82                     | 0.62              |
| 1:A:7:LEU:HD23    | 1:A:8:GLY:N       | 2.14                     | 0.62              |
| 1:A:63:LYS:CB     | 1:A:64:PRO:HD2    | 2.29                     | 0.62              |
| 1:A:527:ARG:O     | 1:A:528:CYS:CB    | 2.47                     | 0.62              |
| 2:B:1776:ARG:HG3  | 2:B:1812:THR:HG21 | 1.80                     | 0.62              |
| 2:B:1777:ASN:O    | 2:B:1778:GLN:HB2  | 1.98                     | 0.62              |
| 2:B:2024:PRO:HA   | 2:B:2167:MET:CB   | 2.27                     | 0.62              |
| 2:B:2225:ASN:ND2  | 2:B:2227:LYS:H    | 1.96                     | 0.62              |
| 2:B:2238:MET:HE1  | 2:B:2326:CYS:H    | 1.64                     | 0.62              |
| 1:A:68:TRP:HB3    | 1:A:244:GLY:HA3   | 1.80                     | 0.62              |
| 1:A:208:TRP:HB3   | 1:A:226:ARG:NH1   | 2.15                     | 0.62              |
| 2:B:1929:LEU:HD23 | 2:B:1932:LEU:HD11 | 1.81                     | 0.62              |
| 2:B:2036:GLN:HE22 | 2:B:2076:LEU:HG   | 1.64                     | 0.62              |
| 2:B:2096:LEU:HB3  | 2:B:2161:THR:CG2  | 2.28                     | 0.62              |
| 1:A:381:THR:HG22  | 1:A:460:THR:HB    | 1.81                     | 0.62              |
| 1:A:390:GLU:HA    | 1:A:426:VAL:HG12  | 1.81                     | 0.62              |
| 1:A:197:LEU:HD21  | 1:A:308:LEU:HD11  | 1.82                     | 0.62              |
| 1:A:383:VAL:O     | 1:A:384:HIS:ND1   | 2.33                     | 0.62              |
| 2:B:1763:ILE:HD13 | 2:B:1764:ARG:O    | 1.99                     | 0.62              |
| 2:B:1870:GLN:HG3  | 2:B:1871:VAL:N    | 2.15                     | 0.62              |
| 2:B:1947:MET:HE2  | 2:B:1948:GLY:N    | 2.15                     | 0.62              |
| 2:B:2038:THR:CG2  | 2:B:2072:LYS:HG2  | 2.26                     | 0.62              |
| 2:B:2156:TYR:CD2  | 2:B:2160:SER:N    | 2.68                     | 0.62              |
| 1:A:18:GLN:O      | 1:A:19:SER:HB3    | 2.00                     | 0.62              |
| 1:A:105:TYR:CE1   | 2:B:1960:GLY:HA2  | 2.35                     | 0.62              |
| 1:A:572:ASN:HB3   | 1:A:637:TRP:CE3   | 2.35                     | 0.62              |
| 1:A:674:SER:C     | 1:A:676:GLU:N     | 2.55                     | 0.62              |
| 2:B:1920:ALA:HB1  | 2:B:1924:TYR:N    | 2.15                     | 0.62              |
| 1:A:271:LEU:HD12  | 1:A:273:GLY:C     | 2.25                     | 0.61              |
| 2:B:1880:PHE:N    | 2:B:1880:PHE:CD1  | 2.68                     | 0.61              |
| 2:B:1996:TRP:HB2  | 2:B:2014:PHE:CE1  | 2.35                     | 0.61              |
| 2:B:2180:MET:HE1  | 2:B:2190:ILE:CD1  | 2.27                     | 0.61              |
| 2:B:2306:LEU:HD23 | 2:B:2307:ARG:N    | 2.15                     | 0.61              |
| 1:A:90:ASN:C      | 1:A:92:ALA:H      | 2.07                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:148:ALA:CA    | 1:A:180:ARG:HH21  | 2.13                     | 0.61              |
| 1:A:565:GLN:HG3   | 1:A:566:ILE:N     | 2.14                     | 0.61              |
| 1:A:663:VAL:HG12  | 1:A:664:TYR:N     | 2.14                     | 0.61              |
| 2:B:1844:GLU:O    | 2:B:1845:LYS:C    | 2.42                     | 0.61              |
| 1:A:453:LEU:HD23  | 1:A:453:LEU:N     | 2.15                     | 0.61              |
| 1:A:578:VAL:CB    | 1:A:644:ALA:H     | 2.13                     | 0.61              |
| 1:A:652:PHE:CE1   | 1:A:682:MET:HG3   | 2.35                     | 0.61              |
| 2:B:1873:VAL:CG1  | 2:B:1939:ARG:HB3  | 2.31                     | 0.61              |
| 2:B:1997:ARG:HD2  | 2:B:2011:SER:HB2  | 1.82                     | 0.61              |
| 2:B:2041:GLY:HA3  | 2:B:2043:TYR:CE1  | 2.35                     | 0.61              |
| 2:B:2053:LEU:H    | 2:B:2163:ARG:HE   | 1.46                     | 0.61              |
| 2:B:2180:MET:HG3  | 2:B:2322:GLU:HA   | 1.82                     | 0.61              |
| 2:B:2224:ASN:ND2  | 2:B:2316:GLN:HE21 | 1.97                     | 0.61              |
| 1:A:716:GLY:O     | 1:A:717:ASP:HB2   | 2.00                     | 0.61              |
| 2:B:2097:TYR:CE2  | 2:B:2130:VAL:HA   | 2.36                     | 0.61              |
| 1:A:474:ASN:HD22  | 1:A:475:ILE:H     | 1.47                     | 0.61              |
| 1:A:670:LEU:HG    | 1:A:672:PRO:HD3   | 1.82                     | 0.61              |
| 2:B:1813:LYS:HD2  | 2:B:1814:THR:H    | 1.66                     | 0.61              |
| 2:B:1881:THR:OG1  | 2:B:1882:ILE:N    | 2.32                     | 0.61              |
| 2:B:2145:ILE:N    | 2:B:2145:ILE:CD1  | 2.57                     | 0.61              |
| 1:A:33:ARG:HB3    | 1:A:35:PRO:HD3    | 1.82                     | 0.61              |
| 1:A:470:SER:HB2   | 1:A:471:ARG:HH11  | 1.66                     | 0.61              |
| 2:B:2130:VAL:O    | 2:B:2131:ASP:HB3  | 2.00                     | 0.61              |
| 1:A:167:ASP:CB    | 1:A:172:LEU:HD22  | 2.25                     | 0.61              |
| 1:A:191:THR:C     | 1:A:193:HIS:H     | 2.07                     | 0.61              |
| 1:A:486:LEU:O     | 1:A:487:TYR:HB2   | 1.98                     | 0.61              |
| 1:A:561:GLN:HG2   | 1:A:562:ARG:N     | 2.10                     | 0.61              |
| 1:A:679:PHE:O     | 1:A:680:MET:HB2   | 2.01                     | 0.61              |
| 2:B:1749:ARG:HG3  | 2:B:1750:GLY:N    | 2.16                     | 0.61              |
| 1:A:106:TRP:C     | 1:A:108:ALA:H     | 2.06                     | 0.61              |
| 2:B:1746:PRO:O    | 2:B:1748:TYR:N    | 2.34                     | 0.61              |
| 2:B:1958:PHE:O    | 2:B:1959:SER:C    | 2.43                     | 0.61              |
| 2:B:2027:MET:HB3  | 2:B:2165:GLU:HA   | 1.83                     | 0.61              |
| 1:A:63:LYS:HB3    | 1:A:64:PRO:HD2    | 1.83                     | 0.60              |
| 2:B:1925:ILE:HG13 | 2:B:2009:GLY:HA3  | 1.83                     | 0.60              |
| 2:B:2194:SER:O    | 2:B:2221:PRO:HA   | 2.01                     | 0.60              |
| 1:A:4:ARG:HG3     | 1:A:85:VAL:HB     | 1.83                     | 0.60              |
| 1:A:448:ILE:CD1   | 1:A:619:GLY:HA3   | 2.30                     | 0.60              |
| 1:A:662:MET:HB2   | 1:A:680:MET:CE    | 2.27                     | 0.60              |
| 2:B:1773:VAL:O    | 2:B:1773:VAL:HG13 | 2.01                     | 0.60              |
| 1:A:102:GLY:O     | 1:A:103:VAL:HG22  | 2.00                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1777:ASN:CG   | 2:B:1809:PRO:HA   | 2.26                     | 0.60              |
| 2:B:1855:LEU:HD23 | 2:B:1855:LEU:C    | 2.25                     | 0.60              |
| 1:A:51:PHE:N      | 1:A:51:PHE:CD1    | 2.65                     | 0.60              |
| 2:B:1943:TYR:C    | 2:B:1944:LEU:HD23 | 2.26                     | 0.60              |
| 2:B:2249:LYS:HA   | 2:B:2254:SER:HA   | 1.83                     | 0.60              |
| 1:A:392:ASP:OD2   | 1:A:392:ASP:N     | 2.30                     | 0.60              |
| 1:A:661:LYS:HE2   | 1:A:665:GLU:OE2   | 2.02                     | 0.60              |
| 2:B:2013:LEU:N    | 2:B:2013:LEU:HD13 | 2.16                     | 0.60              |
| 1:A:474:ASN:HD22  | 1:A:475:ILE:N     | 1.99                     | 0.60              |
| 1:A:552:LEU:HD12  | 1:A:552:LEU:H     | 1.64                     | 0.60              |
| 1:A:570:LYS:HG2   | 1:A:638:TYR:CE2   | 2.36                     | 0.60              |
| 1:A:578:VAL:HB    | 1:A:644:ALA:N     | 2.17                     | 0.60              |
| 2:B:1946:SER:OG   | 2:B:1947:MET:N    | 2.32                     | 0.60              |
| 2:B:2006:LEU:O    | 2:B:2008:ALA:N    | 2.27                     | 0.60              |
| 2:B:2032:ILE:HA   | 2:B:2036:GLN:OE1  | 2.01                     | 0.60              |
| 1:A:489:ARG:HH11  | 1:A:489:ARG:CB    | 2.14                     | 0.60              |
| 2:B:2232:VAL:O    | 2:B:2234:PHE:N    | 2.28                     | 0.60              |
| 1:A:541:ARG:O     | 1:A:542:ASP:C     | 2.44                     | 0.60              |
| 2:B:2044:GLY:O    | 2:B:2046:TRP:N    | 2.35                     | 0.60              |
| 2:B:2178:LEU:HD21 | 2:B:2325:GLY:O    | 2.00                     | 0.60              |
| 2:B:2217:ASN:O    | 2:B:2218:ALA:HB2  | 2.01                     | 0.60              |
| 2:B:2253:THR:HG23 | 2:B:2253:THR:O    | 2.00                     | 0.60              |
| 1:A:661:LYS:HE2   | 1:A:665:GLU:CD    | 2.26                     | 0.60              |
| 1:A:698:ARG:HD2   | 1:A:702:MET:HE1   | 1.83                     | 0.60              |
| 2:B:1954:HIS:HE1  | 2:B:2005:HIS:ND1  | 2.00                     | 0.60              |
| 1:A:68:TRP:O      | 1:A:69:MET:HB2    | 2.01                     | 0.60              |
| 1:A:501:PHE:HB2   | 1:A:502:PRO:HD3   | 1.82                     | 0.60              |
| 2:B:1846:ASP:O    | 2:B:1848:HIS:N    | 2.35                     | 0.60              |
| 1:A:47:LYS:CD     | 1:A:225:ALA:HB1   | 2.32                     | 0.59              |
| 1:A:130:PRO:C     | 1:A:132:GLY:H     | 2.09                     | 0.59              |
| 1:A:690:LEU:HB2   | 1:A:708:VAL:HB    | 1.83                     | 0.59              |
| 2:B:1942:TRP:CE3  | 2:B:1958:PHE:HZ   | 2.20                     | 0.59              |
| 2:B:2116:ARG:HH21 | 2:B:2120:THR:C    | 2.10                     | 0.59              |
| 2:B:2196:PHE:HZ   | 2:B:2198:ASN:HD22 | 1.49                     | 0.59              |
| 1:A:267:HIS:CE1   | 1:A:320:MET:HG3   | 2.37                     | 0.59              |
| 1:A:577:SER:OG    | 1:A:642:ILE:HB    | 2.03                     | 0.59              |
| 1:A:651:VAL:C     | 1:A:693:HIS:HB2   | 2.27                     | 0.59              |
| 2:B:1694:LYS:HB3  | 2:B:1769:ASP:HB3  | 1.83                     | 0.59              |
| 2:B:1934:MET:O    | 2:B:1935:ALA:CB   | 2.51                     | 0.59              |
| 2:B:2186:SER:C    | 2:B:2188:ALA:H    | 2.09                     | 0.59              |
| 2:B:2199:MET:HG2  | 2:B:2199:MET:O    | 2.03                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:24:LEU:O      | 1:A:29:ARG:HG3    | 2.03                     | 0.59              |
| 1:A:96:VAL:HB     | 1:A:160:SER:OG    | 2.02                     | 0.59              |
| 1:A:278:VAL:O     | 1:A:279:ARG:C     | 2.45                     | 0.59              |
| 2:B:1855:LEU:HD23 | 2:B:1856:LEU:O    | 2.02                     | 0.59              |
| 2:B:2097:TYR:CZ   | 2:B:2130:VAL:HG23 | 2.37                     | 0.59              |
| 2:B:2144:ILE:CG2  | 2:B:2145:ILE:H    | 2.15                     | 0.59              |
| 2:B:2220:ARG:HH11 | 2:B:2220:ARG:HB2  | 1.67                     | 0.59              |
| 1:A:234:VAL:O     | 1:A:236:GLY:N     | 2.35                     | 0.59              |
| 2:B:1733:VAL:HG22 | 2:B:1851:LEU:HD12 | 1.83                     | 0.59              |
| 2:B:1770:ASN:OD1  | 2:B:1818:LYS:HA   | 2.01                     | 0.59              |
| 2:B:1771:ILE:HD12 | 2:B:1817:TRP:NE1  | 2.17                     | 0.59              |
| 1:A:180:ARG:O     | 1:A:181:GLU:O     | 2.21                     | 0.59              |
| 1:A:576:PHE:HB3   | 1:A:617:ILE:HD13  | 1.82                     | 0.59              |
| 1:A:654:SER:H     | 1:A:657:THR:HA    | 1.68                     | 0.59              |
| 2:B:1772:MET:HE2  | 2:B:1774:THR:HG23 | 1.83                     | 0.59              |
| 2:B:2023:THR:O    | 2:B:2168:GLY:O    | 2.21                     | 0.59              |
| 1:A:588:THR:HA    | 1:A:591:ILE:CG2   | 2.32                     | 0.59              |
| 1:A:713:LYS:O     | 1:A:714:ASN:HB2   | 2.02                     | 0.59              |
| 2:B:1781:ARG:NH2  | 2:B:1845:LYS:HE2  | 2.18                     | 0.59              |
| 2:B:1801:GLU:H    | 2:B:1802:PRO:CD   | 2.14                     | 0.59              |
| 2:B:1823:MET:O    | 2:B:1824:ALA:HB2  | 2.03                     | 0.59              |
| 2:B:1954:HIS:CD2  | 2:B:2010:MET:HE1  | 2.36                     | 0.59              |
| 1:A:705:LEU:C     | 1:A:706:LEU:HD22  | 2.28                     | 0.59              |
| 2:B:1820:GLN:N    | 2:B:1823:MET:HE2  | 2.17                     | 0.59              |
| 2:B:1834:ALA:HB2  | 2:B:1985:THR:HG22 | 1.84                     | 0.59              |
| 2:B:2105:TYR:CE2  | 2:B:2144:ILE:HD13 | 2.37                     | 0.59              |
| 2:B:2209:ARG:HG2  | 2:B:2209:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:284:ALA:O     | 1:A:285:SER:HB2   | 2.02                     | 0.59              |
| 1:A:434:GLU:CB    | 1:A:466:LYS:HE3   | 2.32                     | 0.59              |
| 1:A:574:ILE:HA    | 1:A:618:ASN:OD1   | 2.03                     | 0.59              |
| 1:A:621:VAL:HG12  | 1:A:622:PHE:N     | 2.16                     | 0.59              |
| 2:B:1833:LYS:HG3  | 2:B:1834:ALA:H    | 1.68                     | 0.59              |
| 2:B:1949:SER:H    | 2:B:1952:ASN:ND2  | 2.01                     | 0.59              |
| 2:B:2224:ASN:HB3  | 2:B:2317:ILE:CD1  | 2.33                     | 0.59              |
| 2:B:2242:GLY:HA2  | 2:B:2297:LEU:HD12 | 1.84                     | 0.59              |
| 2:B:2260:PHE:HB3  | 2:B:2310:PRO:HA   | 1.85                     | 0.59              |
| 1:A:158:TYR:O     | 1:A:159:LEU:HB3   | 2.02                     | 0.59              |
| 1:A:181:GLU:O     | 1:A:183:SER:N     | 2.36                     | 0.59              |
| 1:A:610:ALA:O     | 1:A:613:ILE:HG12  | 2.03                     | 0.59              |
| 1:A:624:SER:C     | 1:A:707:LYS:HZ1   | 2.10                     | 0.59              |
| 1:A:663:VAL:HA    | 2:B:1968:LYS:HZ2  | 1.66                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:667:THR:OG1   | 1:A:668:LEU:N     | 2.34                     | 0.59              |
| 2:B:2027:MET:SD   | 2:B:2164:MET:HE3  | 2.42                     | 0.59              |
| 2:B:2060:ASN:H    | 2:B:2060:ASN:HD22 | 1.50                     | 0.59              |
| 1:A:228:TRP:CB    | 1:A:229:PRO:CD    | 2.72                     | 0.58              |
| 1:A:651:VAL:CG1   | 1:A:652:PHE:H     | 1.96                     | 0.58              |
| 2:B:1753:ASN:HB3  | 2:B:1756:LEU:CD1  | 2.33                     | 0.58              |
| 2:B:2015:LEU:H    | 2:B:2015:LEU:HD12 | 1.68                     | 0.58              |
| 2:B:2233:ASP:O    | 2:B:2235:GLN:N    | 2.36                     | 0.58              |
| 1:A:5:TYR:CD2     | 1:A:76:ILE:HG12   | 2.38                     | 0.58              |
| 1:A:71:LEU:HD11   | 1:A:202:PHE:CE2   | 2.38                     | 0.58              |
| 1:A:71:LEU:HD11   | 1:A:202:PHE:HE2   | 1.69                     | 0.58              |
| 1:A:89:LYS:HA     | 1:A:133:SER:CB    | 2.33                     | 0.58              |
| 1:A:575:LEU:HB3   | 1:A:640:LEU:HD21  | 1.85                     | 0.58              |
| 1:A:591:ILE:O     | 1:A:593:ARG:N     | 2.35                     | 0.58              |
| 1:A:605:ASP:HB2   | 1:A:606:PRO:HD2   | 1.85                     | 0.58              |
| 1:A:663:VAL:HG13  | 2:B:1968:LYS:CD   | 2.34                     | 0.58              |
| 2:B:2052:ARG:NH2  | 2:B:2087:GLN:HE22 | 2.01                     | 0.58              |
| 1:A:8:GLY:O       | 1:A:9:ALA:HB2     | 2.03                     | 0.58              |
| 1:A:164:LEU:H     | 1:A:164:LEU:CD1   | 2.16                     | 0.58              |
| 1:A:279:ARG:HH21  | 2:B:1971:TYR:HB3  | 1.68                     | 0.58              |
| 1:A:565:GLN:HE21  | 1:A:566:ILE:HG23  | 1.68                     | 0.58              |
| 2:B:1764:ARG:HG3  | 2:B:1764:ARG:HH11 | 1.68                     | 0.58              |
| 2:B:2132:SER:O    | 2:B:2133:SER:HB2  | 2.03                     | 0.58              |
| 2:B:2243:VAL:HG23 | 2:B:2321:MET:HE1  | 1.83                     | 0.58              |
| 2:B:2282:VAL:O    | 2:B:2282:VAL:HG13 | 2.04                     | 0.58              |
| 1:A:404:ASP:O     | 1:A:406:SER:N     | 2.36                     | 0.58              |
| 2:B:1790:ILE:HG22 | 2:B:1817:TRP:HZ3  | 1.67                     | 0.58              |
| 2:B:1837:TYR:CZ   | 2:B:1853:GLY:HA3  | 2.38                     | 0.58              |
| 2:B:1873:VAL:HG12 | 2:B:1939:ARG:HB3  | 1.85                     | 0.58              |
| 2:B:2150:ARG:HB3  | 2:B:2152:HIS:CE1  | 2.38                     | 0.58              |
| 2:B:1733:VAL:CG2  | 2:B:1851:LEU:HD12 | 2.34                     | 0.58              |
| 2:B:2210:LEU:C    | 2:B:2212:LEU:H    | 2.10                     | 0.58              |
| 1:A:575:LEU:HD23  | 1:A:575:LEU:N     | 2.19                     | 0.58              |
| 1:A:614:MET:SD    | 1:A:614:MET:N     | 2.68                     | 0.58              |
| 2:B:1736:GLN:HG2  | 2:B:1747:LEU:HG   | 1.84                     | 0.58              |
| 1:A:98:LEU:HB3    | 1:A:136:TYR:CZ    | 2.39                     | 0.58              |
| 1:A:497:HIS:CG    | 1:A:499:LYS:HG2   | 2.38                     | 0.58              |
| 2:B:1719:ARG:HA   | 2:B:1719:ARG:NE   | 2.18                     | 0.58              |
| 2:B:1774:THR:HA   | 2:B:1814:THR:HG22 | 1.86                     | 0.58              |
| 2:B:2012:THR:HG22 | 2:B:2013:LEU:N    | 2.17                     | 0.58              |
| 2:B:2097:TYR:CD2  | 2:B:2130:VAL:HA   | 2.38                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:331:GLU:HG3   | 1:A:333:PRO:HD3   | 1.85                     | 0.58              |
| 1:A:629:VAL:HG11  | 1:A:684:ASN:ND2   | 2.19                     | 0.58              |
| 1:A:657:THR:HG1   | 2:B:1786:TYR:HE1  | 1.52                     | 0.58              |
| 1:A:687:LEU:C     | 1:A:710:SER:OG    | 2.47                     | 0.58              |
| 1:A:687:LEU:HD21  | 2:B:1795:ASP:HB2  | 1.85                     | 0.58              |
| 2:B:1956:ILE:HD11 | 2:B:1978:LEU:CD1  | 2.34                     | 0.58              |
| 2:B:1992:LYS:CD   | 2:B:1993:ALA:H    | 2.17                     | 0.58              |
| 2:B:2178:LEU:HD11 | 2:B:2325:GLY:CA   | 2.33                     | 0.58              |
| 2:B:2232:VAL:HG22 | 2:B:2306:LEU:O    | 2.04                     | 0.58              |
| 1:A:304:GLY:O     | 1:A:326:VAL:HG12  | 2.04                     | 0.58              |
| 1:A:475:ILE:C     | 1:A:475:ILE:HD13  | 2.29                     | 0.58              |
| 1:A:522:THR:OG1   | 1:A:523:LYS:N     | 2.34                     | 0.58              |
| 2:B:1741:GLY:O    | 2:B:1742:SER:O    | 2.22                     | 0.58              |
| 2:B:1848:HIS:CE1  | 2:B:1883:PHE:HA   | 2.39                     | 0.58              |
| 2:B:1940:ILE:HG22 | 2:B:1941:ARG:N    | 2.18                     | 0.58              |
| 2:B:2048:PRO:HD3  | 2:B:2062:TRP:CD1  | 2.39                     | 0.58              |
| 2:B:2124:MET:HE3  | 2:B:2125:VAL:H    | 1.67                     | 0.58              |
| 1:A:382:TRP:HB2   | 1:A:461:LEU:HD12  | 1.86                     | 0.58              |
| 1:A:660:HIS:HB2   | 1:A:680:MET:HG3   | 1.85                     | 0.58              |
| 2:B:2050:LEU:HD22 | 2:B:2054:HIS:CD2  | 2.38                     | 0.58              |
| 1:A:161:HIS:O     | 1:A:163:ASP:N     | 2.37                     | 0.57              |
| 1:A:237:TYR:CD2   | 1:A:242:LEU:HD13  | 2.39                     | 0.57              |
| 1:A:411:TYR:HB3   | 1:A:614:MET:HE3   | 1.85                     | 0.57              |
| 1:A:451:PRO:O     | 1:A:453:LEU:CD2   | 2.52                     | 0.57              |
| 1:A:581:GLU:C     | 1:A:583:ARG:H     | 2.12                     | 0.57              |
| 2:B:1832:CYS:SG   | 2:B:1941:ARG:NH1  | 2.77                     | 0.57              |
| 2:B:1962:VAL:O    | 2:B:1963:PHE:HB3  | 2.04                     | 0.57              |
| 2:B:2006:LEU:C    | 2:B:2008:ALA:H    | 2.11                     | 0.57              |
| 2:B:2145:ILE:O    | 2:B:2146:ALA:HB2  | 2.02                     | 0.57              |
| 2:B:2198:ASN:HB3  | 2:B:2201:ALA:HB3  | 1.85                     | 0.57              |
| 1:A:497:HIS:CE1   | 1:A:499:LYS:HG2   | 2.39                     | 0.57              |
| 2:B:1715:PRO:CB   | 2:B:1718:LEU:HB2  | 2.30                     | 0.57              |
| 2:B:1819:VAL:O    | 2:B:1819:VAL:HG12 | 2.04                     | 0.57              |
| 2:B:2125:VAL:HG23 | 2:B:2125:VAL:O    | 2.04                     | 0.57              |
| 1:A:497:HIS:NE2   | 1:A:499:LYS:HE3   | 2.19                     | 0.57              |
| 1:A:587:LEU:O     | 1:A:591:ILE:HG22  | 2.03                     | 0.57              |
| 2:B:1934:MET:HG3  | 2:B:2016:VAL:HB   | 1.85                     | 0.57              |
| 2:B:2190:ILE:HG12 | 2:B:2232:VAL:HG12 | 1.86                     | 0.57              |
| 2:B:2242:GLY:O    | 2:B:2324:LEU:HB2  | 2.04                     | 0.57              |
| 1:A:71:LEU:O      | 1:A:72:LEU:C      | 2.46                     | 0.57              |
| 1:A:121:ARG:HA    | 1:A:124:GLU:HB2   | 1.85                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:494:GLY:O     | 1:A:495:VAL:HB    | 2.04                     | 0.57              |
| 2:B:1777:ASN:ND2  | 2:B:1778:GLN:H    | 2.02                     | 0.57              |
| 2:B:1785:PHE:HE1  | 2:B:1837:TYR:CD1  | 2.23                     | 0.57              |
| 2:B:1839:SER:OG   | 2:B:1841:VAL:HG23 | 2.04                     | 0.57              |
| 2:B:2053:LEU:O    | 2:B:2054:HIS:C    | 2.45                     | 0.57              |
| 2:B:2060:ASN:ND2  | 2:B:2060:ASN:N    | 2.51                     | 0.57              |
| 1:A:526:PRO:HD2   | 1:A:679:PHE:HZ    | 1.70                     | 0.57              |
| 2:B:1926:MET:H    | 2:B:2009:GLY:HA2  | 1.69                     | 0.57              |
| 2:B:2107:LEU:HG   | 2:B:2146:ALA:HA   | 1.85                     | 0.57              |
| 2:B:2129:ASN:N    | 2:B:2129:ASN:OD1  | 2.37                     | 0.57              |
| 1:A:683:GLU:O     | 1:A:683:GLU:OE2   | 2.23                     | 0.57              |
| 2:B:1730:PHE:CE2  | 2:B:1885:GLU:HG3  | 2.40                     | 0.57              |
| 2:B:2129:ASN:O    | 2:B:2130:VAL:HB   | 2.03                     | 0.57              |
| 2:B:2165:GLU:O    | 2:B:2166:LEU:C    | 2.47                     | 0.57              |
| 1:A:114:TYR:HD1   | 2:B:1997:ARG:HD3  | 1.70                     | 0.57              |
| 1:A:535:SER:O     | 1:A:536:PHE:CD1   | 2.58                     | 0.57              |
| 2:B:1979:TYR:O    | 2:B:1982:VAL:HG12 | 2.04                     | 0.57              |
| 2:B:2080:ILE:HG22 | 2:B:2145:ILE:HG23 | 1.85                     | 0.57              |
| 2:B:2161:THR:O    | 2:B:2162:LEU:HB3  | 2.04                     | 0.57              |
| 1:A:114:TYR:CD1   | 2:B:1997:ARG:HD3  | 2.39                     | 0.57              |
| 1:A:147:MET:HB2   | 1:A:150:ASP:OD2   | 2.04                     | 0.57              |
| 1:A:244:GLY:O     | 1:A:245:LEU:HB2   | 2.04                     | 0.57              |
| 2:B:1848:HIS:CE1  | 2:B:1884:ASP:H    | 2.22                     | 0.57              |
| 1:A:208:TRP:O     | 1:A:209:HIS:O     | 2.23                     | 0.57              |
| 1:A:291:ILE:HG13  | 1:A:291:ILE:O     | 2.05                     | 0.57              |
| 1:A:653:PHE:O     | 1:A:691:GLY:N     | 2.37                     | 0.57              |
| 2:B:1751:GLU:CG   | 2:B:2116:ARG:HB3  | 2.35                     | 0.57              |
| 2:B:1953:ILE:HG13 | 2:B:1980:PRO:HD3  | 1.86                     | 0.57              |
| 2:B:2096:LEU:HD11 | 2:B:2158:ILE:CG2  | 2.34                     | 0.57              |
| 2:B:2237:THR:HA   | 2:B:2304:ARG:CA   | 2.35                     | 0.57              |
| 1:A:69:MET:HA     | 1:A:235:ASN:OD1   | 2.05                     | 0.57              |
| 1:A:159:LEU:N     | 1:A:159:LEU:HD23  | 2.20                     | 0.57              |
| 1:A:606:PRO:HA    | 1:A:609:GLN:NE2   | 2.20                     | 0.57              |
| 1:A:687:LEU:HD11  | 2:B:1795:ASP:CB   | 2.35                     | 0.57              |
| 2:B:1924:TYR:CD2  | 2:B:1930:PRO:HD3  | 2.40                     | 0.57              |
| 2:B:2151:LEU:HD23 | 2:B:2152:HIS:N    | 2.20                     | 0.57              |
| 2:B:1949:SER:H    | 2:B:1952:ASN:HD21 | 1.52                     | 0.56              |
| 2:B:1956:ILE:HD11 | 2:B:1978:LEU:HD11 | 1.87                     | 0.56              |
| 2:B:2141:ASN:CA   | 2:B:2142:PRO:C    | 2.78                     | 0.56              |
| 1:A:3:ARG:CZ      | 1:A:184:LEU:HD12  | 2.35                     | 0.56              |
| 1:A:58:LEU:CD1    | 1:A:58:LEU:H      | 2.18                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:128:VAL:HG13  | 1:A:134:HIS:HD2   | 1.69                     | 0.56              |
| 2:B:2124:MET:HE3  | 2:B:2125:VAL:N    | 2.21                     | 0.56              |
| 1:A:394:ASP:OD2   | 1:A:421:ARG:HD2   | 2.05                     | 0.56              |
| 1:A:414:ASN:HB3   | 1:A:419:ILE:O     | 2.04                     | 0.56              |
| 1:A:658:PHE:C     | 1:A:659:LYS:HD3   | 2.29                     | 0.56              |
| 2:B:1714:SER:OG   | 2:B:1724:SER:HB3  | 2.05                     | 0.56              |
| 2:B:2116:ARG:NH2  | 2:B:2120:THR:HA   | 2.16                     | 0.56              |
| 2:B:2263:SER:OG   | 2:B:2309:HIS:NE2  | 2.38                     | 0.56              |
| 1:A:18:GLN:O      | 1:A:19:SER:CB     | 2.53                     | 0.56              |
| 1:A:111:GLY:O     | 1:A:161:HIS:HB3   | 2.04                     | 0.56              |
| 1:A:604:GLU:HA    | 1:A:608:PHE:CE1   | 2.40                     | 0.56              |
| 2:B:2037:ILE:HB   | 2:B:2048:PRO:HB3  | 1.86                     | 0.56              |
| 2:B:2052:ARG:NH2  | 2:B:2053:LEU:CG   | 2.69                     | 0.56              |
| 2:B:2104:MET:HE2  | 2:B:2114:THR:HG22 | 1.86                     | 0.56              |
| 1:A:152:LEU:O     | 1:A:153:CYS:HB2   | 2.03                     | 0.56              |
| 1:A:385:TYR:CZ    | 1:A:437:LYS:HD2   | 2.40                     | 0.56              |
| 1:A:396:ALA:HB2   | 1:A:421:ARG:NH1   | 2.19                     | 0.56              |
| 1:A:656:TYR:HE2   | 1:A:685:PRO:HG2   | 1.70                     | 0.56              |
| 2:B:1737:GLU:C    | 2:B:1738:PHE:HD2  | 2.13                     | 0.56              |
| 2:B:1882:ILE:O    | 2:B:1882:ILE:CG2  | 2.54                     | 0.56              |
| 2:B:2023:THR:CG2  | 2:B:2024:PRO:HD2  | 2.34                     | 0.56              |
| 2:B:2256:TYR:CE2  | 2:B:2314:VAL:HG21 | 2.41                     | 0.56              |
| 1:A:33:ARG:HD2    | 1:A:35:PRO:HG2    | 1.87                     | 0.56              |
| 1:A:427:ARG:HD2   | 1:A:448:ILE:O     | 2.05                     | 0.56              |
| 1:A:432:THR:HA    | 1:A:438:THR:HB    | 1.88                     | 0.56              |
| 1:A:480:ILE:HG22  | 1:A:481:THR:N     | 2.21                     | 0.56              |
| 1:A:624:SER:HB2   | 1:A:625:LEU:HD12  | 1.86                     | 0.56              |
| 2:B:1965:VAL:HG12 | 2:B:1971:TYR:O    | 2.05                     | 0.56              |
| 2:B:2043:TYR:CD1  | 2:B:2064:THR:HA   | 2.41                     | 0.56              |
| 1:A:501:PHE:O     | 1:A:503:ILE:HG13  | 2.06                     | 0.56              |
| 1:A:621:VAL:O     | 1:A:623:ASP:N     | 2.39                     | 0.56              |
| 2:B:1880:PHE:O    | 2:B:1881:THR:HB   | 2.03                     | 0.56              |
| 2:B:1936:GLN:OE1  | 2:B:1992:LYS:HA   | 2.06                     | 0.56              |
| 2:B:2006:LEU:C    | 2:B:2008:ALA:N    | 2.64                     | 0.56              |
| 2:B:2195:TYR:O    | 2:B:2195:TYR:CG   | 2.58                     | 0.56              |
| 1:A:232:HIS:HB3   | 1:A:320:MET:CG    | 2.36                     | 0.56              |
| 1:A:292:THR:HG23  | 2:B:1977:ASN:HD21 | 1.69                     | 0.56              |
| 1:A:408:LYS:HG3   | 1:A:622:PHE:CE2   | 2.41                     | 0.56              |
| 1:A:588:THR:CA    | 1:A:591:ILE:HG22  | 2.36                     | 0.56              |
| 1:A:625:LEU:O     | 1:A:627:LEU:N     | 2.39                     | 0.56              |
| 2:B:2032:ILE:HG22 | 2:B:2036:GLN:HG3  | 1.86                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2050:LEU:O    | 2:B:2051:ALA:HB2  | 2.06                     | 0.56              |
| 2:B:2083:GLY:HA2  | 2:B:2140:PHE:CD2  | 2.41                     | 0.56              |
| 1:A:56:ASP:CG     | 1:A:57:HIS:ND1    | 2.64                     | 0.56              |
| 1:A:125:ASP:C     | 1:A:127:LYS:H     | 2.14                     | 0.56              |
| 1:A:374:VAL:HG23  | 1:A:374:VAL:O     | 2.06                     | 0.56              |
| 2:B:1820:GLN:NE2  | 2:B:1822:HIS:N    | 2.41                     | 0.56              |
| 2:B:2036:GLN:HE22 | 2:B:2076:LEU:CG   | 2.19                     | 0.56              |
| 2:B:2144:ILE:HG22 | 2:B:2145:ILE:H    | 1.65                     | 0.56              |
| 2:B:2165:GLU:O    | 2:B:2166:LEU:O    | 2.23                     | 0.56              |
| 2:B:2266:GLN:O    | 2:B:2267:ASP:HB3  | 2.05                     | 0.56              |
| 1:A:61:ILE:O      | 1:A:62:ALA:HB2    | 2.06                     | 0.56              |
| 1:A:309:PHE:HB2   | 1:A:321:GLU:HG2   | 1.88                     | 0.56              |
| 1:A:453:LEU:O     | 1:A:551:LEU:HD12  | 2.05                     | 0.56              |
| 1:A:640:LEU:HB3   | 1:A:677:THR:OG1   | 2.06                     | 0.56              |
| 2:B:1834:ALA:HB1  | 2:B:1945:LEU:HD11 | 1.86                     | 0.56              |
| 2:B:1880:PHE:N    | 2:B:1880:PHE:HD1  | 2.04                     | 0.56              |
| 2:B:1924:TYR:CE2  | 2:B:1930:PRO:HD3  | 2.41                     | 0.55              |
| 2:B:1932:LEU:CD1  | 2:B:2014:PHE:HB3  | 2.32                     | 0.55              |
| 2:B:2052:ARG:HH22 | 2:B:2053:LEU:HG   | 1.70                     | 0.55              |
| 1:A:419:ILE:O     | 1:A:420:GLY:O     | 2.24                     | 0.55              |
| 1:A:440:GLU:OE1   | 1:A:441:ALA:N     | 2.38                     | 0.55              |
| 1:A:495:VAL:CG2   | 1:A:496:LYS:H     | 2.17                     | 0.55              |
| 1:A:659:LYS:CE    | 1:A:659:LYS:H     | 2.19                     | 0.55              |
| 1:A:667:THR:O     | 1:A:669:THR:N     | 2.39                     | 0.55              |
| 1:A:705:LEU:O     | 1:A:706:LEU:HB2   | 2.06                     | 0.55              |
| 2:B:2181:GLU:C    | 2:B:2183:LYS:H    | 2.13                     | 0.55              |
| 1:A:434:GLU:HG3   | 1:A:466:LYS:NZ    | 2.21                     | 0.55              |
| 2:B:1938:GLN:O    | 2:B:1939:ARG:C    | 2.48                     | 0.55              |
| 2:B:2180:MET:HB2  | 2:B:2322:GLU:HG3  | 1.87                     | 0.55              |
| 1:A:126:ASP:O     | 1:A:127:LYS:HB2   | 2.07                     | 0.55              |
| 1:A:160:SER:CB    | 1:A:172:LEU:HD23  | 2.26                     | 0.55              |
| 1:A:164:LEU:HD12  | 1:A:164:LEU:N     | 2.20                     | 0.55              |
| 1:A:308:LEU:HD23  | 1:A:309:PHE:N     | 2.21                     | 0.55              |
| 2:B:2012:THR:CG2  | 2:B:2013:LEU:N    | 2.69                     | 0.55              |
| 1:A:89:LYS:HG3    | 1:A:133:SER:CB    | 2.36                     | 0.55              |
| 1:A:260:MET:HE2   | 1:A:261:GLY:N     | 2.22                     | 0.55              |
| 1:A:467:ASN:CG    | 1:A:468:GLN:H     | 2.14                     | 0.55              |
| 2:B:2060:ASN:O    | 2:B:2061:ALA:HB2  | 2.07                     | 0.55              |
| 2:B:2178:LEU:HD11 | 2:B:2325:GLY:HA3  | 1.88                     | 0.55              |
| 1:A:88:LEU:HD23   | 1:A:88:LEU:C      | 2.32                     | 0.55              |
| 1:A:141:LEU:HD22  | 1:A:142:LYS:HG2   | 1.89                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:480:ILE:HD11  | 1:A:553:ILE:HD11  | 1.89                     | 0.55              |
| 1:A:495:VAL:HG21  | 1:A:502:PRO:HD3   | 1.88                     | 0.55              |
| 1:A:552:LEU:C     | 1:A:553:ILE:HG12  | 2.32                     | 0.55              |
| 2:B:2154:THR:O    | 2:B:2155:HIS:ND1  | 2.40                     | 0.55              |
| 2:B:2237:THR:HA   | 2:B:2304:ARG:HB3  | 1.88                     | 0.55              |
| 1:A:38:PHE:HB3    | 1:A:39:PRO:CD     | 2.36                     | 0.55              |
| 1:A:259:GLY:O     | 1:A:260:MET:HB2   | 2.07                     | 0.55              |
| 1:A:574:ILE:O     | 1:A:639:ILE:HA    | 2.07                     | 0.55              |
| 1:A:713:LYS:CE    | 1:A:714:ASN:H     | 2.19                     | 0.55              |
| 2:B:1821:HIS:O    | 2:B:1823:MET:N    | 2.39                     | 0.55              |
| 1:A:27:ASP:O      | 1:A:28:ALA:HB3    | 2.06                     | 0.55              |
| 1:A:118:THR:HG22  | 1:A:123:LYS:CE    | 2.37                     | 0.55              |
| 1:A:319:GLY:O     | 1:A:320:MET:HB2   | 2.06                     | 0.55              |
| 2:B:1709:TYR:OH   | 2:B:1918:PHE:HD2  | 1.90                     | 0.55              |
| 1:A:201:VAL:O     | 1:A:201:VAL:HG12  | 2.06                     | 0.55              |
| 1:A:656:TYR:O     | 1:A:658:PHE:N     | 2.39                     | 0.55              |
| 1:A:63:LYS:CB     | 1:A:64:PRO:CD     | 2.84                     | 0.55              |
| 1:A:682:MET:SD    | 1:A:684:ASN:OD1   | 2.65                     | 0.55              |
| 2:B:1848:HIS:HE1  | 2:B:1883:PHE:HA   | 1.72                     | 0.55              |
| 2:B:2027:MET:N    | 2:B:2165:GLU:HG3  | 2.22                     | 0.55              |
| 2:B:2075:LEU:O    | 2:B:2076:LEU:HB2  | 2.07                     | 0.55              |
| 2:B:2081:ILE:HG12 | 2:B:2144:ILE:O    | 2.07                     | 0.55              |
| 2:B:2149:ILE:HD12 | 2:B:2166:LEU:HD22 | 1.89                     | 0.55              |
| 2:B:2259:GLU:HG2  | 2:B:2284:GLN:HE22 | 1.71                     | 0.55              |
| 1:A:384:HIS:HB3   | 1:A:386:ILE:HG23  | 1.89                     | 0.54              |
| 1:A:543:LEU:HD23  | 1:A:543:LEU:C     | 2.32                     | 0.54              |
| 2:B:1821:HIS:C    | 2:B:1823:MET:N    | 2.60                     | 0.54              |
| 2:B:2021:CYS:O    | 2:B:2023:THR:N    | 2.41                     | 0.54              |
| 1:A:399:VAL:C     | 1:A:400:LEU:HD23  | 2.33                     | 0.54              |
| 1:A:552:LEU:O     | 1:A:553:ILE:HG12  | 2.08                     | 0.54              |
| 2:B:1738:PHE:HE1  | 2:B:1742:SER:CA   | 2.18                     | 0.54              |
| 2:B:1778:GLN:O    | 2:B:1779:ALA:HB2  | 2.06                     | 0.54              |
| 2:B:1919:HIS:O    | 2:B:2010:MET:N    | 2.40                     | 0.54              |
| 2:B:2017:TYR:HA   | 2:B:2173:SER:OG   | 2.07                     | 0.54              |
| 2:B:2255:MET:HB2  | 2:B:2314:VAL:O    | 2.07                     | 0.54              |
| 1:A:276:PHE:CD2   | 1:A:286:LEU:HG    | 2.42                     | 0.54              |
| 1:A:378:HIS:HB2   | 1:A:379:PRO:CD    | 2.35                     | 0.54              |
| 1:A:440:GLU:O     | 1:A:441:ALA:HB3   | 2.06                     | 0.54              |
| 1:A:625:LEU:C     | 1:A:627:LEU:N     | 2.66                     | 0.54              |
| 1:A:663:VAL:HG11  | 2:B:1967:LYS:O    | 2.07                     | 0.54              |
| 2:B:1942:TRP:HB3  | 2:B:1944:LEU:HD21 | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2237:THR:N    | 2:B:2330:ASP:OD2  | 2.39                     | 0.54              |
| 1:A:434:GLU:C     | 1:A:434:GLU:OE1   | 2.51                     | 0.54              |
| 2:B:1743:PHE:O    | 2:B:1744:THR:C    | 2.50                     | 0.54              |
| 2:B:1757:GLY:CA   | 2:B:1922:ASN:HB3  | 2.30                     | 0.54              |
| 2:B:1825:PRO:HD3  | 2:B:1833:LYS:HB2  | 1.90                     | 0.54              |
| 2:B:1977:ASN:O    | 2:B:1978:LEU:C    | 2.51                     | 0.54              |
| 2:B:1997:ARG:HG2  | 2:B:1998:VAL:H    | 1.71                     | 0.54              |
| 2:B:2273:LEU:HD23 | 2:B:2274:PHE:H    | 1.71                     | 0.54              |
| 1:A:141:LEU:HD22  | 1:A:143:GLU:H     | 1.72                     | 0.54              |
| 1:A:141:LEU:HB2   | 1:A:144:ASN:ND2   | 2.22                     | 0.54              |
| 1:A:533:TYR:O     | 1:A:534:SER:HB2   | 2.07                     | 0.54              |
| 1:A:654:SER:CB    | 1:A:690:LEU:HA    | 2.36                     | 0.54              |
| 1:A:662:MET:O     | 1:A:663:VAL:CB    | 2.54                     | 0.54              |
| 2:B:1736:GLN:CG   | 2:B:1747:LEU:HG   | 2.37                     | 0.54              |
| 2:B:2021:CYS:HA   | 2:B:2176:MET:SD   | 2.48                     | 0.54              |
| 1:A:57:HIS:O      | 1:A:58:LEU:O      | 2.25                     | 0.54              |
| 1:A:90:ASN:O      | 1:A:92:ALA:N      | 2.39                     | 0.54              |
| 1:A:529:LEU:HD13  | 1:A:553:ILE:HB    | 1.88                     | 0.54              |
| 1:A:543:LEU:C     | 1:A:543:LEU:CD2   | 2.81                     | 0.54              |
| 1:A:657:THR:CG2   | 2:B:1788:SER:HA   | 2.37                     | 0.54              |
| 2:B:2002:ILE:O    | 2:B:2003:GLY:C    | 2.50                     | 0.54              |
| 1:A:641:SER:C     | 1:A:642:ILE:HG12  | 2.32                     | 0.54              |
| 1:A:661:LYS:HG2   | 1:A:665:GLU:CG    | 2.35                     | 0.54              |
| 2:B:1763:ILE:HD13 | 2:B:1763:ILE:C    | 2.33                     | 0.54              |
| 2:B:1864:ASN:ND2  | 2:B:1867:HIS:O    | 2.41                     | 0.54              |
| 2:B:2052:ARG:CZ   | 2:B:2053:LEU:HB2  | 2.37                     | 0.54              |
| 1:A:543:LEU:O     | 1:A:544:ALA:C     | 2.51                     | 0.54              |
| 1:A:623:ASP:O     | 1:A:624:SER:OG    | 2.16                     | 0.54              |
| 1:A:655:GLY:O     | 1:A:656:TYR:HB2   | 2.07                     | 0.54              |
| 2:B:1698:TYR:CD2  | 2:B:1763:ILE:HG12 | 2.42                     | 0.54              |
| 2:B:1758:LEU:H    | 2:B:1758:LEU:CD2  | 2.16                     | 0.54              |
| 2:B:2036:GLN:C    | 2:B:2037:ILE:HG13 | 2.32                     | 0.54              |
| 2:B:2151:LEU:C    | 2:B:2152:HIS:HD1  | 2.15                     | 0.54              |
| 2:B:2191:THR:O    | 2:B:2231:GLN:HB3  | 2.08                     | 0.54              |
| 1:A:63:LYS:HG2    | 1:A:64:PRO:HD2    | 1.90                     | 0.54              |
| 2:B:2048:PRO:O    | 2:B:2049:LYS:HB2  | 2.08                     | 0.54              |
| 1:A:98:LEU:HD23   | 1:A:99:HIS:N      | 2.23                     | 0.54              |
| 1:A:260:MET:HE2   | 1:A:261:GLY:H     | 1.73                     | 0.54              |
| 1:A:280:ASN:HB3   | 1:A:524:SER:OG    | 2.08                     | 0.54              |
| 1:A:662:MET:N     | 1:A:680:MET:HE1   | 2.23                     | 0.54              |
| 1:A:694:ASN:ND2   | 1:A:699:ASN:HB3   | 2.22                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1694:LYS:N    | 2:B:1694:LYS:HD2  | 2.23                     | 0.54              |
| 2:B:1793:GLU:OE1  | 2:B:1800:ALA:HB1  | 2.08                     | 0.54              |
| 2:B:1835:TRP:O    | 2:B:1945:LEU:HD21 | 2.07                     | 0.54              |
| 2:B:1863:LEU:O    | 2:B:1864:ASN:C    | 2.52                     | 0.54              |
| 1:A:147:MET:H     | 1:A:150:ASP:HB2   | 1.72                     | 0.53              |
| 1:A:155:THR:CG2   | 1:A:295:THR:HG23  | 2.38                     | 0.53              |
| 1:A:193:HIS:N     | 1:A:193:HIS:CD2   | 2.76                     | 0.53              |
| 1:A:196:ILE:HG23  | 1:A:256:HIS:HB3   | 1.91                     | 0.53              |
| 1:A:237:TYR:HB2   | 1:A:242:LEU:HB2   | 1.90                     | 0.53              |
| 1:A:447:GLY:HA3   | 1:A:618:ASN:O     | 2.08                     | 0.53              |
| 1:A:465:PHE:CD2   | 1:A:475:ILE:HG21  | 2.43                     | 0.53              |
| 1:A:650:SER:OG    | 1:A:670:LEU:HB3   | 2.08                     | 0.53              |
| 2:B:1759:LEU:H    | 2:B:1759:LEU:HD12 | 1.73                     | 0.53              |
| 2:B:1927:ASP:HB3  | 2:B:2013:LEU:HD11 | 1.91                     | 0.53              |
| 2:B:2127:PHE:O    | 2:B:2136:LYS:HG3  | 2.09                     | 0.53              |
| 1:A:106:TRP:HA    | 1:A:106:TRP:CE3   | 2.43                     | 0.53              |
| 1:A:470:SER:CB    | 1:A:471:ARG:HH11  | 2.21                     | 0.53              |
| 2:B:2177:PRO:O    | 2:B:2178:LEU:HD23 | 2.08                     | 0.53              |
| 1:A:99:HIS:O      | 1:A:100:ALA:HB2   | 2.08                     | 0.53              |
| 1:A:434:GLU:OE1   | 1:A:434:GLU:O     | 2.26                     | 0.53              |
| 1:A:460:THR:HG23  | 1:A:514:THR:HA    | 1.90                     | 0.53              |
| 1:A:476:TYR:CZ    | 1:A:483:VAL:HG21  | 2.44                     | 0.53              |
| 1:A:484:ARG:HD2   | 1:A:484:ARG:O     | 2.07                     | 0.53              |
| 1:A:593:ARG:HD2   | 1:A:594:PHE:CZ    | 2.43                     | 0.53              |
| 1:A:674:SER:C     | 1:A:676:GLU:H     | 2.16                     | 0.53              |
| 2:B:1764:ARG:HD2  | 2:B:1869:ARG:HG2  | 1.88                     | 0.53              |
| 2:B:1861:ASN:N    | 2:B:1861:ASN:ND2  | 2.54                     | 0.53              |
| 2:B:1884:ASP:O    | 2:B:1885:GLU:HB2  | 2.07                     | 0.53              |
| 2:B:2256:TYR:CD2  | 2:B:2314:VAL:HG21 | 2.43                     | 0.53              |
| 1:A:3:ARG:NH1     | 1:A:184:LEU:HD12  | 2.23                     | 0.53              |
| 1:A:467:ASN:HB3   | 1:A:506:GLY:HA2   | 1.90                     | 0.53              |
| 1:A:615:HIS:HB2   | 1:A:703:THR:CG2   | 2.35                     | 0.53              |
| 1:A:690:LEU:CB    | 1:A:708:VAL:HB    | 2.38                     | 0.53              |
| 2:B:1732:LYS:HA   | 2:B:1849:SER:OG   | 2.08                     | 0.53              |
| 2:B:2191:THR:HG23 | 2:B:2231:GLN:HB3  | 1.90                     | 0.53              |
| 2:B:2259:GLU:HG2  | 2:B:2284:GLN:NE2  | 2.23                     | 0.53              |
| 3:C:1:NAG:O6      | 3:C:2:NAG:H83     | 2.08                     | 0.53              |
| 1:A:306:PHE:N     | 1:A:306:PHE:HD1   | 2.05                     | 0.53              |
| 1:A:394:ASP:HB2   | 1:A:422:LYS:HB2   | 1.89                     | 0.53              |
| 1:A:427:ARG:NH1   | 1:A:448:ILE:HA    | 2.12                     | 0.53              |
| 1:A:527:ARG:HD2   | 1:A:527:ARG:N     | 2.23                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:535:SER:C     | 1:A:536:PHE:CD1   | 2.87                     | 0.53              |
| 1:A:698:ARG:HH11  | 1:A:698:ARG:HG3   | 1.72                     | 0.53              |
| 2:B:1749:ARG:NH1  | 2:B:1756:LEU:HD13 | 2.24                     | 0.53              |
| 1:A:432:THR:HA    | 1:A:438:THR:HG1   | 1.74                     | 0.53              |
| 1:A:463:ILE:HD13  | 1:A:463:ILE:N     | 2.23                     | 0.53              |
| 1:A:523:LYS:HD2   | 1:A:523:LYS:H     | 1.74                     | 0.53              |
| 1:A:576:PHE:HA    | 1:A:617:ILE:HA    | 1.91                     | 0.53              |
| 1:A:659:LYS:HE3   | 2:B:1822:HIS:CD2  | 2.43                     | 0.53              |
| 2:B:1738:PHE:HB2  | 2:B:1746:PRO:CD   | 2.39                     | 0.53              |
| 2:B:1934:MET:HB2  | 2:B:2016:VAL:CB   | 2.39                     | 0.53              |
| 2:B:2046:TRP:HE3  | 2:B:2061:ALA:O    | 1.92                     | 0.53              |
| 2:B:2115:TYR:CG   | 2:B:2144:ILE:HD11 | 2.44                     | 0.53              |
| 2:B:2174:CYS:O    | 2:B:2175:SER:HB3  | 2.09                     | 0.53              |
| 2:B:2198:ASN:CB   | 2:B:2201:ALA:HB3  | 2.38                     | 0.53              |
| 1:A:386:ILE:HD12  | 1:A:387:ALA:CA    | 2.38                     | 0.53              |
| 1:A:415:GLY:N     | 1:A:418:ARG:HB2   | 2.24                     | 0.53              |
| 1:A:420:GLY:HA2   | 1:A:614:MET:HE2   | 1.91                     | 0.53              |
| 1:A:472:PRO:HB2   | 1:A:503:ILE:CG2   | 2.30                     | 0.53              |
| 1:A:610:ALA:HA    | 1:A:613:ILE:HD13  | 1.90                     | 0.53              |
| 2:B:1829:GLU:O    | 2:B:1830:PHE:HB2  | 2.06                     | 0.53              |
| 1:A:196:ILE:HG23  | 1:A:256:HIS:CB    | 2.39                     | 0.53              |
| 1:A:291:ILE:HG23  | 2:B:1955:SER:CB   | 2.38                     | 0.53              |
| 2:B:1740:ASP:HA   | 2:B:1776:ARG:NH2  | 2.23                     | 0.53              |
| 2:B:2129:ASN:HB3  | 2:B:2134:GLY:HA3  | 1.90                     | 0.53              |
| 2:B:1806:PHE:HD1  | 2:B:1806:PHE:H    | 1.57                     | 0.53              |
| 2:B:2064:THR:O    | 2:B:2159:ARG:HD2  | 2.09                     | 0.53              |
| 2:B:2165:GLU:O    | 2:B:2165:GLU:HG2  | 2.07                     | 0.53              |
| 2:B:2245:THR:HG22 | 2:B:2319:LEU:HD11 | 1.91                     | 0.53              |
| 2:B:2256:TYR:CE1  | 2:B:2288:ASP:HA   | 2.44                     | 0.53              |
| 1:A:152:LEU:O     | 1:A:153:CYS:CB    | 2.56                     | 0.53              |
| 1:A:485:PRO:O     | 1:A:486:LEU:O     | 2.26                     | 0.53              |
| 1:A:649:LEU:N     | 1:A:649:LEU:CD1   | 2.72                     | 0.53              |
| 1:A:690:LEU:HD23  | 1:A:690:LEU:C     | 2.34                     | 0.53              |
| 2:B:1830:PHE:CZ   | 2:B:1986:VAL:HA   | 2.44                     | 0.53              |
| 2:B:1947:MET:HE2  | 2:B:1948:GLY:CA   | 2.39                     | 0.53              |
| 1:A:311:HIS:C     | 1:A:312:ILE:CG1   | 2.82                     | 0.52              |
| 1:A:444:HIS:C     | 1:A:446:SER:H     | 2.16                     | 0.52              |
| 2:B:1764:ARG:HD2  | 2:B:1869:ARG:CG   | 2.38                     | 0.52              |
| 2:B:1824:ALA:HB1  | 2:B:1825:PRO:HD2  | 1.91                     | 0.52              |
| 2:B:1953:ILE:H    | 2:B:1953:ILE:CD1  | 2.21                     | 0.52              |
| 1:A:69:MET:HG3    | 1:A:72:LEU:HB3    | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:116:ASP:OD1   | 1:A:123:LYS:HE2   | 2.08                     | 0.52              |
| 1:A:171:GLY:C     | 1:A:172:LEU:HD12  | 2.35                     | 0.52              |
| 1:A:302:ASP:O     | 1:A:303:LEU:HB2   | 2.07                     | 0.52              |
| 1:A:311:HIS:C     | 1:A:312:ILE:HG12  | 2.34                     | 0.52              |
| 1:A:491:LEU:O     | 1:A:493:LYS:N     | 2.41                     | 0.52              |
| 2:B:1772:MET:HE3  | 2:B:1772:MET:C    | 2.34                     | 0.52              |
| 2:B:1830:PHE:CD1  | 2:B:1966:ARG:NH1  | 2.77                     | 0.52              |
| 2:B:1965:VAL:HG22 | 2:B:1966:ARG:N    | 2.23                     | 0.52              |
| 2:B:2052:ARG:CA   | 2:B:2163:ARG:HB3  | 2.39                     | 0.52              |
| 2:B:2071:ILE:O    | 2:B:2150:ARG:HA   | 2.09                     | 0.52              |
| 2:B:2116:ARG:CD   | 2:B:2117:GLY:H    | 2.22                     | 0.52              |
| 1:A:14:TRP:HA     | 1:A:14:TRP:CE3    | 2.45                     | 0.52              |
| 1:A:262:THR:O     | 1:A:263:THR:HB    | 2.09                     | 0.52              |
| 1:A:441:ALA:O     | 1:A:442:ILE:HG23  | 2.09                     | 0.52              |
| 1:A:471:ARG:HG2   | 1:A:585:TRP:CZ3   | 2.45                     | 0.52              |
| 1:A:484:ARG:NH1   | 1:A:486:LEU:HA    | 2.19                     | 0.52              |
| 1:A:640:LEU:N     | 1:A:640:LEU:CD2   | 2.72                     | 0.52              |
| 2:B:1693:LYS:O    | 2:B:1694:LYS:HB2  | 2.09                     | 0.52              |
| 2:B:1709:TYR:HH   | 2:B:1918:PHE:HD2  | 1.53                     | 0.52              |
| 2:B:1949:SER:OG   | 2:B:1950:ASN:N    | 2.43                     | 0.52              |
| 2:B:1966:ARG:HG3  | 2:B:1966:ARG:HH11 | 1.74                     | 0.52              |
| 2:B:2098:ILE:N    | 2:B:2098:ILE:CD1  | 2.68                     | 0.52              |
| 2:B:2130:VAL:O    | 2:B:2130:VAL:HG13 | 2.09                     | 0.52              |
| 1:A:242:LEU:HD23  | 1:A:322:ALA:HB1   | 1.90                     | 0.52              |
| 1:A:382:TRP:HB2   | 1:A:461:LEU:CD1   | 2.39                     | 0.52              |
| 1:A:713:LYS:HA    | 1:A:713:LYS:HZ2   | 1.75                     | 0.52              |
| 1:A:119:SER:O     | 1:A:122:GLU:HB2   | 2.09                     | 0.52              |
| 1:A:387:ALA:HB1   | 1:A:466:LYS:O     | 2.09                     | 0.52              |
| 1:A:617:ILE:HG21  | 1:A:706:LEU:CD2   | 2.39                     | 0.52              |
| 2:B:1943:TYR:N    | 2:B:1943:TYR:CD1  | 2.76                     | 0.52              |
| 2:B:1946:SER:CB   | 2:B:1978:LEU:HB3  | 2.40                     | 0.52              |
| 2:B:1968:LYS:O    | 2:B:1969:GLU:CG   | 2.55                     | 0.52              |
| 1:A:267:HIS:HE1   | 1:A:315:HIS:HB3   | 1.72                     | 0.52              |
| 1:A:400:LEU:O     | 1:A:401:ALA:HB2   | 2.10                     | 0.52              |
| 1:A:426:VAL:HG11  | 1:A:586:TYR:OH    | 2.08                     | 0.52              |
| 1:A:548:ILE:HG13  | 1:A:549:GLY:N     | 2.23                     | 0.52              |
| 2:B:2000:CYS:CB   | 2:B:2010:MET:SD   | 2.98                     | 0.52              |
| 2:B:2104:MET:HA   | 2:B:2113:GLN:O    | 2.08                     | 0.52              |
| 2:B:2151:LEU:HD23 | 2:B:2151:LEU:C    | 2.35                     | 0.52              |
| 2:B:2243:VAL:O    | 2:B:2294:VAL:HG23 | 2.08                     | 0.52              |
| 1:A:39:PRO:C      | 1:A:41:ASN:N      | 2.68                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:383:VAL:C     | 1:A:384:HIS:ND1   | 2.68                     | 0.52              |
| 1:A:654:SER:HB2   | 1:A:690:LEU:CB    | 2.39                     | 0.52              |
| 2:B:2052:ARG:HA   | 2:B:2163:ARG:HB3  | 1.92                     | 0.52              |
| 2:B:2074:ASP:C    | 2:B:2076:LEU:H    | 2.17                     | 0.52              |
| 2:B:2116:ARG:HH21 | 2:B:2121:GLY:N    | 2.07                     | 0.52              |
| 2:B:2217:ASN:HD22 | 2:B:2320:ARG:NH1  | 2.07                     | 0.52              |
| 2:B:2225:ASN:ND2  | 2:B:2228:GLU:N    | 2.56                     | 0.52              |
| 1:A:167:ASP:O     | 1:A:168:LEU:C     | 2.53                     | 0.52              |
| 1:A:283:GLN:O     | 1:A:284:ALA:C     | 2.53                     | 0.52              |
| 1:A:308:LEU:C     | 1:A:308:LEU:CD2   | 2.82                     | 0.52              |
| 1:A:430:ALA:O     | 1:A:431:TYR:O     | 2.27                     | 0.52              |
| 1:A:666:ASP:HB3   | 1:A:669:THR:CG2   | 2.39                     | 0.52              |
| 1:A:690:LEU:HD23  | 1:A:691:GLY:C     | 2.34                     | 0.52              |
| 1:A:690:LEU:H     | 1:A:708:VAL:H     | 1.57                     | 0.52              |
| 2:B:1717:VAL:CG1  | 2:B:1720:ASN:HA   | 2.35                     | 0.52              |
| 2:B:1766:GLU:HB3  | 2:B:1863:LEU:HD11 | 1.91                     | 0.52              |
| 2:B:1809:PRO:O    | 2:B:1811:GLU:N    | 2.43                     | 0.52              |
| 2:B:1943:TYR:N    | 2:B:1943:TYR:HD1  | 2.08                     | 0.52              |
| 2:B:1973:MET:HE2  | 2:B:1975:LEU:O    | 2.10                     | 0.52              |
| 2:B:2021:CYS:O    | 2:B:2022:GLN:C    | 2.53                     | 0.52              |
| 2:B:2134:GLY:O    | 2:B:2135:ILE:HB   | 2.10                     | 0.52              |
| 1:A:529:LEU:HD12  | 1:A:529:LEU:H     | 1.72                     | 0.52              |
| 1:A:656:TYR:CG    | 1:A:686:GLY:CA    | 2.92                     | 0.52              |
| 2:B:1767:VAL:O    | 2:B:1768:GLU:HB2  | 2.09                     | 0.52              |
| 2:B:2116:ARG:CZ   | 2:B:2121:GLY:O    | 2.57                     | 0.52              |
| 2:B:2186:SER:HG   | 2:B:2189:GLN:HG3  | 1.69                     | 0.52              |
| 1:A:576:PHE:CD1   | 1:A:617:ILE:HG23  | 2.45                     | 0.52              |
| 1:A:601:VAL:HG22  | 1:A:602:GLN:N     | 2.24                     | 0.52              |
| 1:A:639:ILE:HD12  | 1:A:679:PHE:HA    | 1.91                     | 0.52              |
| 1:A:658:PHE:HA    | 1:A:659:LYS:HD3   | 1.92                     | 0.52              |
| 2:B:2199:MET:O    | 2:B:2200:PHE:HB2  | 2.10                     | 0.52              |
| 1:A:52:VAL:HG21   | 1:A:54:PHE:CE2    | 2.45                     | 0.51              |
| 1:A:167:ASP:C     | 1:A:172:LEU:HD13  | 2.35                     | 0.51              |
| 1:A:451:PRO:O     | 1:A:453:LEU:HD22  | 2.10                     | 0.51              |
| 2:B:1785:PHE:HD2  | 2:B:1815:TYR:HD2  | 1.58                     | 0.51              |
| 1:A:240:ARG:HD2   | 1:A:323:TYR:CE1   | 2.43                     | 0.51              |
| 1:A:452:LEU:H     | 1:A:452:LEU:CD1   | 2.21                     | 0.51              |
| 2:B:1870:GLN:NE2  | 2:B:1941:ARG:HH22 | 2.08                     | 0.51              |
| 2:B:2217:ASN:O    | 2:B:2218:ALA:CB   | 2.57                     | 0.51              |
| 2:B:2314:VAL:O    | 2:B:2316:GLN:N    | 2.35                     | 0.51              |
| 1:A:34:VAL:O      | 1:A:34:VAL:HG12   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:53:GLU:OE2    | 1:A:65:ARG:NH1    | 2.44                     | 0.51              |
| 1:A:448:ILE:O     | 1:A:449:LEU:O     | 2.27                     | 0.51              |
| 1:A:657:THR:HB    | 2:B:1788:SER:O    | 2.10                     | 0.51              |
| 2:B:2025:LEU:HD12 | 2:B:2166:LEU:CD1  | 2.39                     | 0.51              |
| 2:B:2237:THR:CG2  | 2:B:2238:MET:N    | 2.74                     | 0.51              |
| 1:A:237:TYR:CB    | 1:A:242:LEU:HB2   | 2.40                     | 0.51              |
| 1:A:268:SER:H     | 1:A:312:ILE:CD1   | 2.20                     | 0.51              |
| 1:A:662:MET:CB    | 1:A:680:MET:HE1   | 2.31                     | 0.51              |
| 1:A:667:THR:N     | 2:B:1835:TRP:HZ3  | 2.09                     | 0.51              |
| 1:A:704:ALA:C     | 1:A:706:LEU:HD22  | 2.34                     | 0.51              |
| 2:B:1769:ASP:O    | 2:B:1819:VAL:HG23 | 2.10                     | 0.51              |
| 2:B:1800:ALA:HA   | 2:B:1804:LYS:NZ   | 2.24                     | 0.51              |
| 2:B:1855:LEU:C    | 2:B:1855:LEU:CD2  | 2.83                     | 0.51              |
| 2:B:2096:LEU:CD1  | 2:B:2157:SER:O    | 2.58                     | 0.51              |
| 2:B:2185:ILE:O    | 2:B:2185:ILE:HG22 | 2.10                     | 0.51              |
| 2:B:2276:GLN:HB2  | 2:B:2281:LYS:HB2  | 1.91                     | 0.51              |
| 1:A:60:ASN:O      | 1:A:61:ILE:CG1    | 2.49                     | 0.51              |
| 1:A:591:ILE:C     | 1:A:593:ARG:N     | 2.68                     | 0.51              |
| 2:B:1781:ARG:NH1  | 2:B:1783:TYR:HE1  | 2.09                     | 0.51              |
| 2:B:2107:LEU:HD23 | 2:B:2147:ARG:CB   | 2.39                     | 0.51              |
| 2:B:2225:ASN:OD1  | 2:B:2226:PRO:N    | 2.43                     | 0.51              |
| 1:A:163:ASP:O     | 1:A:167:ASP:CG    | 2.53                     | 0.51              |
| 1:A:308:LEU:HD23  | 1:A:308:LEU:C     | 2.36                     | 0.51              |
| 1:A:407:TYR:C     | 1:A:409:SER:N     | 2.69                     | 0.51              |
| 1:A:481:THR:HG22  | 1:A:519:ASP:OD1   | 2.09                     | 0.51              |
| 2:B:1721:ARG:O    | 2:B:1722:ALA:HB2  | 2.11                     | 0.51              |
| 2:B:1929:LEU:HD21 | 2:B:1932:LEU:HD21 | 1.91                     | 0.51              |
| 2:B:2313:TRP:CG   | 2:B:2317:ILE:HG12 | 2.46                     | 0.51              |
| 1:A:104:SER:O     | 1:A:138:TRP:HB2   | 2.10                     | 0.51              |
| 1:A:168:LEU:O     | 1:A:170:SER:N     | 2.44                     | 0.51              |
| 1:A:275:THR:OG1   | 1:A:282:ARG:NH1   | 2.44                     | 0.51              |
| 1:A:417:GLN:O     | 1:A:418:ARG:CD    | 2.59                     | 0.51              |
| 1:A:713:LYS:HG3   | 1:A:714:ASN:N     | 2.26                     | 0.51              |
| 2:B:1830:PHE:O    | 2:B:1832:CYS:N    | 2.44                     | 0.51              |
| 2:B:1832:CYS:HB3  | 2:B:1857:VAL:O    | 2.10                     | 0.51              |
| 1:A:3:ARG:NH2     | 1:A:184:LEU:HD12  | 2.25                     | 0.51              |
| 1:A:187:GLU:OE1   | 1:A:194:LYS:HD3   | 2.11                     | 0.51              |
| 1:A:435:THR:O     | 1:A:436:PHE:HB2   | 2.10                     | 0.51              |
| 1:A:575:LEU:HB3   | 1:A:640:LEU:CD2   | 2.40                     | 0.51              |
| 2:B:1886:THR:O    | 2:B:1888:SER:N    | 2.43                     | 0.51              |
| 2:B:1901:ALA:H    | 2:B:1912:PHE:HZ   | 1.57                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2034:ASP:O    | 2:B:2037:ILE:HG13 | 2.11                     | 0.51              |
| 2:B:2084:ILE:HG12 | 2:B:2085:LYS:O    | 2.11                     | 0.51              |
| 2:B:2084:ILE:CG1  | 2:B:2166:LEU:HB3  | 2.39                     | 0.51              |
| 2:B:2097:TYR:C    | 2:B:2098:ILE:HD13 | 2.35                     | 0.51              |
| 2:B:2097:TYR:OH   | 2:B:2130:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:58:LEU:CD1    | 1:A:58:LEU:N      | 2.74                     | 0.51              |
| 1:A:280:ASN:HB3   | 1:A:524:SER:CB    | 2.41                     | 0.51              |
| 1:A:492:PRO:O     | 1:A:493:LYS:C     | 2.53                     | 0.51              |
| 1:A:658:PHE:CD1   | 1:A:682:MET:HE1   | 2.45                     | 0.51              |
| 1:A:676:GLU:CD    | 1:A:677:THR:H     | 2.19                     | 0.51              |
| 2:B:1871:VAL:C    | 2:B:1873:VAL:N    | 2.67                     | 0.51              |
| 2:B:1958:PHE:HE1  | 2:B:1998:VAL:HG21 | 1.76                     | 0.51              |
| 2:B:2052:ARG:HH21 | 2:B:2087:GLN:HE22 | 1.58                     | 0.51              |
| 2:B:2264:SER:OG   | 2:B:2301:LEU:HD21 | 2.11                     | 0.51              |
| 2:B:2313:TRP:CB   | 2:B:2317:ILE:HG12 | 2.41                     | 0.51              |
| 1:A:446:SER:CA    | 1:A:449:LEU:HD21  | 2.40                     | 0.51              |
| 2:B:1709:TYR:HE1  | 2:B:1923:GLY:O    | 1.94                     | 0.51              |
| 2:B:1755:HIS:C    | 2:B:1757:GLY:H    | 2.18                     | 0.51              |
| 2:B:1771:ILE:O    | 2:B:1816:PHE:HD1  | 1.94                     | 0.51              |
| 2:B:1921:ILE:C    | 2:B:1923:GLY:N    | 2.68                     | 0.51              |
| 2:B:1945:LEU:HD12 | 2:B:1945:LEU:H    | 1.75                     | 0.51              |
| 2:B:2096:LEU:HD13 | 2:B:2157:SER:O    | 2.11                     | 0.51              |
| 2:B:2130:VAL:O    | 2:B:2131:ASP:CB   | 2.59                     | 0.51              |
| 2:B:2141:ASN:HA   | 2:B:2143:PRO:N    | 2.25                     | 0.51              |
| 2:B:2224:ASN:HD22 | 2:B:2317:ILE:HG13 | 1.75                     | 0.51              |
| 1:A:452:LEU:O     | 1:A:452:LEU:HD22  | 2.11                     | 0.50              |
| 1:A:461:LEU:O     | 1:A:512:LYS:HA    | 2.11                     | 0.50              |
| 1:A:587:LEU:HD23  | 1:A:587:LEU:H     | 1.76                     | 0.50              |
| 2:B:2018:SER:O    | 2:B:2020:LYS:N    | 2.44                     | 0.50              |
| 2:B:2229:TRP:HB2  | 2:B:2307:ARG:HG3  | 1.93                     | 0.50              |
| 1:A:18:GLN:HE21   | 1:A:33:ARG:HH22   | 1.59                     | 0.50              |
| 1:A:159:LEU:CD1   | 1:A:168:LEU:HD21  | 2.41                     | 0.50              |
| 1:A:446:SER:O     | 1:A:449:LEU:HD11  | 2.10                     | 0.50              |
| 2:B:1891:PHE:O    | 2:B:1895:MET:HG3  | 2.11                     | 0.50              |
| 2:B:2107:LEU:O    | 2:B:2108:ASP:HB3  | 2.10                     | 0.50              |
| 2:B:2263:SER:O    | 2:B:2264:SER:CB   | 2.59                     | 0.50              |
| 1:A:5:TYR:HE2     | 1:A:76:ILE:HA     | 1.76                     | 0.50              |
| 1:A:289:SER:CB    | 1:A:290:PRO:HD2   | 2.35                     | 0.50              |
| 1:A:543:LEU:HD22  | 1:A:544:ALA:N     | 2.26                     | 0.50              |
| 2:B:2034:ASP:CG   | 2:B:2049:LYS:HG2  | 2.37                     | 0.50              |
| 2:B:2237:THR:HA   | 2:B:2304:ARG:HA   | 1.92                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:170:SER:OG    | 1:A:172:LEU:HD11  | 2.12                     | 0.50              |
| 1:A:226:ARG:HE    | 1:A:226:ARG:H     | 1.60                     | 0.50              |
| 1:A:269:ILE:HD12  | 1:A:286:LEU:HD12  | 1.91                     | 0.50              |
| 1:A:538:ASN:HD21  | 1:A:541:ARG:HB3   | 1.76                     | 0.50              |
| 1:A:645:GLN:O     | 1:A:646:THR:CB    | 2.59                     | 0.50              |
| 1:A:652:PHE:C     | 1:A:657:THR:O     | 2.55                     | 0.50              |
| 2:B:1762:TYR:OH   | 2:B:1877:ALA:N    | 2.45                     | 0.50              |
| 2:B:1771:ILE:HD12 | 2:B:1817:TRP:CZ2  | 2.46                     | 0.50              |
| 2:B:1781:ARG:HB3  | 2:B:1783:TYR:CE1  | 2.46                     | 0.50              |
| 2:B:1874:GLN:HG3  | 2:B:1938:GLN:NE2  | 2.26                     | 0.50              |
| 2:B:1901:ALA:CB   | 2:B:1902:PRO:HD2  | 2.22                     | 0.50              |
| 2:B:1946:SER:HB3  | 2:B:1978:LEU:HB3  | 1.94                     | 0.50              |
| 2:B:1947:MET:HE2  | 2:B:1948:GLY:HA2  | 1.93                     | 0.50              |
| 2:B:2112:TRP:HA   | 2:B:2112:TRP:CE3  | 2.47                     | 0.50              |
| 1:A:260:MET:SD    | 1:A:260:MET:C     | 2.95                     | 0.50              |
| 1:A:385:TYR:CE1   | 1:A:464:ILE:HD12  | 2.46                     | 0.50              |
| 2:B:1703:VAL:HG22 | 2:B:1704:GLU:H    | 1.76                     | 0.50              |
| 2:B:1767:VAL:HG22 | 2:B:1768:GLU:N    | 2.26                     | 0.50              |
| 2:B:1820:GLN:HE22 | 2:B:1822:HIS:HB3  | 1.77                     | 0.50              |
| 2:B:2035:PHE:HD1  | 2:B:2035:PHE:C    | 2.20                     | 0.50              |
| 2:B:2084:ILE:HG13 | 2:B:2166:LEU:CA   | 2.41                     | 0.50              |
| 2:B:2192:ALA:CB   | 2:B:2230:LEU:HD12 | 2.39                     | 0.50              |
| 2:B:2205:PRO:C    | 2:B:2207:LYS:N    | 2.68                     | 0.50              |
| 1:A:438:THR:OG1   | 1:A:439:ARG:N     | 2.44                     | 0.50              |
| 1:A:657:THR:CB    | 2:B:1788:SER:HA   | 2.42                     | 0.50              |
| 2:B:1776:ARG:HG3  | 2:B:1812:THR:HG22 | 1.91                     | 0.50              |
| 2:B:1897:ARG:HB3  | 2:B:1897:ARG:CZ   | 2.42                     | 0.50              |
| 1:A:90:ASN:C      | 1:A:90:ASN:HD22   | 2.19                     | 0.50              |
| 1:A:197:LEU:HD12  | 1:A:197:LEU:N     | 2.26                     | 0.50              |
| 1:A:278:VAL:HG12  | 1:A:296:ALA:HB2   | 1.94                     | 0.50              |
| 1:A:696:ASP:O     | 1:A:697:PHE:C     | 2.54                     | 0.50              |
| 2:B:1992:LYS:HE3  | 2:B:1993:ALA:N    | 2.23                     | 0.50              |
| 2:B:2302:LEU:N    | 2:B:2302:LEU:CD2  | 2.75                     | 0.50              |
| 1:A:394:ASP:OD1   | 1:A:396:ALA:HB3   | 2.12                     | 0.50              |
| 2:B:1927:ASP:HB3  | 2:B:2013:LEU:CD2  | 2.40                     | 0.50              |
| 2:B:2233:ASP:C    | 2:B:2235:GLN:N    | 2.70                     | 0.50              |
| 2:B:2307:ARG:HG2  | 2:B:2308:ILE:N    | 2.25                     | 0.50              |
| 1:A:96:VAL:HG11   | 1:A:172:LEU:HD21  | 1.94                     | 0.50              |
| 1:A:168:LEU:C     | 1:A:170:SER:H     | 2.20                     | 0.50              |
| 1:A:263:THR:O     | 1:A:265:GLU:N     | 2.45                     | 0.50              |
| 1:A:292:THR:O     | 1:A:293:PHE:HD2   | 1.95                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:481:THR:HG22  | 1:A:519:ASP:OD2   | 2.12                     | 0.50              |
| 1:A:648:PHE:CZ    | 1:A:696:ASP:HB2   | 2.46                     | 0.50              |
| 1:A:702:MET:C     | 1:A:703:THR:HG22  | 2.36                     | 0.50              |
| 2:B:1704:GLU:HG2  | 2:B:1733:VAL:HB   | 1.94                     | 0.50              |
| 2:B:1955:SER:HA   | 2:B:1977:ASN:HA   | 1.94                     | 0.50              |
| 2:B:2035:PHE:C    | 2:B:2035:PHE:CD1  | 2.90                     | 0.50              |
| 2:B:2205:PRO:HB3  | 2:B:2230:LEU:HD11 | 1.92                     | 0.50              |
| 2:B:2264:SER:O    | 2:B:2271:TRP:HA   | 2.12                     | 0.50              |
| 1:A:158:TYR:C     | 1:A:158:TYR:HD1   | 2.17                     | 0.49              |
| 1:A:158:TYR:C     | 1:A:159:LEU:HD23  | 2.37                     | 0.49              |
| 1:A:414:ASN:CB    | 1:A:419:ILE:HA    | 2.42                     | 0.49              |
| 1:A:659:LYS:H     | 1:A:659:LYS:HE2   | 1.77                     | 0.49              |
| 1:A:674:SER:O     | 1:A:676:GLU:N     | 2.44                     | 0.49              |
| 2:B:1764:ARG:O    | 2:B:1765:ALA:CB   | 2.60                     | 0.49              |
| 2:B:1780:SER:O    | 2:B:1809:PRO:HG3  | 2.12                     | 0.49              |
| 2:B:2191:THR:HG23 | 2:B:2231:GLN:NE2  | 2.27                     | 0.49              |
| 2:B:2279:LYS:H    | 2:B:2279:LYS:CD   | 2.22                     | 0.49              |
| 1:A:167:ASP:O     | 1:A:172:LEU:HD13  | 2.12                     | 0.49              |
| 1:A:304:GLY:N     | 1:A:326:VAL:HG13  | 2.25                     | 0.49              |
| 1:A:575:LEU:N     | 1:A:618:ASN:OD1   | 2.43                     | 0.49              |
| 1:A:698:ARG:HB3   | 1:A:702:MET:SD    | 2.52                     | 0.49              |
| 2:B:1857:VAL:HG23 | 2:B:1858:CYS:H    | 1.76                     | 0.49              |
| 2:B:1944:LEU:O    | 2:B:1978:LEU:HD13 | 2.12                     | 0.49              |
| 2:B:2203:TRP:HZ3  | 2:B:2217:ASN:C    | 2.19                     | 0.49              |
| 2:B:2225:ASN:OD1  | 2:B:2227:LYS:N    | 2.45                     | 0.49              |
| 2:B:2288:ASP:OD1  | 2:B:2289:SER:N    | 2.45                     | 0.49              |
| 1:A:50:LEU:HA     | 1:A:171:GLY:O     | 2.12                     | 0.49              |
| 1:A:81:TYR:O      | 1:A:82:ASP:C      | 2.55                     | 0.49              |
| 1:A:162:VAL:O     | 1:A:162:VAL:CG2   | 2.57                     | 0.49              |
| 1:A:239:ASN:ND2   | 3:C:1:NAG:C7      | 2.75                     | 0.49              |
| 1:A:307:LEU:CD2   | 1:A:309:PHE:HB3   | 2.27                     | 0.49              |
| 1:A:565:GLN:HG3   | 1:A:566:ILE:HG12  | 1.92                     | 0.49              |
| 2:B:2170:ASP:OD1  | 2:B:2171:LEU:N    | 2.45                     | 0.49              |
| 2:B:2181:GLU:C    | 2:B:2183:LYS:N    | 2.70                     | 0.49              |
| 1:A:56:ASP:C      | 1:A:57:HIS:ND1    | 2.71                     | 0.49              |
| 1:A:522:THR:H     | 1:A:525:ASP:CG    | 2.20                     | 0.49              |
| 1:A:621:VAL:CG1   | 1:A:622:PHE:N     | 2.74                     | 0.49              |
| 1:A:671:PHE:CD1   | 1:A:671:PHE:N     | 2.78                     | 0.49              |
| 1:A:674:SER:O     | 1:A:675:GLY:C     | 2.55                     | 0.49              |
| 2:B:1794:GLU:CG   | 2:B:1795:ASP:H    | 2.19                     | 0.49              |
| 2:B:1879:PHE:O    | 2:B:1879:PHE:CG   | 2.64                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1898:ASN:O    | 2:B:1899:CYS:CB   | 2.51                     | 0.49              |
| 2:B:2016:VAL:HG22 | 2:B:2017:TYR:N    | 2.27                     | 0.49              |
| 2:B:2134:GLY:O    | 2:B:2135:ILE:CB   | 2.60                     | 0.49              |
| 1:A:7:LEU:HD21    | 1:A:51:PHE:HB3    | 1.93                     | 0.49              |
| 1:A:53:GLU:O      | 1:A:54:PHE:HB2    | 2.12                     | 0.49              |
| 1:A:457:VAL:C     | 1:A:459:ASP:H     | 2.20                     | 0.49              |
| 1:A:574:ILE:CB    | 1:A:639:ILE:HG23  | 2.19                     | 0.49              |
| 2:B:1880:PHE:HD1  | 2:B:1880:PHE:H    | 1.60                     | 0.49              |
| 1:A:116:ASP:HA    | 2:B:1995:ILE:HG13 | 1.94                     | 0.49              |
| 1:A:360:PHE:O     | 1:A:361:ASP:HB3   | 2.13                     | 0.49              |
| 1:A:527:ARG:CD    | 1:A:527:ARG:N     | 2.75                     | 0.49              |
| 1:A:615:HIS:ND1   | 1:A:615:HIS:N     | 2.59                     | 0.49              |
| 1:A:626:GLN:HA    | 1:A:707:LYS:O     | 2.12                     | 0.49              |
| 2:B:2078:PRO:O    | 2:B:2079:MET:HG3  | 2.12                     | 0.49              |
| 1:A:423:TYR:HE1   | 1:A:614:MET:HE2   | 1.78                     | 0.49              |
| 1:A:427:ARG:HD2   | 1:A:448:ILE:CA    | 2.43                     | 0.49              |
| 1:A:650:SER:HA    | 1:A:693:HIS:O     | 2.13                     | 0.49              |
| 1:A:688:TRP:HH2   | 2:B:1797:ARG:H    | 1.61                     | 0.49              |
| 2:B:2027:MET:H    | 2:B:2165:GLU:CG   | 2.22                     | 0.49              |
| 2:B:2162:LEU:HD12 | 2:B:2163:ARG:N    | 2.28                     | 0.49              |
| 2:B:2193:SER:HB3  | 2:B:2229:TRP:HE1  | 1.78                     | 0.49              |
| 1:A:63:LYS:HB3    | 1:A:64:PRO:CD     | 2.42                     | 0.49              |
| 1:A:89:LYS:HA     | 1:A:133:SER:HB3   | 1.94                     | 0.49              |
| 1:A:273:GLY:C     | 1:A:274:HIS:ND1   | 2.71                     | 0.49              |
| 1:A:566:ILE:HG13  | 1:A:567:MET:CE    | 2.43                     | 0.49              |
| 2:B:1738:PHE:HB2  | 2:B:1746:PRO:HG2  | 1.93                     | 0.49              |
| 2:B:2124:MET:HE2  | 2:B:2125:VAL:O    | 2.13                     | 0.49              |
| 2:B:2302:LEU:N    | 2:B:2302:LEU:HD23 | 2.28                     | 0.49              |
| 1:A:269:ILE:HD11  | 1:A:308:LEU:HD21  | 1.95                     | 0.49              |
| 1:A:371:ILE:HB    | 1:A:374:VAL:CG1   | 2.43                     | 0.49              |
| 2:B:2064:THR:O    | 2:B:2065:LYS:HG2  | 2.12                     | 0.49              |
| 2:B:2180:MET:O    | 2:B:2209:ARG:HG2  | 2.13                     | 0.49              |
| 1:A:461:LEU:N     | 1:A:513:TRP:O     | 2.41                     | 0.49              |
| 1:A:573:VAL:C     | 1:A:574:ILE:HG13  | 2.38                     | 0.49              |
| 2:B:1780:SER:O    | 2:B:1781:ARG:C    | 2.56                     | 0.49              |
| 2:B:2100:GLN:HG2  | 2:B:2155:HIS:HB2  | 1.94                     | 0.49              |
| 2:B:2116:ARG:NH1  | 2:B:2116:ARG:CG   | 2.72                     | 0.49              |
| 2:B:2141:ASN:HA   | 2:B:2142:PRO:C    | 2.37                     | 0.49              |
| 2:B:2296:SER:O    | 2:B:2297:LEU:CB   | 2.60                     | 0.49              |
| 1:A:114:TYR:O     | 1:A:116:ASP:N     | 2.46                     | 0.48              |
| 1:A:439:ARG:NE    | 1:A:439:ARG:O     | 2.46                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:591:ILE:C     | 1:A:593:ARG:H     | 2.21                     | 0.48              |
| 2:B:1738:PHE:HB3  | 2:B:1747:LEU:CA   | 2.39                     | 0.48              |
| 2:B:1751:GLU:HG3  | 2:B:2116:ARG:HB3  | 1.95                     | 0.48              |
| 2:B:1764:ARG:HG3  | 2:B:1764:ARG:NH1  | 2.28                     | 0.48              |
| 2:B:1946:SER:O    | 2:B:1947:MET:CB   | 2.56                     | 0.48              |
| 2:B:2018:SER:C    | 2:B:2020:LYS:N    | 2.71                     | 0.48              |
| 2:B:2078:PRO:HB3  | 2:B:2107:LEU:CD2  | 2.34                     | 0.48              |
| 2:B:2135:ILE:O    | 2:B:2137:HIS:N    | 2.45                     | 0.48              |
| 2:B:2220:ARG:HH11 | 2:B:2220:ARG:CB   | 2.26                     | 0.48              |
| 2:B:2259:GLU:CG   | 2:B:2284:GLN:HE22 | 2.25                     | 0.48              |
| 2:B:2274:PHE:HZ   | 2:B:2299:PRO:HD2  | 1.78                     | 0.48              |
| 5:E:3:BMA:O3      | 5:E:5:MAN:C1      | 2.60                     | 0.48              |
| 1:A:159:LEU:HD13  | 1:A:168:LEU:HD21  | 1.95                     | 0.48              |
| 1:A:400:LEU:C     | 1:A:405:ARG:NH2   | 2.71                     | 0.48              |
| 1:A:426:VAL:HG23  | 1:A:426:VAL:O     | 2.12                     | 0.48              |
| 1:A:435:THR:O     | 1:A:436:PHE:CB    | 2.61                     | 0.48              |
| 1:A:559:VAL:HG23  | 1:A:559:VAL:O     | 2.13                     | 0.48              |
| 2:B:2151:LEU:HD13 | 2:B:2162:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:255:TRP:CE3   | 1:A:255:TRP:HA    | 2.48                     | 0.48              |
| 1:A:467:ASN:CG    | 1:A:468:GLN:N     | 2.70                     | 0.48              |
| 1:A:489:ARG:CB    | 1:A:489:ARG:NH1   | 2.77                     | 0.48              |
| 2:B:1789:LEU:HD11 | 2:B:1835:TRP:CG   | 2.48                     | 0.48              |
| 2:B:1929:LEU:CB   | 2:B:2012:THR:HG21 | 2.26                     | 0.48              |
| 2:B:2162:LEU:HD13 | 2:B:2163:ARG:O    | 2.14                     | 0.48              |
| 2:B:2273:LEU:HD22 | 2:B:2280:VAL:HG12 | 1.95                     | 0.48              |
| 1:A:26:VAL:O      | 1:A:26:VAL:HG13   | 2.13                     | 0.48              |
| 1:A:147:MET:HE3   | 2:B:1972:LYS:HE3  | 1.96                     | 0.48              |
| 1:A:498:LEU:O     | 1:A:502:PRO:HD2   | 2.13                     | 0.48              |
| 2:B:1762:TYR:CD2  | 2:B:1764:ARG:NH2  | 2.81                     | 0.48              |
| 2:B:1767:VAL:HA   | 2:B:1819:VAL:CG1  | 2.35                     | 0.48              |
| 2:B:2000:CYS:SG   | 2:B:2002:ILE:CD1  | 2.99                     | 0.48              |
| 2:B:2102:ILE:C    | 2:B:2103:ILE:HD12 | 2.38                     | 0.48              |
| 2:B:2105:TYR:O    | 2:B:2106:SER:HB2  | 2.13                     | 0.48              |
| 1:A:18:GLN:NE2    | 1:A:33:ARG:HH22   | 2.12                     | 0.48              |
| 1:A:309:PHE:CD1   | 1:A:309:PHE:C     | 2.91                     | 0.48              |
| 2:B:1927:ASP:CG   | 2:B:2013:LEU:HD11 | 2.38                     | 0.48              |
| 1:A:51:PHE:HD1    | 1:A:51:PHE:N      | 2.00                     | 0.48              |
| 1:A:83:THR:HG22   | 1:A:84:VAL:N      | 2.27                     | 0.48              |
| 1:A:106:TRP:O     | 1:A:107:LYS:HG2   | 2.13                     | 0.48              |
| 1:A:626:GLN:O     | 1:A:708:VAL:HA    | 2.13                     | 0.48              |
| 1:A:660:HIS:N     | 1:A:660:HIS:CD2   | 2.81                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1787:SER:O    | 2:B:1790:ILE:HG23 | 2.14                     | 0.48              |
| 2:B:1911:THR:HG23 | 2:B:1912:PHE:N    | 2.29                     | 0.48              |
| 2:B:1982:VAL:O    | 2:B:1983:PHE:CB   | 2.61                     | 0.48              |
| 2:B:2105:TYR:CD2  | 2:B:2144:ILE:HD13 | 2.49                     | 0.48              |
| 1:A:292:THR:HG23  | 2:B:1977:ASN:CG   | 2.38                     | 0.48              |
| 1:A:467:ASN:ND2   | 1:A:506:GLY:HA2   | 2.13                     | 0.48              |
| 1:A:584:SER:C     | 1:A:586:TYR:H     | 2.22                     | 0.48              |
| 1:A:608:PHE:O     | 1:A:609:GLN:C     | 2.56                     | 0.48              |
| 2:B:1883:PHE:O    | 2:B:1917:ARG:HA   | 2.13                     | 0.48              |
| 2:B:1997:ARG:HG2  | 2:B:1998:VAL:N    | 2.28                     | 0.48              |
| 2:B:2081:ILE:O    | 2:B:2081:ILE:HG13 | 2.14                     | 0.48              |
| 2:B:2115:TYR:CD1  | 2:B:2144:ILE:HD11 | 2.48                     | 0.48              |
| 1:A:77:GLN:HB3    | 1:A:177:LEU:HD12  | 1.96                     | 0.48              |
| 1:A:387:ALA:HA    | 1:A:465:PHE:HD1   | 1.79                     | 0.48              |
| 1:A:437:LYS:O     | 1:A:438:THR:CB    | 2.61                     | 0.48              |
| 1:A:465:PHE:CD2   | 1:A:475:ILE:CG2   | 2.97                     | 0.48              |
| 2:B:1697:HIS:CA   | 2:B:1772:MET:HB3  | 2.39                     | 0.48              |
| 2:B:1737:GLU:C    | 2:B:1738:PHE:CD2  | 2.92                     | 0.48              |
| 2:B:1741:GLY:O    | 2:B:1742:SER:C    | 2.56                     | 0.48              |
| 2:B:1756:LEU:O    | 2:B:1757:GLY:C    | 2.56                     | 0.48              |
| 2:B:1813:LYS:HG3  | 2:B:1814:THR:N    | 2.28                     | 0.48              |
| 2:B:1819:VAL:HA   | 2:B:1823:MET:CE   | 2.43                     | 0.48              |
| 2:B:2033:ARG:N    | 2:B:2036:GLN:OE1  | 2.47                     | 0.48              |
| 2:B:2036:GLN:NE2  | 2:B:2076:LEU:HD21 | 2.28                     | 0.48              |
| 2:B:2225:ASN:ND2  | 2:B:2228:GLU:H    | 2.09                     | 0.48              |
| 1:A:29:ARG:O      | 1:A:30:PHE:HB2    | 2.12                     | 0.48              |
| 1:A:126:ASP:O     | 1:A:127:LYS:CB    | 2.62                     | 0.48              |
| 1:A:169:ASN:OD1   | 1:A:203:ASP:HB3   | 2.14                     | 0.48              |
| 1:A:310:CYS:SG    | 1:A:312:ILE:HG13  | 2.53                     | 0.48              |
| 1:A:471:ARG:HD2   | 1:A:471:ARG:N     | 2.28                     | 0.48              |
| 1:A:586:TYR:N     | 1:A:586:TYR:CD1   | 2.82                     | 0.48              |
| 2:B:1913:LYS:C    | 2:B:1915:ASN:H    | 2.22                     | 0.48              |
| 1:A:90:ASN:C      | 1:A:92:ALA:N      | 2.72                     | 0.48              |
| 1:A:213:LYS:O     | 1:A:214:ASN:C     | 2.56                     | 0.48              |
| 1:A:269:ILE:HD13  | 1:A:269:ILE:C     | 2.38                     | 0.48              |
| 1:A:398:LEU:HD22  | 1:A:623:ASP:HB2   | 1.96                     | 0.48              |
| 2:B:1830:PHE:CE2  | 2:B:1986:VAL:HA   | 2.49                     | 0.48              |
| 2:B:2081:ILE:HD11 | 2:B:2144:ILE:CB   | 2.30                     | 0.48              |
| 2:B:2123:LEU:HD12 | 2:B:2123:LEU:O    | 2.13                     | 0.48              |
| 2:B:2179:GLY:HA3  | 2:B:2185:ILE:HG13 | 1.96                     | 0.48              |
| 2:B:2258:LYS:HE3  | 2:B:2284:GLN:CD   | 2.38                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:2304:ARG:O    | 2:B:2305:TYR:CD1 | 2.67                     | 0.48              |
| 2:B:2323:VAL:HG12 | 2:B:2324:LEU:N   | 2.25                     | 0.48              |
| 1:A:65:ARG:H      | 1:A:70:GLY:HA2   | 1.79                     | 0.47              |
| 1:A:96:VAL:HB     | 1:A:160:SER:CB   | 2.42                     | 0.47              |
| 1:A:254:TYR:HE1   | 1:A:297:GLN:CD   | 2.22                     | 0.47              |
| 1:A:375:ALA:O     | 1:A:376:LYS:HB2  | 2.14                     | 0.47              |
| 1:A:621:VAL:O     | 1:A:622:PHE:C    | 2.57                     | 0.47              |
| 1:A:657:THR:O     | 1:A:658:PHE:CB   | 2.62                     | 0.47              |
| 2:B:1947:MET:HA   | 2:B:1981:GLY:N   | 2.29                     | 0.47              |
| 2:B:1964:THR:OG1  | 2:B:1965:VAL:N   | 2.47                     | 0.47              |
| 2:B:1982:VAL:HG13 | 2:B:1983:PHE:N   | 2.29                     | 0.47              |
| 1:A:1:ALA:O       | 1:A:2:THR:HG23   | 2.14                     | 0.47              |
| 1:A:35:PRO:O      | 1:A:36:LYS:HB2   | 2.15                     | 0.47              |
| 1:A:48:LYS:HZ2    | 1:A:204:GLU:HB2  | 1.78                     | 0.47              |
| 1:A:271:LEU:C     | 1:A:273:GLY:N    | 2.72                     | 0.47              |
| 1:A:282:ARG:HH22  | 1:A:299:LEU:HD13 | 1.79                     | 0.47              |
| 1:A:307:LEU:HD21  | 1:A:321:GLU:HB3  | 1.96                     | 0.47              |
| 1:A:534:SER:OG    | 1:A:535:SER:N    | 2.46                     | 0.47              |
| 1:A:542:ASP:O     | 1:A:543:LEU:C    | 2.56                     | 0.47              |
| 2:B:2043:TYR:CG   | 2:B:2064:THR:HA  | 2.50                     | 0.47              |
| 2:B:2078:PRO:HA   | 2:B:2146:ALA:O   | 2.13                     | 0.47              |
| 2:B:2237:THR:HA   | 2:B:2304:ARG:CB  | 2.44                     | 0.47              |
| 1:A:481:THR:HG22  | 1:A:519:ASP:CG   | 2.39                     | 0.47              |
| 1:A:527:ARG:HH12  | 1:A:556:LYS:HD3  | 1.79                     | 0.47              |
| 2:B:1762:TYR:HD2  | 2:B:1764:ARG:NH2 | 2.12                     | 0.47              |
| 2:B:2276:GLN:O    | 2:B:2278:GLY:N   | 2.47                     | 0.47              |
| 1:A:7:LEU:CD1     | 1:A:51:PHE:HB3   | 2.41                     | 0.47              |
| 1:A:639:ILE:N     | 1:A:639:ILE:CD1  | 2.63                     | 0.47              |
| 1:A:682:MET:O     | 1:A:682:MET:SD   | 2.73                     | 0.47              |
| 2:B:2237:THR:CG2  | 2:B:2238:MET:H   | 2.23                     | 0.47              |
| 1:A:651:VAL:HG21  | 1:A:668:LEU:HB3  | 1.97                     | 0.47              |
| 1:A:654:SER:OG    | 1:A:688:TRP:O    | 2.31                     | 0.47              |
| 1:A:663:VAL:HA    | 2:B:1968:LYS:CE  | 2.45                     | 0.47              |
| 1:A:713:LYS:HA    | 1:A:713:LYS:HZ1  | 1.77                     | 0.47              |
| 2:B:1830:PHE:CD1  | 2:B:1987:GLU:OE1 | 2.68                     | 0.47              |
| 2:B:2116:ARG:HD3  | 2:B:2117:GLY:N   | 2.29                     | 0.47              |
| 2:B:2180:MET:O    | 2:B:2209:ARG:NH1 | 2.47                     | 0.47              |
| 1:A:50:LEU:HD22   | 1:A:171:GLY:HA3  | 1.96                     | 0.47              |
| 1:A:68:TRP:CD1    | 1:A:68:TRP:H     | 2.33                     | 0.47              |
| 1:A:679:PHE:CD2   | 1:A:680:MET:N    | 2.83                     | 0.47              |
| 2:B:1715:PRO:O    | 2:B:1716:HIS:C   | 2.57                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1761:PRO:O    | 2:B:1763:ILE:N    | 2.47                     | 0.47              |
| 2:B:1789:LEU:C    | 2:B:1791:SER:N    | 2.61                     | 0.47              |
| 2:B:1790:ILE:HA   | 2:B:1817:TRP:CZ3  | 2.47                     | 0.47              |
| 2:B:1855:LEU:HD23 | 2:B:1856:LEU:N    | 2.29                     | 0.47              |
| 2:B:1947:MET:HG2  | 2:B:1948:GLY:H    | 1.78                     | 0.47              |
| 2:B:1989:LEU:C    | 2:B:1989:LEU:CD2  | 2.84                     | 0.47              |
| 2:B:1997:ARG:CG   | 2:B:1998:VAL:H    | 2.26                     | 0.47              |
| 1:A:22:GLY:O      | 1:A:23:GLU:CB     | 2.63                     | 0.47              |
| 1:A:104:SER:OG    | 1:A:139:GLN:N     | 2.46                     | 0.47              |
| 1:A:118:THR:OG1   | 1:A:122:GLU:OE1   | 2.29                     | 0.47              |
| 1:A:196:ILE:HD12  | 1:A:196:ILE:N     | 2.29                     | 0.47              |
| 1:A:233:THR:HB    | 1:A:237:TYR:O     | 2.15                     | 0.47              |
| 1:A:295:THR:O     | 1:A:296:ALA:HB2   | 2.15                     | 0.47              |
| 1:A:440:GLU:O     | 1:A:441:ALA:CB    | 2.62                     | 0.47              |
| 1:A:476:TYR:OH    | 1:A:483:VAL:HG21  | 2.14                     | 0.47              |
| 1:A:548:ILE:CG1   | 1:A:549:GLY:N     | 2.78                     | 0.47              |
| 1:A:581:GLU:C     | 1:A:583:ARG:N     | 2.72                     | 0.47              |
| 1:A:605:ASP:O     | 1:A:607:GLU:N     | 2.48                     | 0.47              |
| 1:A:617:ILE:HG21  | 1:A:706:LEU:HD21  | 1.96                     | 0.47              |
| 1:A:652:PHE:O     | 1:A:657:THR:O     | 2.33                     | 0.47              |
| 2:B:1704:GLU:HG3  | 2:B:1779:ALA:HB2  | 1.97                     | 0.47              |
| 2:B:1763:ILE:O    | 2:B:1763:ILE:HD13 | 2.15                     | 0.47              |
| 2:B:1774:THR:HG22 | 2:B:1814:THR:CG2  | 2.45                     | 0.47              |
| 2:B:1790:ILE:O    | 2:B:1791:SER:O    | 2.33                     | 0.47              |
| 2:B:2000:CYS:SG   | 2:B:2002:ILE:CG1  | 3.03                     | 0.47              |
| 2:B:2037:ILE:O    | 2:B:2038:THR:CB   | 2.60                     | 0.47              |
| 2:B:2112:TRP:HA   | 2:B:2112:TRP:HE3  | 1.80                     | 0.47              |
| 2:B:2112:TRP:NE1  | 2:B:2150:ARG:NH1  | 2.62                     | 0.47              |
| 2:B:2243:VAL:CG2  | 2:B:2321:MET:HE1  | 2.44                     | 0.47              |
| 1:A:172:LEU:O     | 1:A:173:ILE:HB    | 2.14                     | 0.47              |
| 1:A:273:GLY:O     | 1:A:274:HIS:CE1   | 2.67                     | 0.47              |
| 1:A:391:GLU:HG2   | 1:A:392:ASP:N     | 2.29                     | 0.47              |
| 1:A:580:ASP:OD1   | 1:A:613:ILE:HG22  | 2.15                     | 0.47              |
| 1:A:696:ASP:O     | 1:A:699:ASN:HB2   | 2.15                     | 0.47              |
| 2:B:1753:ASN:HB3  | 2:B:1756:LEU:HD12 | 1.96                     | 0.47              |
| 2:B:1924:TYR:CD2  | 2:B:1929:LEU:HA   | 2.50                     | 0.47              |
| 2:B:2190:ILE:HA   | 2:B:2231:GLN:O    | 2.14                     | 0.47              |
| 2:B:2194:SER:HB2  | 2:B:2222:GLN:H    | 1.75                     | 0.47              |
| 1:A:12:LEU:CD2    | 1:A:61:ILE:HG12   | 2.43                     | 0.47              |
| 1:A:89:LYS:HA     | 1:A:133:SER:HA    | 1.97                     | 0.47              |
| 1:A:105:TYR:O     | 1:A:106:TRP:CB    | 2.61                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:208:TRP:CB    | 1:A:226:ARG:NH1   | 2.78                     | 0.47              |
| 1:A:242:LEU:HD23  | 1:A:322:ALA:CB    | 2.45                     | 0.47              |
| 1:A:507:GLU:CG    | 1:A:508:ILE:N     | 2.63                     | 0.47              |
| 1:A:543:LEU:O     | 1:A:546:GLY:N     | 2.47                     | 0.47              |
| 1:A:657:THR:HG21  | 2:B:1788:SER:CA   | 2.43                     | 0.47              |
| 2:B:1947:MET:HA   | 2:B:1981:GLY:H    | 1.79                     | 0.47              |
| 2:B:1992:LYS:HA   | 2:B:1992:LYS:HD2  | 1.73                     | 0.47              |
| 2:B:2075:LEU:O    | 2:B:2076:LEU:CB   | 2.63                     | 0.47              |
| 2:B:2260:PHE:CE1  | 2:B:2283:PHE:CB   | 2.98                     | 0.47              |
| 2:B:2264:SER:OG   | 2:B:2303:THR:HG21 | 2.15                     | 0.47              |
| 2:B:2311:GLN:O    | 2:B:2313:TRP:CD1  | 2.67                     | 0.47              |
| 2:B:2332:TYR:CD1  | 2:B:2332:TYR:O    | 2.67                     | 0.47              |
| 1:A:106:TRP:C     | 1:A:107:LYS:HG2   | 2.40                     | 0.47              |
| 1:A:158:TYR:O     | 1:A:173:ILE:HG13  | 2.15                     | 0.47              |
| 1:A:578:VAL:HG21  | 1:A:644:ALA:HB3   | 1.97                     | 0.47              |
| 2:B:1708:ASP:C    | 2:B:1709:TYR:CD2  | 2.93                     | 0.47              |
| 2:B:1820:GLN:HE21 | 2:B:1822:HIS:N    | 2.10                     | 0.47              |
| 2:B:1929:LEU:HB3  | 2:B:2012:THR:CB   | 2.45                     | 0.47              |
| 2:B:2053:LEU:N    | 2:B:2163:ARG:HH21 | 2.13                     | 0.47              |
| 2:B:2237:THR:CA   | 2:B:2304:ARG:HB3  | 2.45                     | 0.47              |
| 1:A:15:ASP:O      | 1:A:16:TYR:CB     | 2.59                     | 0.46              |
| 2:B:2000:CYS:C    | 2:B:2002:ILE:H    | 2.23                     | 0.46              |
| 2:B:2043:TYR:CD2  | 2:B:2065:LYS:HB2  | 2.51                     | 0.46              |
| 2:B:2258:LYS:HA   | 2:B:2285:GLY:O    | 2.15                     | 0.46              |
| 2:B:2297:LEU:O    | 2:B:2298:ASP:C    | 2.58                     | 0.46              |
| 1:A:156:TYR:HA    | 1:A:293:PHE:CE1   | 2.50                     | 0.46              |
| 1:A:156:TYR:HB2   | 1:A:176:LEU:O     | 2.15                     | 0.46              |
| 1:A:275:THR:CA    | 1:A:284:ALA:HB2   | 2.30                     | 0.46              |
| 1:A:399:VAL:HG22  | 1:A:400:LEU:N     | 2.31                     | 0.46              |
| 1:A:475:ILE:O     | 1:A:475:ILE:HD13  | 2.15                     | 0.46              |
| 1:A:543:LEU:CD2   | 1:A:544:ALA:N     | 2.78                     | 0.46              |
| 2:B:1797:ARG:HG2  | 2:B:1797:ARG:O    | 2.15                     | 0.46              |
| 2:B:1977:ASN:OD1  | 2:B:1977:ASN:N    | 2.48                     | 0.46              |
| 2:B:1982:VAL:HG13 | 2:B:1983:PHE:H    | 1.80                     | 0.46              |
| 2:B:2145:ILE:O    | 2:B:2146:ALA:CB   | 2.63                     | 0.46              |
| 2:B:2218:ALA:HA   | 2:B:2320:ARG:HG2  | 1.98                     | 0.46              |
| 2:B:1927:ASP:HA   | 2:B:2011:SER:O    | 2.15                     | 0.46              |
| 2:B:2150:ARG:HE   | 2:B:2152:HIS:CE1  | 2.33                     | 0.46              |
| 2:B:2273:LEU:CD2  | 2:B:2280:VAL:HG12 | 2.44                     | 0.46              |
| 1:A:71:LEU:C      | 1:A:71:LEU:CD2    | 2.88                     | 0.46              |
| 1:A:88:LEU:C      | 1:A:88:LEU:CD2    | 2.88                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:105:TYR:CE1   | 2:B:1960:GLY:CA   | 2.98                     | 0.46              |
| 1:A:261:GLY:O     | 1:A:263:THR:HG22  | 2.15                     | 0.46              |
| 1:A:647:ASP:O     | 1:A:648:PHE:HD1   | 1.98                     | 0.46              |
| 1:A:687:LEU:HD21  | 2:B:1795:ASP:CB   | 2.45                     | 0.46              |
| 2:B:1719:ARG:O    | 2:B:1721:ARG:N    | 2.48                     | 0.46              |
| 2:B:1957:HIS:ND1  | 2:B:1958:PHE:N    | 2.64                     | 0.46              |
| 2:B:2257:VAL:O    | 2:B:2286:ASN:HB2  | 2.15                     | 0.46              |
| 2:B:2265:SER:OG   | 2:B:2271:TRP:CE3  | 2.68                     | 0.46              |
| 1:A:385:TYR:HE1   | 1:A:464:ILE:HD12  | 1.81                     | 0.46              |
| 1:A:633:GLU:O     | 1:A:634:VAL:C     | 2.58                     | 0.46              |
| 2:B:1697:HIS:N    | 2:B:1697:HIS:ND1  | 2.64                     | 0.46              |
| 2:B:1743:PHE:O    | 2:B:1745:GLN:N    | 2.49                     | 0.46              |
| 2:B:1847:VAL:HG11 | 2:B:1947:MET:CE   | 2.37                     | 0.46              |
| 2:B:2156:TYR:CE2  | 2:B:2159:ARG:HA   | 2.50                     | 0.46              |
| 2:B:2191:THR:HG23 | 2:B:2231:GLN:CD   | 2.40                     | 0.46              |
| 2:B:2304:ARG:C    | 2:B:2305:TYR:HD1  | 2.24                     | 0.46              |
| 1:A:5:TYR:HD2     | 1:A:76:ILE:HG12   | 1.79                     | 0.46              |
| 1:A:86:ILE:HB     | 1:A:136:TYR:HB2   | 1.97                     | 0.46              |
| 1:A:460:THR:HG21  | 1:A:512:LYS:HZ3   | 1.77                     | 0.46              |
| 1:A:652:PHE:O     | 1:A:657:THR:CG2   | 2.64                     | 0.46              |
| 2:B:2000:CYS:O    | 2:B:2006:LEU:HB2  | 2.16                     | 0.46              |
| 2:B:2036:GLN:HG2  | 2:B:2036:GLN:H    | 1.51                     | 0.46              |
| 1:A:7:LEU:HD21    | 1:A:51:PHE:CB     | 2.46                     | 0.46              |
| 1:A:58:LEU:H      | 1:A:58:LEU:HD12   | 1.80                     | 0.46              |
| 1:A:106:TRP:C     | 1:A:108:ALA:N     | 2.74                     | 0.46              |
| 1:A:121:ARG:HA    | 1:A:124:GLU:OE1   | 2.16                     | 0.46              |
| 1:A:623:ASP:C     | 1:A:624:SER:HG    | 2.17                     | 0.46              |
| 1:A:661:LYS:O     | 1:A:680:MET:SD    | 2.74                     | 0.46              |
| 2:B:1709:TYR:HE1  | 2:B:1924:TYR:HA   | 1.80                     | 0.46              |
| 2:B:1956:ILE:HG22 | 2:B:1957:HIS:N    | 2.30                     | 0.46              |
| 2:B:2238:MET:SD   | 2:B:2327:GLU:HA   | 2.56                     | 0.46              |
| 2:B:2296:SER:O    | 2:B:2297:LEU:CG   | 2.63                     | 0.46              |
| 1:A:267:HIS:CE1   | 1:A:315:HIS:CG    | 3.00                     | 0.46              |
| 1:A:371:ILE:O     | 1:A:371:ILE:HG22  | 2.16                     | 0.46              |
| 1:A:394:ASP:CG    | 1:A:396:ALA:H     | 2.24                     | 0.46              |
| 1:A:676:GLU:CG    | 1:A:677:THR:N     | 2.79                     | 0.46              |
| 2:B:1882:ILE:HG22 | 2:B:1952:ASN:HD21 | 1.79                     | 0.46              |
| 2:B:1927:ASP:CB   | 2:B:2013:LEU:HD11 | 2.46                     | 0.46              |
| 2:B:1993:ALA:CA   | 2:B:2016:VAL:HG13 | 2.42                     | 0.46              |
| 2:B:2279:LYS:O    | 2:B:2280:VAL:O    | 2.33                     | 0.46              |
| 2:B:2322:GLU:HG2  | 2:B:2323:VAL:N    | 2.31                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:8:GLY:CA      | 1:A:52:VAL:HG22  | 2.45                     | 0.46              |
| 1:A:95:PRO:O      | 1:A:96:VAL:O     | 2.34                     | 0.46              |
| 1:A:424:LYS:HD2   | 1:A:593:ARG:NH2  | 2.27                     | 0.46              |
| 1:A:704:ALA:O     | 1:A:706:LEU:CD2  | 2.64                     | 0.46              |
| 2:B:1755:HIS:HB3  | 2:B:1931:GLY:O   | 2.15                     | 0.46              |
| 2:B:1772:MET:HE1  | 2:B:1814:THR:HB  | 1.98                     | 0.46              |
| 2:B:1773:VAL:HG11 | 2:B:1785:PHE:HE2 | 1.81                     | 0.46              |
| 2:B:1777:ASN:ND2  | 2:B:1778:GLN:N   | 2.64                     | 0.46              |
| 2:B:1781:ARG:HG2  | 2:B:1783:TYR:CE1 | 2.51                     | 0.46              |
| 2:B:1833:LYS:HD2  | 2:B:1833:LYS:HA  | 1.82                     | 0.46              |
| 2:B:2263:SER:OG   | 2:B:2309:HIS:CE1 | 2.69                     | 0.46              |
| 2:B:2271:TRP:CD1  | 2:B:2271:TRP:N   | 2.84                     | 0.46              |
| 2:B:2306:LEU:HD23 | 2:B:2307:ARG:O   | 2.16                     | 0.46              |
| 1:A:106:TRP:O     | 1:A:107:LYS:CB   | 2.64                     | 0.46              |
| 1:A:118:THR:O     | 1:A:119:SER:HB2  | 2.16                     | 0.46              |
| 1:A:235:ASN:OD1   | 1:A:235:ASN:O    | 2.34                     | 0.46              |
| 1:A:286:LEU:O     | 1:A:287:GLU:C    | 2.59                     | 0.46              |
| 1:A:290:PRO:C     | 1:A:291:ILE:HG22 | 2.39                     | 0.46              |
| 1:A:490:ARG:O     | 1:A:491:LEU:HD23 | 2.16                     | 0.46              |
| 1:A:522:THR:HB    | 1:A:523:LYS:HD2  | 1.97                     | 0.46              |
| 1:A:552:LEU:HD21  | 1:A:638:TYR:CD2  | 2.51                     | 0.46              |
| 1:A:647:ASP:C     | 1:A:647:ASP:OD1  | 2.59                     | 0.46              |
| 2:B:2128:GLY:O    | 2:B:2136:LYS:HG3 | 2.16                     | 0.46              |
| 1:A:199:PHE:N     | 1:A:199:PHE:CD1  | 2.84                     | 0.45              |
| 1:A:267:HIS:CE1   | 1:A:315:HIS:CB   | 2.98                     | 0.45              |
| 1:A:461:LEU:CD2   | 1:A:513:TRP:HE3  | 2.25                     | 0.45              |
| 1:A:605:ASP:C     | 1:A:607:GLU:H    | 2.24                     | 0.45              |
| 2:B:1700:ILE:HG12 | 2:B:1701:ALA:N   | 2.32                     | 0.45              |
| 2:B:1982:VAL:CG2  | 2:B:1983:PHE:H   | 2.18                     | 0.45              |
| 2:B:2116:ARG:NH2  | 2:B:2121:GLY:N   | 2.63                     | 0.45              |
| 2:B:2152:HIS:N    | 2:B:2152:HIS:HD1 | 2.14                     | 0.45              |
| 2:B:2205:PRO:C    | 2:B:2207:LYS:H   | 2.23                     | 0.45              |
| 2:B:2233:ASP:O    | 2:B:2234:PHE:C   | 2.58                     | 0.45              |
| 1:A:65:ARG:CG     | 1:A:66:PRO:CD    | 2.86                     | 0.45              |
| 1:A:203:ASP:O     | 1:A:204:GLU:C    | 2.59                     | 0.45              |
| 1:A:384:HIS:O     | 1:A:386:ILE:N    | 2.49                     | 0.45              |
| 1:A:450:GLY:O     | 1:A:451:PRO:C    | 2.59                     | 0.45              |
| 1:A:473:TYR:HA    | 1:A:537:VAL:HG22 | 1.95                     | 0.45              |
| 1:A:526:PRO:HB2   | 1:A:679:PHE:HE2  | 1.76                     | 0.45              |
| 1:A:632:HIS:O     | 1:A:634:VAL:N    | 2.49                     | 0.45              |
| 1:A:676:GLU:HG3   | 1:A:677:THR:N    | 2.31                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1782:PRO:CB   | 2:B:1809:PRO:HD3  | 2.39                     | 0.45              |
| 1:A:8:GLY:HA3     | 1:A:52:VAL:HG22   | 1.98                     | 0.45              |
| 1:A:77:GLN:OE1    | 1:A:194:LYS:HD2   | 2.16                     | 0.45              |
| 1:A:90:ASN:C      | 1:A:90:ASN:ND2    | 2.73                     | 0.45              |
| 1:A:105:TYR:HD2   | 1:A:110:GLU:N     | 2.14                     | 0.45              |
| 1:A:156:TYR:HD1   | 1:A:293:PHE:CD1   | 2.29                     | 0.45              |
| 1:A:173:ILE:HG12  | 1:A:174:GLY:N     | 2.30                     | 0.45              |
| 1:A:446:SER:HB3   | 1:A:449:LEU:HD21  | 1.98                     | 0.45              |
| 2:B:1870:GLN:HE21 | 2:B:1941:ARG:HH22 | 1.63                     | 0.45              |
| 2:B:1996:TRP:O    | 2:B:2013:LEU:CA   | 2.57                     | 0.45              |
| 2:B:2162:LEU:C    | 2:B:2162:LEU:CD1  | 2.86                     | 0.45              |
| 2:B:2224:ASN:HB3  | 2:B:2317:ILE:HG13 | 1.99                     | 0.45              |
| 2:B:2224:ASN:HD22 | 2:B:2317:ILE:N    | 2.14                     | 0.45              |
| 1:A:2:THR:O       | 1:A:3:ARG:O       | 2.34                     | 0.45              |
| 1:A:386:ILE:C     | 1:A:386:ILE:CD1   | 2.82                     | 0.45              |
| 1:A:417:GLN:OE1   | 1:A:601:VAL:HG23  | 2.16                     | 0.45              |
| 1:A:624:SER:CB    | 1:A:625:LEU:HD12  | 2.46                     | 0.45              |
| 1:A:665:GLU:C     | 1:A:666:ASP:OD1   | 2.59                     | 0.45              |
| 2:B:1770:ASN:CB   | 2:B:1816:PHE:HE1  | 2.23                     | 0.45              |
| 2:B:1776:ARG:HA   | 2:B:1812:THR:HB   | 1.99                     | 0.45              |
| 2:B:1820:GLN:NE2  | 2:B:1822:HIS:HB3  | 2.31                     | 0.45              |
| 2:B:2201:ALA:O    | 2:B:2202:THR:CG2  | 2.60                     | 0.45              |
| 1:A:63:LYS:HG2    | 1:A:64:PRO:CD     | 2.46                     | 0.45              |
| 1:A:84:VAL:HG12   | 1:A:85:VAL:N      | 2.32                     | 0.45              |
| 1:A:607:GLU:HG2   | 1:A:608:PHE:N     | 2.32                     | 0.45              |
| 1:A:655:GLY:O     | 1:A:656:TYR:CB    | 2.64                     | 0.45              |
| 1:A:705:LEU:O     | 1:A:706:LEU:HD22  | 2.17                     | 0.45              |
| 2:B:1970:GLU:O    | 2:B:1971:TYR:C    | 2.60                     | 0.45              |
| 2:B:2018:SER:C    | 2:B:2020:LYS:H    | 2.25                     | 0.45              |
| 2:B:2049:LYS:O    | 2:B:2050:LEU:HD23 | 2.17                     | 0.45              |
| 2:B:2327:GLU:HG3  | 2:B:2328:ALA:N    | 2.32                     | 0.45              |
| 1:A:109:SER:OG    | 1:A:137:VAL:O     | 2.33                     | 0.45              |
| 1:A:115:ASP:OD1   | 1:A:115:ASP:O     | 2.34                     | 0.45              |
| 1:A:181:GLU:HG3   | 1:A:182:GLY:N     | 2.31                     | 0.45              |
| 1:A:442:ILE:HD12  | 1:A:442:ILE:N     | 2.31                     | 0.45              |
| 1:A:486:LEU:HB3   | 1:A:512:LYS:HD3   | 1.97                     | 0.45              |
| 1:A:515:VAL:O     | 1:A:515:VAL:HG12  | 2.16                     | 0.45              |
| 1:A:527:ARG:NH1   | 1:A:556:LYS:HD3   | 2.32                     | 0.45              |
| 1:A:703:THR:O     | 1:A:704:ALA:HB2   | 2.17                     | 0.45              |
| 1:A:723:TYR:CD1   | 1:A:723:TYR:C     | 2.94                     | 0.45              |
| 2:B:1782:PRO:HB3  | 2:B:1808:LYS:CA   | 2.41                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1804:LYS:O    | 2:B:1805:ASN:O    | 2.35                     | 0.45              |
| 2:B:2080:ILE:HG12 | 2:B:2170:ASP:N    | 2.32                     | 0.45              |
| 2:B:2129:ASN:HB2  | 2:B:2130:VAL:H    | 1.52                     | 0.45              |
| 2:B:2217:ASN:HD22 | 2:B:2320:ARG:HH11 | 1.64                     | 0.45              |
| 2:B:2243:VAL:HG23 | 2:B:2321:MET:CE   | 2.47                     | 0.45              |
| 1:A:97:SER:N      | 1:A:160:SER:OG    | 2.45                     | 0.45              |
| 1:A:286:LEU:O     | 1:A:288:ILE:N     | 2.49                     | 0.45              |
| 1:A:405:ARG:HD2   | 1:A:408:LYS:HB3   | 1.97                     | 0.45              |
| 1:A:483:VAL:HG13  | 1:A:513:TRP:CD1   | 2.51                     | 0.45              |
| 1:A:515:VAL:HG12  | 1:A:516:THR:O     | 2.17                     | 0.45              |
| 1:A:518:GLU:CD    | 1:A:518:GLU:N     | 2.74                     | 0.45              |
| 2:B:1758:LEU:O    | 2:B:1759:LEU:O    | 2.35                     | 0.45              |
| 2:B:1762:TYR:HB3  | 2:B:1764:ARG:CZ   | 2.47                     | 0.45              |
| 2:B:2002:ILE:O    | 2:B:2004:GLU:N    | 2.50                     | 0.45              |
| 2:B:2250:SER:O    | 2:B:2251:LEU:C    | 2.59                     | 0.45              |
| 2:B:2275:PHE:CD1  | 2:B:2280:VAL:N    | 2.82                     | 0.45              |
| 1:A:66:PRO:HA     | 1:A:67:PRO:HD2    | 1.85                     | 0.45              |
| 1:A:141:LEU:CB    | 1:A:144:ASN:ND2   | 2.80                     | 0.45              |
| 1:A:191:THR:C     | 1:A:193:HIS:N     | 2.75                     | 0.45              |
| 1:A:246:ILE:HA    | 1:A:325:LYS:O     | 2.16                     | 0.45              |
| 1:A:570:LYS:CG    | 1:A:638:TYR:HE2   | 2.28                     | 0.45              |
| 2:B:1734:VAL:CG1  | 2:B:1758:LEU:HB3  | 2.47                     | 0.45              |
| 2:B:1799:GLY:CA   | 2:B:1803:ARG:HD3  | 2.46                     | 0.45              |
| 2:B:2050:LEU:HD12 | 2:B:2061:ALA:O    | 2.16                     | 0.45              |
| 1:A:27:ASP:O      | 1:A:28:ALA:CB     | 2.65                     | 0.45              |
| 1:A:279:ARG:NH2   | 2:B:1971:TYR:CB   | 2.71                     | 0.45              |
| 1:A:327:ASP:OD1   | 1:A:328:SER:N     | 2.50                     | 0.45              |
| 1:A:486:LEU:N     | 1:A:486:LEU:CD1   | 2.77                     | 0.45              |
| 1:A:605:ASP:CG    | 1:A:607:GLU:HB3   | 2.42                     | 0.45              |
| 1:A:657:THR:OG1   | 2:B:1786:TYR:HE1  | 1.99                     | 0.45              |
| 2:B:1871:VAL:O    | 2:B:1871:VAL:HG12 | 2.17                     | 0.45              |
| 2:B:1880:PHE:CZ   | 2:B:1956:ILE:HD13 | 2.51                     | 0.45              |
| 2:B:1896:GLU:O    | 2:B:1897:ARG:HB3  | 2.17                     | 0.45              |
| 2:B:2014:PHE:CD1  | 2:B:2014:PHE:N    | 2.84                     | 0.45              |
| 2:B:2033:ARG:O    | 2:B:2034:ASP:C    | 2.60                     | 0.45              |
| 1:A:9:ALA:O       | 1:A:10:VAL:C      | 2.60                     | 0.45              |
| 1:A:12:LEU:HD22   | 1:A:61:ILE:HG23   | 1.98                     | 0.45              |
| 1:A:331:GLU:HA    | 1:A:331:GLU:OE2   | 2.15                     | 0.45              |
| 2:B:1944:LEU:HB2  | 2:B:1978:LEU:HD21 | 1.99                     | 0.45              |
| 2:B:2036:GLN:O    | 2:B:2037:ILE:CG2  | 2.60                     | 0.45              |
| 2:B:2084:ILE:HG13 | 2:B:2166:LEU:CB   | 2.43                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:2097:TYR:CZ   | 2:B:2157:SER:HB2 | 2.51                     | 0.45              |
| 1:A:141:LEU:O     | 1:A:144:ASN:HB2  | 2.16                     | 0.44              |
| 1:A:401:ALA:HB3   | 1:A:405:ARG:CZ   | 2.47                     | 0.44              |
| 1:A:439:ARG:HH11  | 1:A:439:ARG:HG3  | 1.82                     | 0.44              |
| 1:A:651:VAL:HG21  | 1:A:668:LEU:CA   | 2.47                     | 0.44              |
| 2:B:1764:ARG:HD2  | 2:B:1869:ARG:HB2 | 1.94                     | 0.44              |
| 2:B:2086:THR:HG21 | 2:B:2101:PHE:CE2 | 2.49                     | 0.44              |
| 2:B:2271:TRP:CZ3  | 2:B:2307:ARG:CB  | 2.99                     | 0.44              |
| 1:A:14:TRP:HA     | 1:A:14:TRP:HE3   | 1.82                     | 0.44              |
| 1:A:152:LEU:HD23  | 1:A:179:CYS:CB   | 2.39                     | 0.44              |
| 1:A:155:THR:O     | 1:A:293:PHE:HB3  | 2.17                     | 0.44              |
| 1:A:184:LEU:O     | 1:A:188:LYS:HB3  | 2.17                     | 0.44              |
| 1:A:199:PHE:HD1   | 1:A:199:PHE:H    | 1.65                     | 0.44              |
| 1:A:240:ARG:O     | 1:A:241:SER:O    | 2.35                     | 0.44              |
| 1:A:530:THR:O     | 1:A:531:ARG:NE   | 2.50                     | 0.44              |
| 1:A:530:THR:HG22  | 1:A:638:TYR:HB3  | 1.99                     | 0.44              |
| 1:A:650:SER:C     | 1:A:651:VAL:CG2  | 2.90                     | 0.44              |
| 1:A:656:TYR:O     | 1:A:657:THR:HB   | 2.16                     | 0.44              |
| 1:A:657:THR:HG21  | 2:B:1786:TYR:OH  | 2.17                     | 0.44              |
| 2:B:1745:GLN:CG   | 2:B:1746:PRO:HB3 | 2.39                     | 0.44              |
| 2:B:1962:VAL:HG23 | 2:B:1963:PHE:N   | 2.31                     | 0.44              |
| 2:B:2301:LEU:CD2  | 2:B:2302:LEU:N   | 2.80                     | 0.44              |
| 1:A:80:VAL:O      | 1:A:81:TYR:CB    | 2.66                     | 0.44              |
| 1:A:159:LEU:HB2   | 1:A:172:LEU:O    | 2.17                     | 0.44              |
| 1:A:255:TRP:HA    | 1:A:255:TRP:HE3  | 1.82                     | 0.44              |
| 1:A:409:SER:C     | 1:A:411:TYR:N    | 2.74                     | 0.44              |
| 1:A:427:ARG:HH11  | 1:A:448:ILE:CA   | 2.14                     | 0.44              |
| 1:A:578:VAL:HG21  | 1:A:644:ALA:H    | 1.76                     | 0.44              |
| 2:B:1882:ILE:HD11 | 2:B:1919:HIS:CE1 | 2.52                     | 0.44              |
| 2:B:1948:GLY:HA3  | 2:B:1952:ASN:ND2 | 2.32                     | 0.44              |
| 2:B:2065:LYS:HE3  | 2:B:2066:GLU:H   | 1.82                     | 0.44              |
| 2:B:2228:GLU:O    | 2:B:2309:HIS:HB3 | 2.17                     | 0.44              |
| 1:A:5:TYR:HE2     | 1:A:76:ILE:HG23  | 1.82                     | 0.44              |
| 1:A:238:VAL:O     | 1:A:239:ASN:C    | 2.60                     | 0.44              |
| 1:A:273:GLY:CA    | 1:A:306:PHE:HD2  | 2.25                     | 0.44              |
| 1:A:407:TYR:O     | 1:A:409:SER:N    | 2.51                     | 0.44              |
| 1:A:419:ILE:HG13  | 1:A:420:GLY:N    | 2.32                     | 0.44              |
| 1:A:529:LEU:HD12  | 1:A:553:ILE:HB   | 1.96                     | 0.44              |
| 2:B:1740:ASP:O    | 2:B:1742:SER:N   | 2.50                     | 0.44              |
| 2:B:1824:ALA:HB1  | 2:B:1825:PRO:CD  | 2.47                     | 0.44              |
| 2:B:1829:GLU:HB2  | 2:B:1966:ARG:NE  | 2.32                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1889:TRP:O    | 2:B:1890:TYR:CB   | 2.59                     | 0.44              |
| 2:B:1933:VAL:O    | 2:B:1933:VAL:CG2  | 2.65                     | 0.44              |
| 2:B:2030:GLY:O    | 2:B:2032:ILE:N    | 2.49                     | 0.44              |
| 2:B:2107:LEU:CD2  | 2:B:2147:ARG:HB2  | 2.42                     | 0.44              |
| 2:B:2260:PHE:HB2  | 2:B:2309:HIS:O    | 2.18                     | 0.44              |
| 2:B:2323:VAL:CG1  | 2:B:2324:LEU:H    | 2.21                     | 0.44              |
| 1:A:2:THR:HG22    | 1:A:82:ASP:HA     | 2.00                     | 0.44              |
| 1:A:523:LYS:N     | 1:A:523:LYS:CD    | 2.72                     | 0.44              |
| 1:A:604:GLU:HA    | 1:A:608:PHE:HE1   | 1.83                     | 0.44              |
| 1:A:646:THR:O     | 1:A:647:ASP:O     | 2.35                     | 0.44              |
| 1:A:651:VAL:O     | 1:A:693:HIS:N     | 2.51                     | 0.44              |
| 1:A:654:SER:HA    | 1:A:689:ILE:O     | 2.17                     | 0.44              |
| 2:B:1999:GLU:HB3  | 2:B:2011:SER:CB   | 2.47                     | 0.44              |
| 2:B:2115:TYR:CE2  | 2:B:2140:PHE:HD1  | 2.36                     | 0.44              |
| 2:B:2330:ASP:C    | 2:B:2332:TYR:N    | 2.75                     | 0.44              |
| 1:A:101:VAL:O     | 1:A:101:VAL:CG1   | 2.63                     | 0.44              |
| 1:A:419:ILE:O     | 1:A:420:GLY:C     | 2.60                     | 0.44              |
| 1:A:423:TYR:CE2   | 1:A:581:GLU:HG3   | 2.51                     | 0.44              |
| 1:A:654:SER:H     | 1:A:657:THR:CA    | 2.30                     | 0.44              |
| 1:A:660:HIS:HB2   | 1:A:680:MET:HG2   | 1.96                     | 0.44              |
| 2:B:1732:LYS:CE   | 2:B:1885:GLU:OE2  | 2.66                     | 0.44              |
| 2:B:1745:GLN:HA   | 2:B:1746:PRO:HA   | 1.65                     | 0.44              |
| 2:B:1767:VAL:HG23 | 2:B:1819:VAL:HG12 | 2.00                     | 0.44              |
| 2:B:2177:PRO:C    | 2:B:2178:LEU:HD23 | 2.43                     | 0.44              |
| 1:A:22:GLY:O      | 1:A:23:GLU:HG3    | 2.17                     | 0.44              |
| 1:A:316:GLN:HG2   | 1:A:317:HIS:N     | 2.29                     | 0.44              |
| 1:A:461:LEU:HD12  | 1:A:461:LEU:HA    | 1.75                     | 0.44              |
| 1:A:461:LEU:CB    | 1:A:463:ILE:HD11  | 2.41                     | 0.44              |
| 1:A:485:PRO:C     | 1:A:486:LEU:HD12  | 2.42                     | 0.44              |
| 1:A:716:GLY:O     | 1:A:717:ASP:CB    | 2.65                     | 0.44              |
| 2:B:1703:VAL:CG2  | 2:B:1704:GLU:N    | 2.79                     | 0.44              |
| 2:B:1871:VAL:O    | 2:B:1871:VAL:CG1  | 2.66                     | 0.44              |
| 2:B:1897:ARG:NH1  | 2:B:1897:ARG:CB   | 2.80                     | 0.44              |
| 2:B:2080:ILE:HD11 | 2:B:2169:CYS:HB3  | 1.99                     | 0.44              |
| 2:B:2179:GLY:O    | 2:B:2181:GLU:N    | 2.51                     | 0.44              |
| 2:B:2317:ILE:O    | 2:B:2317:ILE:HG22 | 2.18                     | 0.44              |
| 1:A:34:VAL:N      | 1:A:35:PRO:CD     | 2.75                     | 0.44              |
| 1:A:64:PRO:CB     | 1:A:70:GLY:HA3    | 2.48                     | 0.44              |
| 1:A:69:MET:HA     | 1:A:235:ASN:HD21  | 1.82                     | 0.44              |
| 1:A:209:HIS:ND1   | 1:A:209:HIS:C     | 2.75                     | 0.44              |
| 1:A:231:MET:O     | 1:A:232:HIS:CG    | 2.71                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:267:HIS:CD2   | 1:A:320:MET:SD    | 3.11                     | 0.44              |
| 1:A:548:ILE:CD1   | 1:A:549:GLY:H     | 2.28                     | 0.44              |
| 1:A:653:PHE:CA    | 1:A:657:THR:HA    | 2.42                     | 0.44              |
| 2:B:1714:SER:HA   | 2:B:1715:PRO:HD3  | 1.86                     | 0.44              |
| 2:B:1924:TYR:HD2  | 2:B:1928:THR:O    | 2.00                     | 0.44              |
| 2:B:1944:LEU:HD23 | 2:B:1944:LEU:N    | 2.33                     | 0.44              |
| 2:B:2096:LEU:HD13 | 2:B:2096:LEU:HA   | 1.80                     | 0.44              |
| 1:A:164:LEU:O     | 1:A:165:VAL:C     | 2.60                     | 0.44              |
| 1:A:271:LEU:HD12  | 1:A:273:GLY:CA    | 2.48                     | 0.44              |
| 1:A:471:ARG:HB2   | 1:A:473:TYR:CE1   | 2.53                     | 0.44              |
| 1:A:646:THR:O     | 1:A:647:ASP:C     | 2.60                     | 0.44              |
| 2:B:1755:HIS:C    | 2:B:1757:GLY:N    | 2.76                     | 0.44              |
| 2:B:1774:THR:HG22 | 2:B:1814:THR:HG21 | 1.99                     | 0.44              |
| 2:B:1924:TYR:CD2  | 2:B:1928:THR:C    | 2.89                     | 0.44              |
| 2:B:2016:VAL:CG2  | 2:B:2017:TYR:N    | 2.81                     | 0.44              |
| 1:A:165:VAL:C     | 1:A:167:ASP:H     | 2.25                     | 0.43              |
| 1:A:396:ALA:CB    | 1:A:397:PRO:CA    | 2.81                     | 0.43              |
| 1:A:426:VAL:HG23  | 1:A:547:LEU:HG    | 1.99                     | 0.43              |
| 1:A:586:TYR:O     | 1:A:590:ASN:HB2   | 2.18                     | 0.43              |
| 1:A:677:THR:OG1   | 1:A:678:VAL:N     | 2.50                     | 0.43              |
| 2:B:1794:GLU:O    | 2:B:1795:ASP:OD1  | 2.35                     | 0.43              |
| 2:B:1940:ILE:CG2  | 2:B:1941:ARG:N    | 2.80                     | 0.43              |
| 2:B:2259:GLU:CD   | 2:B:2312:SER:HG   | 2.26                     | 0.43              |
| 1:A:46:TYR:HE1    | 1:A:227:ALA:CB    | 2.26                     | 0.43              |
| 1:A:172:LEU:N     | 1:A:172:LEU:CD1   | 2.81                     | 0.43              |
| 1:A:270:PHE:HD1   | 1:A:285:SER:HA    | 1.83                     | 0.43              |
| 1:A:573:VAL:HG22  | 1:A:574:ILE:N     | 2.33                     | 0.43              |
| 1:A:605:ASP:C     | 1:A:607:GLU:N     | 2.74                     | 0.43              |
| 1:A:663:VAL:O     | 2:B:1968:LYS:HE3  | 2.18                     | 0.43              |
| 2:B:2042:GLN:O    | 2:B:2046:TRP:O    | 2.35                     | 0.43              |
| 2:B:2044:GLY:C    | 2:B:2046:TRP:N    | 2.71                     | 0.43              |
| 2:B:2065:LYS:HD3  | 2:B:2159:ARG:HD3  | 2.00                     | 0.43              |
| 1:A:65:ARG:HD2    | 1:A:65:ARG:HA     | 1.80                     | 0.43              |
| 1:A:254:TYR:HD1   | 1:A:297:GLN:HB3   | 1.83                     | 0.43              |
| 1:A:266:VAL:HG22  | 1:A:290:PRO:HD3   | 2.01                     | 0.43              |
| 1:A:518:GLU:CD    | 1:A:518:GLU:H     | 2.27                     | 0.43              |
| 1:A:663:VAL:CG2   | 2:B:1968:LYS:HD2  | 2.41                     | 0.43              |
| 2:B:1934:MET:SD   | 2:B:2014:PHE:HD2  | 2.41                     | 0.43              |
| 2:B:2233:ASP:OD1  | 2:B:2305:TYR:CZ   | 2.71                     | 0.43              |
| 2:B:2304:ARG:C    | 2:B:2305:TYR:CD1  | 2.96                     | 0.43              |
| 1:A:507:GLU:OE2   | 1:A:508:ILE:HG22  | 2.17                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1763:ILE:HG22 | 2:B:1837:TYR:CE2  | 2.54                     | 0.43              |
| 2:B:1771:ILE:HD12 | 2:B:1817:TRP:CE2  | 2.53                     | 0.43              |
| 2:B:1813:LYS:CG   | 2:B:1814:THR:N    | 2.81                     | 0.43              |
| 2:B:1893:GLU:C    | 2:B:1895:MET:H    | 2.26                     | 0.43              |
| 2:B:1914:GLU:HA   | 2:B:1917:ARG:HG3  | 2.00                     | 0.43              |
| 2:B:1923:GLY:O    | 2:B:1924:TYR:CD1  | 2.72                     | 0.43              |
| 2:B:2043:TYR:CE2  | 2:B:2065:LYS:HB2  | 2.52                     | 0.43              |
| 1:A:7:LEU:O       | 1:A:88:LEU:HA     | 2.19                     | 0.43              |
| 1:A:446:SER:CB    | 1:A:449:LEU:HD21  | 2.48                     | 0.43              |
| 1:A:508:ILE:HG23  | 1:A:508:ILE:O     | 2.18                     | 0.43              |
| 1:A:598:PRO:CG    | 1:A:599:ALA:H     | 2.25                     | 0.43              |
| 1:A:608:PHE:HA    | 1:A:611:SER:HB2   | 2.00                     | 0.43              |
| 1:A:698:ARG:HG3   | 1:A:698:ARG:NH1   | 2.33                     | 0.43              |
| 2:B:1777:ASN:ND2  | 2:B:1809:PRO:HA   | 2.33                     | 0.43              |
| 2:B:1844:GLU:C    | 2:B:1846:ASP:N    | 2.77                     | 0.43              |
| 2:B:1859:HIS:O    | 2:B:1862:THR:CG2  | 2.66                     | 0.43              |
| 2:B:1919:HIS:CD2  | 2:B:1919:HIS:N    | 2.87                     | 0.43              |
| 2:B:2052:ARG:H    | 2:B:2163:ARG:CG   | 2.29                     | 0.43              |
| 1:A:104:SER:C     | 1:A:105:TYR:HD1   | 2.27                     | 0.43              |
| 1:A:230:LYS:O     | 1:A:231:MET:HG2   | 2.19                     | 0.43              |
| 1:A:246:ILE:N     | 1:A:246:ILE:CD1   | 2.75                     | 0.43              |
| 1:A:285:SER:O     | 1:A:286:LEU:C     | 2.61                     | 0.43              |
| 1:A:289:SER:O     | 1:A:291:ILE:N     | 2.52                     | 0.43              |
| 2:B:1719:ARG:HG2  | 2:B:1723:GLN:HE21 | 1.83                     | 0.43              |
| 2:B:1829:GLU:HB3  | 2:B:1830:PHE:H    | 1.52                     | 0.43              |
| 2:B:2074:ASP:O    | 2:B:2076:LEU:N    | 2.51                     | 0.43              |
| 2:B:2259:GLU:O    | 2:B:2260:PHE:HB3  | 2.17                     | 0.43              |
| 1:A:289:SER:HB3   | 1:A:290:PRO:CD    | 2.45                     | 0.43              |
| 1:A:619:GLY:O     | 1:A:620:TYR:CG    | 2.72                     | 0.43              |
| 2:B:1696:ARG:HH11 | 2:B:1696:ARG:HG3  | 1.84                     | 0.43              |
| 2:B:1708:ASP:CG   | 2:B:1709:TYR:N    | 2.75                     | 0.43              |
| 2:B:1734:VAL:HG11 | 2:B:1758:LEU:HB3  | 2.00                     | 0.43              |
| 2:B:2203:TRP:CZ3  | 2:B:2218:ALA:HB3  | 2.53                     | 0.43              |
| 2:B:2225:ASN:CG   | 2:B:2226:PRO:N    | 2.73                     | 0.43              |
| 1:A:76:ILE:O      | 1:A:176:LEU:HD12  | 2.18                     | 0.43              |
| 1:A:386:ILE:O     | 1:A:465:PHE:HA    | 2.19                     | 0.43              |
| 1:A:428:PHE:CE1   | 1:A:547:LEU:HD22  | 2.54                     | 0.43              |
| 1:A:461:LEU:CB    | 1:A:513:TRP:HB2   | 2.41                     | 0.43              |
| 2:B:1725:GLY:O    | 2:B:1726:SER:O    | 2.35                     | 0.43              |
| 2:B:1957:HIS:HB2  | 2:B:2001:LEU:HD13 | 2.01                     | 0.43              |
| 2:B:2075:LEU:HD13 | 2:B:2079:MET:HB2  | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:104:SER:C    | 1:A:105:TYR:CD1   | 2.97                     | 0.43              |
| 1:A:168:LEU:C    | 1:A:170:SER:N     | 2.77                     | 0.43              |
| 1:A:180:ARG:O    | 1:A:181:GLU:C     | 2.61                     | 0.43              |
| 1:A:420:GLY:HA2  | 1:A:614:MET:CE    | 2.48                     | 0.43              |
| 1:A:493:LYS:HB3  | 1:A:494:GLY:H     | 1.62                     | 0.43              |
| 1:A:616:SER:C    | 1:A:619:GLY:H     | 2.26                     | 0.43              |
| 1:A:652:PHE:HB2  | 1:A:658:PHE:HB2   | 2.01                     | 0.43              |
| 2:B:1846:ASP:O   | 2:B:1847:VAL:C    | 2.62                     | 0.43              |
| 2:B:1880:PHE:CG  | 2:B:1921:ILE:HG22 | 2.53                     | 0.43              |
| 2:B:1912:PHE:HB3 | 2:B:1915:ASN:HB2  | 2.01                     | 0.43              |
| 2:B:1940:ILE:CD1 | 2:B:1990:PRO:HD3  | 2.46                     | 0.43              |
| 2:B:1989:LEU:HA  | 2:B:1990:PRO:HD3  | 1.77                     | 0.43              |
| 2:B:2084:ILE:CG1 | 2:B:2085:LYS:N    | 2.63                     | 0.43              |
| 2:B:2249:LYS:HA  | 2:B:2254:SER:CB   | 2.49                     | 0.43              |
| 2:B:2279:LYS:O   | 2:B:2280:VAL:C    | 2.62                     | 0.43              |
| 1:A:203:ASP:O    | 1:A:203:ASP:CG    | 2.62                     | 0.43              |
| 1:A:280:ASN:HB3  | 1:A:524:SER:HB2   | 2.00                     | 0.43              |
| 1:A:409:SER:C    | 1:A:411:TYR:H     | 2.25                     | 0.43              |
| 1:A:475:ILE:O    | 1:A:475:ILE:CG2   | 2.66                     | 0.43              |
| 1:A:498:LEU:HA   | 1:A:502:PRO:CG    | 2.47                     | 0.43              |
| 1:A:572:ASN:HB2  | 1:A:636:TYR:O     | 2.19                     | 0.43              |
| 1:A:702:MET:O    | 1:A:703:THR:CB    | 2.66                     | 0.43              |
| 2:B:1704:GLU:CD  | 2:B:1779:ALA:HB1  | 2.44                     | 0.43              |
| 2:B:2096:LEU:CD1 | 2:B:2159:ARG:H    | 2.32                     | 0.43              |
| 2:B:2232:VAL:C   | 2:B:2234:PHE:N    | 2.77                     | 0.43              |
| 2:B:2243:VAL:C   | 2:B:2294:VAL:HG23 | 2.44                     | 0.43              |
| 1:A:426:VAL:O    | 1:A:547:LEU:HD23  | 2.19                     | 0.42              |
| 1:A:555:TYR:CD1  | 1:A:556:LYS:N     | 2.87                     | 0.42              |
| 1:A:692:CYS:HB3  | 1:A:706:LEU:HB2   | 2.00                     | 0.42              |
| 2:B:1722:ALA:O   | 2:B:1723:GLN:HG3  | 2.18                     | 0.42              |
| 2:B:2194:SER:HB2 | 2:B:2221:PRO:CB   | 2.49                     | 0.42              |
| 1:A:29:ARG:N     | 1:A:29:ARG:HD2    | 2.34                     | 0.42              |
| 1:A:68:TRP:O     | 1:A:68:TRP:CE3    | 2.73                     | 0.42              |
| 1:A:105:TYR:CZ   | 2:B:1960:GLY:HA2  | 2.54                     | 0.42              |
| 1:A:400:LEU:HA   | 1:A:405:ARG:NH2   | 2.34                     | 0.42              |
| 1:A:428:PHE:HE1  | 1:A:547:LEU:CB    | 2.26                     | 0.42              |
| 1:A:631:LEU:O    | 1:A:632:HIS:HB2   | 2.18                     | 0.42              |
| 1:A:662:MET:N    | 1:A:680:MET:SD    | 2.92                     | 0.42              |
| 2:B:1779:ALA:O   | 2:B:1809:PRO:HB3  | 2.19                     | 0.42              |
| 2:B:1784:SER:O   | 2:B:1839:SER:CA   | 2.59                     | 0.42              |
| 2:B:1797:ARG:O   | 2:B:1797:ARG:CG   | 2.68                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1959:SER:HB3  | 2:B:1997:ARG:H    | 1.84                     | 0.42              |
| 2:B:2139:ILE:HG23 | 2:B:2139:ILE:O    | 2.19                     | 0.42              |
| 2:B:2212:LEU:O    | 2:B:2320:ARG:NH1  | 2.52                     | 0.42              |
| 1:A:5:TYR:CE2     | 1:A:76:ILE:HG12   | 2.55                     | 0.42              |
| 1:A:35:PRO:O      | 1:A:36:LYS:HE3    | 2.20                     | 0.42              |
| 1:A:393:TRP:CZ2   | 1:A:448:ILE:HG23  | 2.54                     | 0.42              |
| 1:A:533:TYR:O     | 1:A:534:SER:CB    | 2.67                     | 0.42              |
| 1:A:658:PHE:HE1   | 1:A:686:GLY:H     | 1.67                     | 0.42              |
| 2:B:2089:ALA:O    | 2:B:2096:LEU:HB2  | 2.19                     | 0.42              |
| 2:B:2130:VAL:C    | 2:B:2131:ASP:OD1  | 2.62                     | 0.42              |
| 2:B:2224:ASN:HA   | 2:B:2317:ILE:HD12 | 2.00                     | 0.42              |
| 2:B:2255:MET:SD   | 2:B:2316:GLN:HB2  | 2.59                     | 0.42              |
| 2:B:2324:LEU:HD23 | 2:B:2324:LEU:HA   | 1.87                     | 0.42              |
| 2:B:2328:ALA:O    | 2:B:2329:GLN:O    | 2.37                     | 0.42              |
| 1:A:75:THR:HG22   | 1:A:175:ALA:CB    | 2.45                     | 0.42              |
| 1:A:83:THR:HG23   | 1:A:138:TRP:O     | 2.19                     | 0.42              |
| 1:A:188:LYS:O     | 1:A:188:LYS:HG2   | 2.19                     | 0.42              |
| 1:A:254:TYR:CD1   | 1:A:297:GLN:HB3   | 2.54                     | 0.42              |
| 1:A:287:GLU:OE2   | 1:A:676:GLU:HG2   | 2.18                     | 0.42              |
| 1:A:310:CYS:HB3   | 1:A:320:MET:HB3   | 2.01                     | 0.42              |
| 1:A:446:SER:HB3   | 1:A:449:LEU:CD1   | 2.45                     | 0.42              |
| 1:A:446:SER:O     | 1:A:447:GLY:O     | 2.37                     | 0.42              |
| 1:A:598:PRO:HG2   | 1:A:599:ALA:N     | 2.31                     | 0.42              |
| 1:A:661:LYS:HE2   | 1:A:665:GLU:CG    | 2.49                     | 0.42              |
| 1:A:663:VAL:HG22  | 2:B:1968:LYS:HZ2  | 1.83                     | 0.42              |
| 2:B:1709:TYR:CE1  | 2:B:1924:TYR:HA   | 2.55                     | 0.42              |
| 2:B:1935:ALA:H    | 2:B:2016:VAL:HG23 | 1.84                     | 0.42              |
| 2:B:1967:LYS:O    | 2:B:1968:LYS:CB   | 2.63                     | 0.42              |
| 2:B:2046:TRP:CZ3  | 2:B:2060:ASN:N    | 2.88                     | 0.42              |
| 2:B:2082:HIS:O    | 2:B:2139:ILE:HD12 | 2.19                     | 0.42              |
| 2:B:2255:MET:O    | 2:B:2255:MET:HG2  | 2.19                     | 0.42              |
| 1:A:7:LEU:HD23    | 1:A:8:GLY:O       | 2.19                     | 0.42              |
| 1:A:53:GLU:CG     | 1:A:54:PHE:N      | 2.58                     | 0.42              |
| 1:A:100:ALA:O     | 1:A:101:VAL:HG12  | 2.20                     | 0.42              |
| 1:A:119:SER:H     | 1:A:123:LYS:HE3   | 1.84                     | 0.42              |
| 1:A:250:ARG:HH11  | 1:A:250:ARG:CG    | 2.32                     | 0.42              |
| 1:A:313:SER:OG    | 1:A:314:SER:N     | 2.51                     | 0.42              |
| 1:A:403:ASP:HB3   | 1:A:404:ASP:H     | 1.72                     | 0.42              |
| 1:A:627:LEU:HD13  | 1:A:637:TRP:CH2   | 2.55                     | 0.42              |
| 2:B:1777:ASN:CG   | 2:B:1778:GLN:H    | 2.27                     | 0.42              |
| 2:B:1832:CYS:CB   | 2:B:1857:VAL:O    | 2.67                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:1911:THR:O    | 2:B:1913:LYS:N   | 2.52                     | 0.42              |
| 2:B:2038:THR:HG21 | 2:B:2072:LYS:HE3 | 2.01                     | 0.42              |
| 2:B:2061:ALA:HB2  | 2:B:2163:ARG:HD2 | 2.00                     | 0.42              |
| 2:B:2116:ARG:O    | 2:B:2124:MET:HB2 | 2.20                     | 0.42              |
| 1:A:100:ALA:HB3   | 1:A:105:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:123:LYS:CA    | 1:A:126:ASP:HB2  | 2.46                     | 0.42              |
| 1:A:161:HIS:O     | 1:A:161:HIS:ND1  | 2.53                     | 0.42              |
| 1:A:584:SER:O     | 1:A:586:TYR:N    | 2.53                     | 0.42              |
| 1:A:690:LEU:O     | 1:A:690:LEU:HD23 | 2.20                     | 0.42              |
| 2:B:2166:LEU:HD12 | 2:B:2166:LEU:C   | 2.43                     | 0.42              |
| 2:B:2224:ASN:ND2  | 2:B:2316:GLN:NE2 | 2.66                     | 0.42              |
| 2:B:2256:TYR:HB2  | 2:B:2257:VAL:H   | 1.46                     | 0.42              |
| 1:A:40:PHE:C      | 1:A:42:THR:N     | 2.78                     | 0.42              |
| 1:A:434:GLU:OE2   | 1:A:436:PHE:C    | 2.62                     | 0.42              |
| 1:A:545:SER:HA    | 1:A:584:SER:OG   | 2.19                     | 0.42              |
| 1:A:584:SER:C     | 1:A:586:TYR:N    | 2.78                     | 0.42              |
| 1:A:604:GLU:HG3   | 1:A:609:GLN:HG2  | 2.02                     | 0.42              |
| 1:A:640:LEU:HD23  | 1:A:640:LEU:H    | 1.81                     | 0.42              |
| 1:A:677:THR:O     | 1:A:678:VAL:HG23 | 2.19                     | 0.42              |
| 2:B:1860:THR:O    | 2:B:1862:THR:N   | 2.52                     | 0.42              |
| 2:B:1889:TRP:HB3  | 2:B:1890:TYR:H   | 1.72                     | 0.42              |
| 2:B:2194:SER:CB   | 2:B:2222:GLN:N   | 2.66                     | 0.42              |
| 1:A:52:VAL:HG23   | 1:A:53:GLU:N     | 2.35                     | 0.42              |
| 1:A:106:TRP:HA    | 1:A:106:TRP:HE3  | 1.84                     | 0.42              |
| 1:A:198:LEU:HD23  | 1:A:198:LEU:C    | 2.44                     | 0.42              |
| 1:A:273:GLY:C     | 1:A:274:HIS:CG   | 2.97                     | 0.42              |
| 1:A:284:ALA:O     | 1:A:285:SER:CB   | 2.67                     | 0.42              |
| 1:A:301:MET:O     | 1:A:302:ASP:HB2  | 2.20                     | 0.42              |
| 1:A:463:ILE:O     | 1:A:465:PHE:N    | 2.51                     | 0.42              |
| 1:A:655:GLY:O     | 1:A:656:TYR:CD1  | 2.73                     | 0.42              |
| 1:A:682:MET:O     | 1:A:682:MET:HE2  | 2.19                     | 0.42              |
| 2:B:1963:PHE:CE2  | 2:B:1986:VAL:HB  | 2.55                     | 0.42              |
| 2:B:2034:ASP:HB3  | 2:B:2049:LYS:HG2 | 2.01                     | 0.42              |
| 2:B:2075:LEU:HB2  | 2:B:2077:ALA:O   | 2.19                     | 0.42              |
| 2:B:2209:ARG:HA   | 2:B:2321:MET:O   | 2.20                     | 0.42              |
| 2:B:2275:PHE:HD1  | 2:B:2279:LYS:C   | 2.27                     | 0.42              |
| 1:A:15:ASP:OD1    | 1:A:17:MET:HG2   | 2.20                     | 0.42              |
| 1:A:22:GLY:O      | 1:A:23:GLU:HB2   | 2.20                     | 0.42              |
| 1:A:50:LEU:C      | 1:A:51:PHE:O     | 2.61                     | 0.42              |
| 1:A:71:LEU:CD1    | 1:A:236:GLY:HA3  | 2.47                     | 0.42              |
| 1:A:424:LYS:H     | 1:A:590:ASN:CG   | 2.26                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:702:MET:O     | 1:A:703:THR:HB    | 2.20                     | 0.42              |
| 2:B:2095:SER:O    | 2:B:2096:LEU:HD22 | 2.18                     | 0.42              |
| 2:B:2276:GLN:C    | 2:B:2278:GLY:N    | 2.62                     | 0.42              |
| 1:A:101:VAL:HG23  | 2:B:1957:HIS:CE1  | 2.55                     | 0.42              |
| 1:A:476:TYR:CE2   | 1:A:497:HIS:HE1   | 2.37                     | 0.42              |
| 1:A:491:LEU:HB3   | 1:A:495:VAL:CG1   | 2.49                     | 0.42              |
| 1:A:658:PHE:HE1   | 1:A:686:GLY:N     | 2.18                     | 0.42              |
| 2:B:1886:THR:C    | 2:B:1888:SER:N    | 2.76                     | 0.42              |
| 2:B:1930:PRO:HB2  | 2:B:1931:GLY:H    | 1.45                     | 0.42              |
| 2:B:2034:ASP:O    | 2:B:2035:PHE:C    | 2.63                     | 0.42              |
| 2:B:2204:SER:O    | 2:B:2206:SER:N    | 2.53                     | 0.42              |
| 2:B:2266:GLN:O    | 2:B:2267:ASP:CB   | 2.67                     | 0.42              |
| 1:A:327:ASP:CG    | 1:A:328:SER:N     | 2.77                     | 0.41              |
| 1:A:552:LEU:N     | 1:A:552:LEU:CD1   | 2.83                     | 0.41              |
| 1:A:595:LEU:O     | 1:A:596:PRO:O     | 2.37                     | 0.41              |
| 1:A:636:TYR:HD2   | 1:A:638:TYR:OH    | 2.03                     | 0.41              |
| 2:B:1835:TRP:N    | 2:B:1855:LEU:O    | 2.53                     | 0.41              |
| 2:B:1840:ASP:O    | 2:B:1840:ASP:OD1  | 2.37                     | 0.41              |
| 2:B:1921:ILE:C    | 2:B:1923:GLY:H    | 2.28                     | 0.41              |
| 2:B:1997:ARG:CG   | 2:B:1998:VAL:N    | 2.83                     | 0.41              |
| 2:B:1998:VAL:C    | 2:B:1999:GLU:HG3  | 2.45                     | 0.41              |
| 2:B:2027:MET:CB   | 2:B:2165:GLU:HA   | 2.47                     | 0.41              |
| 2:B:2074:ASP:C    | 2:B:2076:LEU:N    | 2.78                     | 0.41              |
| 2:B:2096:LEU:HD22 | 2:B:2096:LEU:N    | 2.33                     | 0.41              |
| 2:B:2103:ILE:HD12 | 2:B:2103:ILE:N    | 2.35                     | 0.41              |
| 1:A:50:LEU:CD2    | 1:A:171:GLY:HA3   | 2.51                     | 0.41              |
| 1:A:137:VAL:O     | 1:A:137:VAL:HG13  | 2.21                     | 0.41              |
| 1:A:415:GLY:H     | 1:A:418:ARG:HB2   | 1.85                     | 0.41              |
| 1:A:587:LEU:H     | 1:A:587:LEU:CD2   | 2.33                     | 0.41              |
| 2:B:1809:PRO:O    | 2:B:1810:ASN:HB3  | 2.20                     | 0.41              |
| 2:B:1848:HIS:C    | 2:B:1850:GLY:H    | 2.28                     | 0.41              |
| 2:B:1876:PHE:HE2  | 2:B:1934:MET:CE   | 2.33                     | 0.41              |
| 2:B:1901:ALA:HB3  | 2:B:1912:PHE:CE1  | 2.55                     | 0.41              |
| 2:B:1992:LYS:CG   | 2:B:1993:ALA:N    | 2.83                     | 0.41              |
| 2:B:2070:TRP:CZ3  | 2:B:2072:LYS:HE2  | 2.54                     | 0.41              |
| 2:B:2107:LEU:O    | 2:B:2108:ASP:CB   | 2.68                     | 0.41              |
| 2:B:2301:LEU:HD23 | 2:B:2302:LEU:N    | 2.23                     | 0.41              |
| 1:A:7:LEU:CD1     | 1:A:51:PHE:HD2    | 2.33                     | 0.41              |
| 1:A:49:THR:C      | 1:A:50:LEU:HD23   | 2.45                     | 0.41              |
| 1:A:89:LYS:O      | 1:A:91:MET:N      | 2.45                     | 0.41              |
| 2:B:1701:ALA:O    | 2:B:1735:PHE:HA   | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1761:PRO:O    | 2:B:1837:TYR:OH   | 2.37                     | 0.41              |
| 2:B:1822:HIS:HD1  | 2:B:1823:MET:HG2  | 1.85                     | 0.41              |
| 2:B:1873:VAL:HG11 | 2:B:1939:ARG:HB3  | 1.99                     | 0.41              |
| 1:A:662:MET:N     | 1:A:680:MET:CE    | 2.83                     | 0.41              |
| 2:B:1700:ILE:HD11 | 2:B:1735:PHE:CB   | 2.37                     | 0.41              |
| 2:B:1888:SER:O    | 2:B:1889:TRP:O    | 2.39                     | 0.41              |
| 2:B:2116:ARG:HD2  | 2:B:2117:GLY:O    | 2.20                     | 0.41              |
| 2:B:2313:TRP:CE2  | 2:B:2317:ILE:HD11 | 2.55                     | 0.41              |
| 1:A:427:ARG:HD2   | 1:A:448:ILE:HA    | 2.03                     | 0.41              |
| 1:A:624:SER:O     | 1:A:625:LEU:HB2   | 2.20                     | 0.41              |
| 1:A:652:PHE:CB    | 1:A:657:THR:O     | 2.69                     | 0.41              |
| 2:B:1822:HIS:ND1  | 2:B:1822:HIS:C    | 2.78                     | 0.41              |
| 2:B:1929:LEU:HA   | 2:B:1930:PRO:HD3  | 1.41                     | 0.41              |
| 2:B:2036:GLN:NE2  | 2:B:2076:LEU:HG   | 2.32                     | 0.41              |
| 1:A:98:LEU:HD21   | 1:A:138:TRP:HH2   | 1.85                     | 0.41              |
| 1:A:199:PHE:HE2   | 1:A:269:ILE:HG13  | 1.85                     | 0.41              |
| 1:A:309:PHE:CD1   | 1:A:309:PHE:O     | 2.73                     | 0.41              |
| 1:A:368:PHE:HB3   | 1:A:369:ILE:H     | 1.71                     | 0.41              |
| 1:A:427:ARG:HD3   | 1:A:448:ILE:CG2   | 2.47                     | 0.41              |
| 2:B:2064:THR:O    | 2:B:2065:LYS:CG   | 2.68                     | 0.41              |
| 2:B:2186:SER:C    | 2:B:2188:ALA:N    | 2.76                     | 0.41              |
| 1:A:184:LEU:O     | 1:A:184:LEU:HD23  | 2.20                     | 0.41              |
| 1:A:281:HIS:ND1   | 1:A:281:HIS:N     | 2.68                     | 0.41              |
| 1:A:316:GLN:CD    | 1:A:316:GLN:N     | 2.71                     | 0.41              |
| 1:A:475:ILE:CD1   | 1:A:513:TRP:HZ2   | 2.33                     | 0.41              |
| 1:A:596:PRO:HB2   | 1:A:597:ASN:H     | 1.69                     | 0.41              |
| 1:A:657:THR:CG2   | 2:B:1786:TYR:OH   | 2.68                     | 0.41              |
| 2:B:1859:HIS:HD2  | 2:B:1862:THR:HG21 | 1.86                     | 0.41              |
| 2:B:2130:VAL:O    | 2:B:2130:VAL:HG22 | 2.19                     | 0.41              |
| 2:B:2141:ASN:N    | 2:B:2142:PRO:C    | 2.78                     | 0.41              |
| 2:B:2163:ARG:O    | 2:B:2164:MET:HB3  | 2.20                     | 0.41              |
| 2:B:2208:ALA:H    | 2:B:2209:ARG:HD2  | 1.85                     | 0.41              |
| 2:B:2330:ASP:CG   | 2:B:2331:LEU:H    | 2.16                     | 0.41              |
| 1:A:658:PHE:CE1   | 1:A:686:GLY:CA    | 2.99                     | 0.41              |
| 2:B:1726:SER:O    | 2:B:1727:VAL:CG2  | 2.66                     | 0.41              |
| 2:B:1740:ASP:CA   | 2:B:1776:ARG:HH22 | 2.27                     | 0.41              |
| 2:B:1956:ILE:O    | 2:B:1975:LEU:HD23 | 2.20                     | 0.41              |
| 2:B:2080:ILE:O    | 2:B:2168:GLY:HA3  | 2.21                     | 0.41              |
| 2:B:2194:SER:HB3  | 2:B:2222:GLN:CB   | 2.50                     | 0.41              |
| 3:C:1:NAG:O6      | 3:C:2:NAG:N2      | 2.54                     | 0.41              |
| 1:A:72:LEU:HD12   | 1:A:198:LEU:HD12  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:90:ASN:HD21  | 1:A:92:ALA:HB3    | 1.85                     | 0.41              |
| 1:A:114:TYR:H    | 1:A:114:TYR:HD2   | 1.68                     | 0.41              |
| 1:A:232:HIS:C    | 1:A:233:THR:CG2   | 2.93                     | 0.41              |
| 1:A:239:ASN:C    | 1:A:241:SER:H     | 2.29                     | 0.41              |
| 1:A:269:ILE:HG23 | 1:A:286:LEU:HB2   | 2.02                     | 0.41              |
| 1:A:383:VAL:HG12 | 1:A:384:HIS:N     | 2.36                     | 0.41              |
| 1:A:385:TYR:CG   | 1:A:436:PHE:O     | 2.73                     | 0.41              |
| 1:A:588:THR:O    | 1:A:591:ILE:HG22  | 2.20                     | 0.41              |
| 1:A:621:VAL:HG13 | 1:A:703:THR:CB    | 2.50                     | 0.41              |
| 1:A:626:GLN:O    | 1:A:627:LEU:O     | 2.39                     | 0.41              |
| 1:A:687:LEU:HD11 | 2:B:1795:ASP:HB2  | 2.03                     | 0.41              |
| 2:B:1771:ILE:CD1 | 2:B:1817:TRP:HE1  | 2.28                     | 0.41              |
| 2:B:1780:SER:HB2 | 2:B:1781:ARG:H    | 1.60                     | 0.41              |
| 2:B:2033:ARG:C   | 2:B:2035:PHE:N    | 2.76                     | 0.41              |
| 2:B:2229:TRP:CD1 | 2:B:2229:TRP:N    | 2.88                     | 0.41              |
| 2:B:2301:LEU:CD2 | 2:B:2303:THR:HG23 | 2.51                     | 0.41              |
| 2:B:2314:VAL:O   | 2:B:2315:HIS:HB2  | 2.21                     | 0.41              |
| 1:A:33:ARG:HB3   | 1:A:34:VAL:H      | 1.55                     | 0.41              |
| 1:A:102:GLY:C    | 1:A:103:VAL:CG2   | 2.80                     | 0.41              |
| 2:B:1832:CYS:HA  | 2:B:1857:VAL:O    | 2.20                     | 0.41              |
| 2:B:1856:LEU:H   | 2:B:1856:LEU:CD2  | 2.26                     | 0.41              |
| 2:B:2013:LEU:N   | 2:B:2013:LEU:CD1  | 2.81                     | 0.41              |
| 2:B:2065:LYS:C   | 2:B:2067:PRO:CD   | 2.93                     | 0.41              |
| 2:B:2077:ALA:HB1 | 2:B:2078:PRO:CD   | 2.45                     | 0.41              |
| 2:B:2289:SER:C   | 2:B:2291:THR:H    | 2.29                     | 0.41              |
| 1:A:54:PHE:HE1   | 1:A:60:ASN:OD1    | 2.04                     | 0.40              |
| 1:A:72:LEU:HG    | 1:A:198:LEU:HD12  | 2.02                     | 0.40              |
| 1:A:232:HIS:HB2  | 1:A:318:ASP:O     | 2.21                     | 0.40              |
| 1:A:238:VAL:HG12 | 1:A:319:GLY:HA3   | 2.02                     | 0.40              |
| 1:A:408:LYS:HG3  | 1:A:622:PHE:CD2   | 2.56                     | 0.40              |
| 1:A:411:TYR:HE1  | 1:A:610:ALA:O     | 2.04                     | 0.40              |
| 1:A:533:TYR:CZ   | 1:A:549:GLY:HA3   | 2.56                     | 0.40              |
| 1:A:654:SER:HG   | 1:A:689:ILE:C     | 2.29                     | 0.40              |
| 2:B:1738:PHE:HB2 | 2:B:1746:PRO:CG   | 2.50                     | 0.40              |
| 2:B:1912:PHE:HB3 | 2:B:1915:ASN:ND2  | 2.36                     | 0.40              |
| 2:B:1957:HIS:O   | 2:B:1998:VAL:HG23 | 2.21                     | 0.40              |
| 2:B:1966:ARG:NH1 | 2:B:1966:ARG:HG3  | 2.35                     | 0.40              |
| 2:B:1979:TYR:O   | 2:B:1980:PRO:C    | 2.65                     | 0.40              |
| 2:B:1999:GLU:HB3 | 2:B:2010:MET:O    | 2.21                     | 0.40              |
| 2:B:2025:LEU:N   | 2:B:2025:LEU:HD23 | 2.36                     | 0.40              |
| 2:B:2134:GLY:C   | 2:B:2135:ILE:HG13 | 2.45                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:7:LEU:HD11    | 1:A:51:PHE:HD2    | 1.85                     | 0.40              |
| 1:A:249:HIS:CE1   | 1:A:302:ASP:O     | 2.75                     | 0.40              |
| 1:A:717:ASP:HB3   | 1:A:718:TYR:H     | 1.71                     | 0.40              |
| 2:B:1701:ALA:HA   | 2:B:1775:PHE:CD1  | 2.57                     | 0.40              |
| 2:B:2010:MET:O    | 2:B:2011:SER:HB3  | 2.21                     | 0.40              |
| 2:B:2065:LYS:O    | 2:B:2067:PRO:CD   | 2.69                     | 0.40              |
| 2:B:2321:MET:HB2  | 2:B:2321:MET:HE3  | 1.62                     | 0.40              |
| 1:A:83:THR:CG2    | 1:A:84:VAL:N      | 2.84                     | 0.40              |
| 1:A:186:LYS:HD2   | 1:A:186:LYS:HA    | 1.69                     | 0.40              |
| 1:A:387:ALA:HA    | 1:A:465:PHE:CD1   | 2.56                     | 0.40              |
| 1:A:553:ILE:C     | 1:A:554:CYS:SG    | 3.04                     | 0.40              |
| 1:A:593:ARG:NH1   | 1:A:594:PHE:CZ    | 2.86                     | 0.40              |
| 1:A:654:SER:OG    | 1:A:688:TRP:C     | 2.64                     | 0.40              |
| 2:B:1972:LYS:C    | 2:B:1973:MET:HG3  | 2.47                     | 0.40              |
| 2:B:2118:ASN:ND2  | 5:E:1:NAG:O7      | 2.54                     | 0.40              |
| 2:B:2149:ILE:HD12 | 2:B:2166:LEU:CD2  | 2.52                     | 0.40              |
| 2:B:2205:PRO:O    | 2:B:2207:LYS:N    | 2.54                     | 0.40              |
| 2:B:2329:GLN:CD   | 2:B:2329:GLN:C    | 2.89                     | 0.40              |
| 1:A:46:TYR:C      | 1:A:47:LYS:HD2    | 2.47                     | 0.40              |
| 1:A:110:GLU:O     | 1:A:112:ALA:N     | 2.55                     | 0.40              |
| 1:A:120:GLN:O     | 1:A:121:ARG:C     | 2.64                     | 0.40              |
| 1:A:304:GLY:N     | 1:A:326:VAL:CG1   | 2.84                     | 0.40              |
| 1:A:305:GLN:C     | 1:A:306:PHE:CD1   | 2.99                     | 0.40              |
| 1:A:467:ASN:O     | 1:A:468:GLN:HB2   | 2.21                     | 0.40              |
| 1:A:625:LEU:O     | 1:A:626:GLN:CG    | 2.61                     | 0.40              |
| 1:A:646:THR:C     | 1:A:647:ASP:O     | 2.63                     | 0.40              |
| 1:A:654:SER:OG    | 1:A:689:ILE:C     | 2.65                     | 0.40              |
| 2:B:1906:GLN:HB3  | 2:B:1910:PRO:CG   | 2.52                     | 0.40              |
| 2:B:1936:GLN:O    | 2:B:1937:ASP:HB2  | 2.21                     | 0.40              |
| 2:B:1951:GLU:C    | 2:B:1953:ILE:HD12 | 2.47                     | 0.40              |
| 2:B:1954:HIS:HB3  | 2:B:2000:CYS:HB2  | 2.04                     | 0.40              |
| 2:B:2060:ASN:HD22 | 2:B:2060:ASN:N    | 2.14                     | 0.40              |
| 2:B:2313:TRP:HB2  | 2:B:2314:VAL:H    | 1.61                     | 0.40              |
| 1:A:83:THR:CG2    | 1:A:139:GLN:HG2   | 2.52                     | 0.40              |
| 1:A:170:SER:OG    | 1:A:172:LEU:CD1   | 2.70                     | 0.40              |
| 1:A:402:PRO:O     | 1:A:403:ASP:C     | 2.64                     | 0.40              |
| 1:A:663:VAL:CA    | 2:B:1968:LYS:HE3  | 2.51                     | 0.40              |
| 2:B:1694:LYS:N    | 2:B:1694:LYS:CD   | 2.84                     | 0.40              |
| 2:B:1953:ILE:HG13 | 2:B:1980:PRO:CD   | 2.51                     | 0.40              |
| 2:B:2047:ALA:CB   | 2:B:2048:PRO:CD   | 2.94                     | 0.40              |
| 2:B:2256:TYR:O    | 2:B:2257:VAL:HG23 | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers  | Percentiles |   |
|-----|-------|-----------------|-----------|-----------|-----------|-------------|---|
| 1   | A     | 687/742 (93%)   | 312 (45%) | 180 (26%) | 195 (28%) | 0           | 0 |
| 2   | B     | 642/770 (83%)   | 316 (49%) | 172 (27%) | 154 (24%) | 0           | 0 |
| All | All   | 1329/1512 (88%) | 628 (47%) | 352 (26%) | 349 (26%) | 0           | 0 |

All (349) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ARG  |
| 1   | A     | 9   | ALA  |
| 1   | A     | 17  | MET  |
| 1   | A     | 19  | SER  |
| 1   | A     | 23  | GLU  |
| 1   | A     | 26  | VAL  |
| 1   | A     | 30  | PHE  |
| 1   | A     | 38  | PHE  |
| 1   | A     | 42  | THR  |
| 1   | A     | 58  | LEU  |
| 1   | A     | 60  | ASN  |
| 1   | A     | 61  | ILE  |
| 1   | A     | 62  | ALA  |
| 1   | A     | 63  | LYS  |
| 1   | A     | 66  | PRO  |
| 1   | A     | 67  | PRO  |
| 1   | A     | 69  | MET  |
| 1   | A     | 87  | THR  |
| 1   | A     | 96  | VAL  |
| 1   | A     | 103 | VAL  |
| 1   | A     | 106 | TRP  |
| 1   | A     | 115 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 122 | GLU  |
| 1   | A     | 127 | LYS  |
| 1   | A     | 148 | ALA  |
| 1   | A     | 153 | CYS  |
| 1   | A     | 165 | VAL  |
| 1   | A     | 181 | GLU  |
| 1   | A     | 182 | GLY  |
| 1   | A     | 190 | GLN  |
| 1   | A     | 204 | GLU  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 207 | SER  |
| 1   | A     | 209 | HIS  |
| 1   | A     | 224 | SER  |
| 1   | A     | 229 | PRO  |
| 1   | A     | 230 | LYS  |
| 1   | A     | 239 | ASN  |
| 1   | A     | 241 | SER  |
| 1   | A     | 285 | SER  |
| 1   | A     | 291 | ILE  |
| 1   | A     | 312 | ILE  |
| 1   | A     | 363 | ASP  |
| 1   | A     | 375 | ALA  |
| 1   | A     | 377 | LYS  |
| 1   | A     | 378 | HIS  |
| 1   | A     | 399 | VAL  |
| 1   | A     | 403 | ASP  |
| 1   | A     | 405 | ARG  |
| 1   | A     | 420 | GLY  |
| 1   | A     | 431 | TYR  |
| 1   | A     | 433 | ASP  |
| 1   | A     | 436 | PHE  |
| 1   | A     | 437 | LYS  |
| 1   | A     | 438 | THR  |
| 1   | A     | 439 | ARG  |
| 1   | A     | 447 | GLY  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 468 | GLN  |
| 1   | A     | 486 | LEU  |
| 1   | A     | 492 | PRO  |
| 1   | A     | 501 | PHE  |
| 1   | A     | 502 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 528  | CYS  |
| 1   | A     | 539  | MET  |
| 1   | A     | 543  | LEU  |
| 1   | A     | 562  | ARG  |
| 1   | A     | 596  | PRO  |
| 1   | A     | 607  | GLU  |
| 1   | A     | 618  | ASN  |
| 1   | A     | 621  | VAL  |
| 1   | A     | 622  | PHE  |
| 1   | A     | 627  | LEU  |
| 1   | A     | 633  | GLU  |
| 1   | A     | 646  | THR  |
| 1   | A     | 656  | TYR  |
| 1   | A     | 663  | VAL  |
| 1   | A     | 667  | THR  |
| 1   | A     | 674  | SER  |
| 1   | A     | 697  | PHE  |
| 1   | A     | 703  | THR  |
| 1   | A     | 704  | ALA  |
| 1   | A     | 717  | ASP  |
| 2   | B     | 1710 | GLY  |
| 2   | B     | 1720 | ASN  |
| 2   | B     | 1726 | SER  |
| 2   | B     | 1740 | ASP  |
| 2   | B     | 1742 | SER  |
| 2   | B     | 1743 | PHE  |
| 2   | B     | 1744 | THR  |
| 2   | B     | 1747 | LEU  |
| 2   | B     | 1751 | GLU  |
| 2   | B     | 1756 | LEU  |
| 2   | B     | 1759 | LEU  |
| 2   | B     | 1762 | TYR  |
| 2   | B     | 1765 | ALA  |
| 2   | B     | 1778 | GLN  |
| 2   | B     | 1780 | SER  |
| 2   | B     | 1791 | SER  |
| 2   | B     | 1794 | GLU  |
| 2   | B     | 1796 | GLN  |
| 2   | B     | 1805 | ASN  |
| 2   | B     | 1829 | GLU  |
| 2   | B     | 1831 | ASP  |
| 2   | B     | 1846 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1847 | VAL  |
| 2   | B     | 1871 | VAL  |
| 2   | B     | 1889 | TRP  |
| 2   | B     | 1890 | TYR  |
| 2   | B     | 1891 | PHE  |
| 2   | B     | 1899 | CYS  |
| 2   | B     | 1909 | ASP  |
| 2   | B     | 1911 | THR  |
| 2   | B     | 1913 | LYS  |
| 2   | B     | 1927 | ASP  |
| 2   | B     | 1930 | PRO  |
| 2   | B     | 1934 | MET  |
| 2   | B     | 1935 | ALA  |
| 2   | B     | 1945 | LEU  |
| 2   | B     | 1947 | MET  |
| 2   | B     | 1968 | LYS  |
| 2   | B     | 1982 | VAL  |
| 2   | B     | 1984 | GLU  |
| 2   | B     | 2008 | ALA  |
| 2   | B     | 2022 | GLN  |
| 2   | B     | 2031 | HIS  |
| 2   | B     | 2037 | ILE  |
| 2   | B     | 2038 | THR  |
| 2   | B     | 2049 | LYS  |
| 2   | B     | 2069 | SER  |
| 2   | B     | 2108 | ASP  |
| 2   | B     | 2120 | THR  |
| 2   | B     | 2130 | VAL  |
| 2   | B     | 2131 | ASP  |
| 2   | B     | 2135 | ILE  |
| 2   | B     | 2139 | ILE  |
| 2   | B     | 2141 | ASN  |
| 2   | B     | 2142 | PRO  |
| 2   | B     | 2146 | ALA  |
| 2   | B     | 2166 | LEU  |
| 2   | B     | 2171 | LEU  |
| 2   | B     | 2173 | SER  |
| 2   | B     | 2193 | SER  |
| 2   | B     | 2200 | PHE  |
| 2   | B     | 2211 | HIS  |
| 2   | B     | 2218 | ALA  |
| 2   | B     | 2224 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2251 | LEU  |
| 2   | B     | 2252 | LEU  |
| 2   | B     | 2264 | SER  |
| 2   | B     | 2267 | ASP  |
| 2   | B     | 2280 | VAL  |
| 2   | B     | 2286 | ASN  |
| 2   | B     | 2296 | SER  |
| 2   | B     | 2297 | LEU  |
| 2   | B     | 2327 | GLU  |
| 2   | B     | 2329 | GLN  |
| 1   | A     | 28   | ALA  |
| 1   | A     | 70   | GLY  |
| 1   | A     | 90   | ASN  |
| 1   | A     | 91   | MET  |
| 1   | A     | 100  | ALA  |
| 1   | A     | 101  | VAL  |
| 1   | A     | 110  | GLU  |
| 1   | A     | 111  | GLY  |
| 1   | A     | 117  | GLN  |
| 1   | A     | 131  | GLY  |
| 1   | A     | 162  | VAL  |
| 1   | A     | 169  | ASN  |
| 1   | A     | 211  | GLU  |
| 1   | A     | 260  | MET  |
| 1   | A     | 272  | GLU  |
| 1   | A     | 284  | ALA  |
| 1   | A     | 391  | GLU  |
| 1   | A     | 495  | VAL  |
| 1   | A     | 497  | HIS  |
| 1   | A     | 499  | LYS  |
| 1   | A     | 500  | ASP  |
| 1   | A     | 540  | GLU  |
| 1   | A     | 557  | GLU  |
| 1   | A     | 569  | ASP  |
| 1   | A     | 592  | GLN  |
| 1   | A     | 598  | PRO  |
| 1   | A     | 601  | VAL  |
| 1   | A     | 620  | TYR  |
| 1   | A     | 626  | GLN  |
| 1   | A     | 647  | ASP  |
| 1   | A     | 658  | PHE  |
| 1   | A     | 670  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 700  | ARG  |
| 2   | B     | 1738 | PHE  |
| 2   | B     | 1809 | PRO  |
| 2   | B     | 1822 | HIS  |
| 2   | B     | 1861 | ASN  |
| 2   | B     | 1886 | THR  |
| 2   | B     | 1931 | GLY  |
| 2   | B     | 1952 | ASN  |
| 2   | B     | 1959 | SER  |
| 2   | B     | 1983 | PHE  |
| 2   | B     | 2003 | GLY  |
| 2   | B     | 2021 | CYS  |
| 2   | B     | 2030 | GLY  |
| 2   | B     | 2040 | SER  |
| 2   | B     | 2045 | GLN  |
| 2   | B     | 2052 | ARG  |
| 2   | B     | 2075 | LEU  |
| 2   | B     | 2093 | PHE  |
| 2   | B     | 2136 | LYS  |
| 2   | B     | 2180 | MET  |
| 2   | B     | 2210 | LEU  |
| 2   | B     | 2228 | GLU  |
| 2   | B     | 2233 | ASP  |
| 2   | B     | 2234 | PHE  |
| 2   | B     | 2235 | GLN  |
| 2   | B     | 2299 | PRO  |
| 1   | A     | 20   | ASP  |
| 1   | A     | 32   | PRO  |
| 1   | A     | 33   | ARG  |
| 1   | A     | 51   | PHE  |
| 1   | A     | 56   | ASP  |
| 1   | A     | 81   | TYR  |
| 1   | A     | 82   | ASP  |
| 1   | A     | 118  | THR  |
| 1   | A     | 163  | ASP  |
| 1   | A     | 235  | ASN  |
| 1   | A     | 290  | PRO  |
| 1   | A     | 362  | ASP  |
| 1   | A     | 408  | LYS  |
| 1   | A     | 421  | ARG  |
| 1   | A     | 441  | ALA  |
| 1   | A     | 464  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 521  | PRO  |
| 1   | A     | 552  | LEU  |
| 1   | A     | 585  | TRP  |
| 1   | A     | 624  | SER  |
| 1   | A     | 642  | ILE  |
| 1   | A     | 706  | LEU  |
| 1   | A     | 711  | CYS  |
| 2   | B     | 1709 | TYR  |
| 2   | B     | 1722 | ALA  |
| 2   | B     | 1766 | GLU  |
| 2   | B     | 1769 | ASP  |
| 2   | B     | 1779 | ALA  |
| 2   | B     | 1801 | GLU  |
| 2   | B     | 1881 | THR  |
| 2   | B     | 1888 | SER  |
| 2   | B     | 1897 | ARG  |
| 2   | B     | 1914 | GLU  |
| 2   | B     | 1963 | PHE  |
| 2   | B     | 2010 | MET  |
| 2   | B     | 2019 | ASN  |
| 2   | B     | 2051 | ALA  |
| 2   | B     | 2057 | GLY  |
| 2   | B     | 2061 | ALA  |
| 2   | B     | 2202 | THR  |
| 2   | B     | 2279 | LYS  |
| 2   | B     | 2313 | TRP  |
| 2   | B     | 2314 | VAL  |
| 2   | B     | 2331 | LEU  |
| 1   | A     | 71   | LEU  |
| 1   | A     | 145  | GLY  |
| 1   | A     | 166  | LYS  |
| 1   | A     | 173  | ILE  |
| 1   | A     | 205  | GLY  |
| 1   | A     | 242  | LEU  |
| 1   | A     | 261  | GLY  |
| 1   | A     | 302  | ASP  |
| 1   | A     | 396  | ALA  |
| 1   | A     | 446  | SER  |
| 1   | A     | 451  | PRO  |
| 1   | A     | 522  | THR  |
| 1   | A     | 534  | SER  |
| 1   | A     | 603  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 614  | MET  |
| 1   | A     | 616  | SER  |
| 1   | A     | 680  | MET  |
| 1   | A     | 723  | TYR  |
| 2   | B     | 1739 | THR  |
| 2   | B     | 1746 | PRO  |
| 2   | B     | 1781 | ARG  |
| 2   | B     | 1782 | PRO  |
| 2   | B     | 1866 | ALA  |
| 2   | B     | 1867 | HIS  |
| 2   | B     | 1870 | GLN  |
| 2   | B     | 1936 | GLN  |
| 2   | B     | 1949 | SER  |
| 2   | B     | 1967 | LYS  |
| 2   | B     | 2001 | LEU  |
| 2   | B     | 2066 | GLU  |
| 2   | B     | 2106 | SER  |
| 2   | B     | 2253 | THR  |
| 1   | A     | 40   | PHE  |
| 1   | A     | 54   | PHE  |
| 1   | A     | 120  | GLN  |
| 1   | A     | 168  | LEU  |
| 1   | A     | 212  | THR  |
| 1   | A     | 238  | VAL  |
| 1   | A     | 263  | THR  |
| 1   | A     | 264  | PRO  |
| 1   | A     | 372  | ARG  |
| 1   | A     | 374  | VAL  |
| 1   | A     | 401  | ALA  |
| 1   | A     | 402  | PRO  |
| 1   | A     | 404  | ASP  |
| 1   | A     | 454  | TYR  |
| 1   | A     | 479  | GLY  |
| 1   | A     | 544  | ALA  |
| 1   | A     | 546  | GLY  |
| 1   | A     | 609  | GLN  |
| 1   | A     | 683  | GLU  |
| 2   | B     | 1694 | LYS  |
| 2   | B     | 1717 | VAL  |
| 2   | B     | 2007 | HIS  |
| 2   | B     | 2161 | THR  |
| 2   | B     | 2205 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2277 | ASN  |
| 2   | B     | 2323 | VAL  |
| 1   | A     | 36   | LYS  |
| 1   | A     | 109  | SER  |
| 1   | A     | 269  | ILE  |
| 1   | A     | 287  | GLU  |
| 1   | A     | 397  | PRO  |
| 1   | A     | 445  | GLU  |
| 1   | A     | 485  | PRO  |
| 1   | A     | 542  | ASP  |
| 1   | A     | 668  | LEU  |
| 2   | B     | 1790 | ILE  |
| 2   | B     | 1854 | PRO  |
| 2   | B     | 1864 | ASN  |
| 2   | B     | 1926 | MET  |
| 2   | B     | 2246 | GLN  |
| 1   | A     | 10   | VAL  |
| 1   | A     | 689  | ILE  |
| 2   | B     | 2292 | PRO  |
| 1   | A     | 619  | GLY  |
| 1   | A     | 651  | VAL  |
| 2   | B     | 1901 | ALA  |
| 2   | B     | 2158 | ILE  |
| 2   | B     | 2248 | VAL  |
| 1   | A     | 52   | VAL  |
| 1   | A     | 258  | ILE  |
| 1   | A     | 273  | GLY  |
| 2   | B     | 1757 | GLY  |
| 2   | B     | 1962 | VAL  |
| 2   | B     | 2048 | PRO  |
| 1   | A     | 371  | ILE  |
| 1   | A     | 475  | ILE  |
| 2   | B     | 2002 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric | Outliers  | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|-------------|----|
| 1   | A     | 616/662 (93%)   | 510 (83%) | 106 (17%) | 2           | 13 |
| 2   | B     | 572/688 (83%)   | 476 (83%) | 96 (17%)  | 2           | 13 |
| All | All   | 1188/1350 (88%) | 986 (83%) | 202 (17%) | 2           | 13 |

All (202) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | TRP  |
| 1   | A     | 38  | PHE  |
| 1   | A     | 50  | LEU  |
| 1   | A     | 51  | PHE  |
| 1   | A     | 58  | LEU  |
| 1   | A     | 66  | PRO  |
| 1   | A     | 67  | PRO  |
| 1   | A     | 88  | LEU  |
| 1   | A     | 89  | LYS  |
| 1   | A     | 98  | LEU  |
| 1   | A     | 103 | VAL  |
| 1   | A     | 106 | TRP  |
| 1   | A     | 107 | LYS  |
| 1   | A     | 113 | GLU  |
| 1   | A     | 114 | TYR  |
| 1   | A     | 120 | GLN  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 164 | LEU  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 179 | CYS  |
| 1   | A     | 191 | THR  |
| 1   | A     | 209 | HIS  |
| 1   | A     | 211 | GLU  |
| 1   | A     | 226 | ARG  |
| 1   | A     | 229 | PRO  |
| 1   | A     | 233 | THR  |
| 1   | A     | 238 | VAL  |
| 1   | A     | 246 | ILE  |
| 1   | A     | 250 | ARG  |
| 1   | A     | 255 | TRP  |
| 1   | A     | 260 | MET  |
| 1   | A     | 269 | ILE  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 288 | ILE  |
| 1   | A     | 291 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 292 | THR  |
| 1   | A     | 295 | THR  |
| 1   | A     | 299 | LEU  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 306 | PHE  |
| 1   | A     | 307 | LEU  |
| 1   | A     | 308 | LEU  |
| 1   | A     | 309 | PHE  |
| 1   | A     | 312 | ILE  |
| 1   | A     | 324 | VAL  |
| 1   | A     | 386 | ILE  |
| 1   | A     | 392 | ASP  |
| 1   | A     | 394 | ASP  |
| 1   | A     | 400 | LEU  |
| 1   | A     | 404 | ASP  |
| 1   | A     | 432 | THR  |
| 1   | A     | 434 | GLU  |
| 1   | A     | 440 | GLU  |
| 1   | A     | 442 | ILE  |
| 1   | A     | 448 | ILE  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 453 | LEU  |
| 1   | A     | 461 | LEU  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 475 | ILE  |
| 1   | A     | 483 | VAL  |
| 1   | A     | 486 | LEU  |
| 1   | A     | 492 | PRO  |
| 1   | A     | 502 | PRO  |
| 1   | A     | 503 | ILE  |
| 1   | A     | 504 | LEU  |
| 1   | A     | 508 | ILE  |
| 1   | A     | 521 | PRO  |
| 1   | A     | 529 | LEU  |
| 1   | A     | 531 | ARG  |
| 1   | A     | 532 | TYR  |
| 1   | A     | 538 | ASN  |
| 1   | A     | 540 | GLU  |
| 1   | A     | 543 | LEU  |
| 1   | A     | 550 | PRO  |
| 1   | A     | 586 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 590  | ASN  |
| 1   | A     | 603  | LEU  |
| 1   | A     | 614  | MET  |
| 1   | A     | 618  | ASN  |
| 1   | A     | 620  | TYR  |
| 1   | A     | 636  | TYR  |
| 1   | A     | 639  | ILE  |
| 1   | A     | 648  | PHE  |
| 1   | A     | 649  | LEU  |
| 1   | A     | 651  | VAL  |
| 1   | A     | 656  | TYR  |
| 1   | A     | 659  | LYS  |
| 1   | A     | 660  | HIS  |
| 1   | A     | 663  | VAL  |
| 1   | A     | 669  | THR  |
| 1   | A     | 671  | PHE  |
| 1   | A     | 682  | MET  |
| 1   | A     | 683  | GLU  |
| 1   | A     | 684  | ASN  |
| 1   | A     | 687  | LEU  |
| 1   | A     | 696  | ASP  |
| 1   | A     | 700  | ARG  |
| 1   | A     | 706  | LEU  |
| 1   | A     | 707  | LYS  |
| 1   | A     | 711  | CYS  |
| 1   | A     | 713  | LYS  |
| 1   | A     | 721  | ASP  |
| 1   | A     | 723  | TYR  |
| 1   | A     | 725  | ASP  |
| 2   | B     | 1689 | ARG  |
| 2   | B     | 1693 | LYS  |
| 2   | B     | 1697 | HIS  |
| 2   | B     | 1711 | MET  |
| 2   | B     | 1717 | VAL  |
| 2   | B     | 1720 | ASN  |
| 2   | B     | 1733 | VAL  |
| 2   | B     | 1737 | GLU  |
| 2   | B     | 1738 | PHE  |
| 2   | B     | 1746 | PRO  |
| 2   | B     | 1758 | LEU  |
| 2   | B     | 1763 | ILE  |
| 2   | B     | 1768 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1780 | SER  |
| 2   | B     | 1789 | LEU  |
| 2   | B     | 1795 | ASP  |
| 2   | B     | 1806 | PHE  |
| 2   | B     | 1812 | THR  |
| 2   | B     | 1820 | GLN  |
| 2   | B     | 1821 | HIS  |
| 2   | B     | 1822 | HIS  |
| 2   | B     | 1825 | PRO  |
| 2   | B     | 1830 | PHE  |
| 2   | B     | 1848 | HIS  |
| 2   | B     | 1852 | ILE  |
| 2   | B     | 1855 | LEU  |
| 2   | B     | 1857 | VAL  |
| 2   | B     | 1859 | HIS  |
| 2   | B     | 1861 | ASN  |
| 2   | B     | 1863 | LEU  |
| 2   | B     | 1878 | LEU  |
| 2   | B     | 1880 | PHE  |
| 2   | B     | 1886 | THR  |
| 2   | B     | 1890 | TYR  |
| 2   | B     | 1893 | GLU  |
| 2   | B     | 1894 | ASN  |
| 2   | B     | 1904 | ASN  |
| 2   | B     | 1905 | ILE  |
| 2   | B     | 1908 | GLU  |
| 2   | B     | 1943 | TYR  |
| 2   | B     | 1947 | MET  |
| 2   | B     | 1950 | ASN  |
| 2   | B     | 1952 | ASN  |
| 2   | B     | 1953 | ILE  |
| 2   | B     | 1958 | PHE  |
| 2   | B     | 1964 | THR  |
| 2   | B     | 1977 | ASN  |
| 2   | B     | 1985 | THR  |
| 2   | B     | 1989 | LEU  |
| 2   | B     | 1995 | ILE  |
| 2   | B     | 1999 | GLU  |
| 2   | B     | 2001 | LEU  |
| 2   | B     | 2013 | LEU  |
| 2   | B     | 2014 | PHE  |
| 2   | B     | 2036 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2038 | THR  |
| 2   | B     | 2045 | GLN  |
| 2   | B     | 2052 | ARG  |
| 2   | B     | 2053 | LEU  |
| 2   | B     | 2060 | ASN  |
| 2   | B     | 2066 | GLU  |
| 2   | B     | 2098 | ILE  |
| 2   | B     | 2101 | PHE  |
| 2   | B     | 2112 | TRP  |
| 2   | B     | 2116 | ARG  |
| 2   | B     | 2123 | LEU  |
| 2   | B     | 2129 | ASN  |
| 2   | B     | 2139 | ILE  |
| 2   | B     | 2145 | ILE  |
| 2   | B     | 2154 | THR  |
| 2   | B     | 2161 | THR  |
| 2   | B     | 2162 | LEU  |
| 2   | B     | 2170 | ASP  |
| 2   | B     | 2191 | THR  |
| 2   | B     | 2194 | SER  |
| 2   | B     | 2205 | PRO  |
| 2   | B     | 2212 | LEU  |
| 2   | B     | 2220 | ARG  |
| 2   | B     | 2224 | ASN  |
| 2   | B     | 2225 | ASN  |
| 2   | B     | 2232 | VAL  |
| 2   | B     | 2245 | THR  |
| 2   | B     | 2251 | LEU  |
| 2   | B     | 2252 | LEU  |
| 2   | B     | 2256 | TYR  |
| 2   | B     | 2276 | GLN  |
| 2   | B     | 2279 | LYS  |
| 2   | B     | 2284 | GLN  |
| 2   | B     | 2290 | PHE  |
| 2   | B     | 2292 | PRO  |
| 2   | B     | 2298 | ASP  |
| 2   | B     | 2302 | LEU  |
| 2   | B     | 2309 | HIS  |
| 2   | B     | 2313 | TRP  |
| 2   | B     | 2321 | MET  |
| 2   | B     | 2323 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54)

such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 18   | GLN  |
| 1   | A     | 60   | ASN  |
| 1   | A     | 90   | ASN  |
| 1   | A     | 134  | HIS  |
| 1   | A     | 169  | ASN  |
| 1   | A     | 193  | HIS  |
| 1   | A     | 214  | ASN  |
| 1   | A     | 232  | HIS  |
| 1   | A     | 249  | HIS  |
| 1   | A     | 280  | ASN  |
| 1   | A     | 283  | GLN  |
| 1   | A     | 305  | GLN  |
| 1   | A     | 317  | HIS  |
| 1   | A     | 410  | GLN  |
| 1   | A     | 467  | ASN  |
| 1   | A     | 474  | ASN  |
| 1   | A     | 565  | GLN  |
| 1   | A     | 592  | GLN  |
| 1   | A     | 660  | HIS  |
| 1   | A     | 684  | ASN  |
| 1   | A     | 693  | HIS  |
| 1   | A     | 694  | ASN  |
| 1   | A     | 699  | ASN  |
| 2   | B     | 1692 | GLN  |
| 2   | B     | 1723 | GLN  |
| 2   | B     | 1736 | GLN  |
| 2   | B     | 1753 | ASN  |
| 2   | B     | 1777 | ASN  |
| 2   | B     | 1778 | GLN  |
| 2   | B     | 1805 | ASN  |
| 2   | B     | 1820 | GLN  |
| 2   | B     | 1848 | HIS  |
| 2   | B     | 1859 | HIS  |
| 2   | B     | 1861 | ASN  |
| 2   | B     | 1864 | ASN  |
| 2   | B     | 1904 | ASN  |
| 2   | B     | 1906 | GLN  |
| 2   | B     | 1915 | ASN  |
| 2   | B     | 1961 | HIS  |
| 2   | B     | 2045 | GLN  |
| 2   | B     | 2054 | HIS  |
| 2   | B     | 2060 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2087 | GLN  |
| 2   | B     | 2100 | GLN  |
| 2   | B     | 2172 | ASN  |
| 2   | B     | 2222 | GLN  |
| 2   | B     | 2224 | ASN  |
| 2   | B     | 2225 | ASN  |
| 2   | B     | 2231 | GLN  |
| 2   | B     | 2284 | GLN  |
| 2   | B     | 2295 | ASN  |
| 2   | B     | 2311 | GLN  |
| 2   | B     | 2316 | GLN  |
| 2   | B     | 2329 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

13 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 3   | NAG  | C     | 1   | 1,3  | 14,14,15     | 0.87 | 1 (7%)      | 17,19,21    | 0.89 | 1 (5%)      |
| 3   | NAG  | C     | 2   | 3    | 14,14,15     | 0.70 | 0           | 17,19,21    | 0.79 | 1 (5%)      |
| 3   | BMA  | C     | 3   | 3    | 11,11,12     | 0.76 | 0           | 15,15,17    | 0.63 | 0           |
| 3   | MAN  | C     | 4   | 3    | 11,11,12     | 0.52 | 0           | 15,15,17    | 0.86 | 1 (6%)      |
| 4   | NAG  | D     | 1   | 4,2  | 14,14,15     | 0.70 | 0           | 17,19,21    | 0.54 | 0           |
| 4   | NAG  | D     | 2   | 4    | 14,14,15     | 0.75 | 0           | 17,19,21    | 0.54 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | NAG  | E     | 1   | 2,5  | 14,14,15     | 0.71 | 0        | 17,19,21    | 1.26 | 3 (17%)  |
| 5   | NAG  | E     | 2   | 5    | 14,14,15     | 0.55 | 0        | 17,19,21    | 0.88 | 1 (5%)   |
| 5   | BMA  | E     | 3   | 5    | 11,11,12     | 1.50 | 3 (27%)  | 15,15,17    | 0.91 | 0        |
| 5   | BMA  | E     | 4   | 5    | 11,11,12     | 1.03 | 1 (9%)   | 15,15,17    | 1.32 | 2 (13%)  |
| 5   | MAN  | E     | 5   | 5    | 11,11,12     | 0.64 | 0        | 15,15,17    | 0.80 | 1 (6%)   |
| 5   | MAN  | E     | 6   | 5    | 11,11,12     | 1.32 | 2 (18%)  | 15,15,17    | 0.74 | 0        |
| 5   | MAN  | E     | 7   | 5    | 11,11,12     | 1.74 | 1 (9%)   | 15,15,17    | 0.85 | 1 (6%)   |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | C     | 1   | 1,3  | -       | 5/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | C     | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | MAN  | C     | 4   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | NAG  | D     | 1   | 4,2  | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | D     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | E     | 1   | 2,5  | -       | 5/6/23/26 | 0/1/1/1 |
| 5   | NAG  | E     | 2   | 5    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | BMA  | E     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | BMA  | E     | 4   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | E     | 5   | 5    | -       | 1/2/19/22 | 0/1/1/1 |
| 5   | MAN  | E     | 6   | 5    | -       | 1/2/19/22 | 0/1/1/1 |
| 5   | MAN  | E     | 7   | 5    | -       | 2/2/19/22 | 0/1/1/1 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 5   | E     | 7   | MAN  | C2-C3 | 4.37 | 1.59        | 1.52     |
| 3   | C     | 1   | NAG  | C1-C2 | 2.57 | 1.55        | 1.52     |
| 5   | E     | 4   | BMA  | C1-C2 | 2.50 | 1.58        | 1.52     |
| 5   | E     | 6   | MAN  | C2-C3 | 2.40 | 1.56        | 1.52     |
| 5   | E     | 6   | MAN  | C4-C5 | 2.33 | 1.58        | 1.53     |
| 5   | E     | 3   | BMA  | C2-C3 | 2.23 | 1.55        | 1.52     |
| 5   | E     | 3   | BMA  | C4-C3 | 2.05 | 1.57        | 1.52     |
| 5   | E     | 3   | BMA  | C4-C5 | 2.04 | 1.57        | 1.53     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | E     | 4   | BMA  | C1-O5-C5 | 3.97  | 117.51      | 112.19   |
| 5   | E     | 1   | NAG  | C2-N2-C7 | -2.79 | 119.17      | 122.90   |
| 5   | E     | 2   | NAG  | C2-N2-C7 | -2.43 | 119.64      | 122.90   |
| 5   | E     | 1   | NAG  | C4-C3-C2 | 2.31  | 114.41      | 111.02   |
| 5   | E     | 1   | NAG  | C3-C4-C5 | 2.28  | 114.38      | 110.23   |
| 3   | C     | 4   | MAN  | C1-O5-C5 | 2.26  | 115.22      | 112.19   |
| 5   | E     | 7   | MAN  | C1-O5-C5 | 2.26  | 115.21      | 112.19   |
| 3   | C     | 2   | NAG  | C2-N2-C7 | -2.18 | 119.97      | 122.90   |
| 5   | E     | 4   | BMA  | C1-C2-C3 | 2.10  | 112.70      | 109.64   |
| 5   | E     | 5   | MAN  | C1-C2-C3 | 2.08  | 112.67      | 109.64   |
| 3   | C     | 1   | NAG  | C2-N2-C7 | -2.00 | 120.22      | 122.90   |

There are no chirality outliers.

All (35) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | C     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | C     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | C     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | C     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | C     | 2   | NAG  | O7-C7-N2-C2 |
| 4   | D     | 1   | NAG  | C8-C7-N2-C2 |
| 4   | D     | 1   | NAG  | O7-C7-N2-C2 |
| 4   | D     | 2   | NAG  | C8-C7-N2-C2 |
| 4   | D     | 2   | NAG  | O7-C7-N2-C2 |
| 5   | E     | 1   | NAG  | C1-C2-N2-C7 |
| 5   | E     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | E     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | E     | 2   | NAG  | C8-C7-N2-C2 |
| 5   | E     | 2   | NAG  | O7-C7-N2-C2 |
| 5   | E     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | E     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | E     | 7   | MAN  | O5-C5-C6-O6 |
| 5   | E     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | C     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | C     | 4   | MAN  | O5-C5-C6-O6 |
| 5   | E     | 7   | MAN  | C4-C5-C6-O6 |
| 5   | E     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | E     | 4   | BMA  | C4-C5-C6-O6 |
| 5   | E     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | E     | 4   | BMA  | O5-C5-C6-O6 |

*Continued on next page...*

*Continued from previous page...*

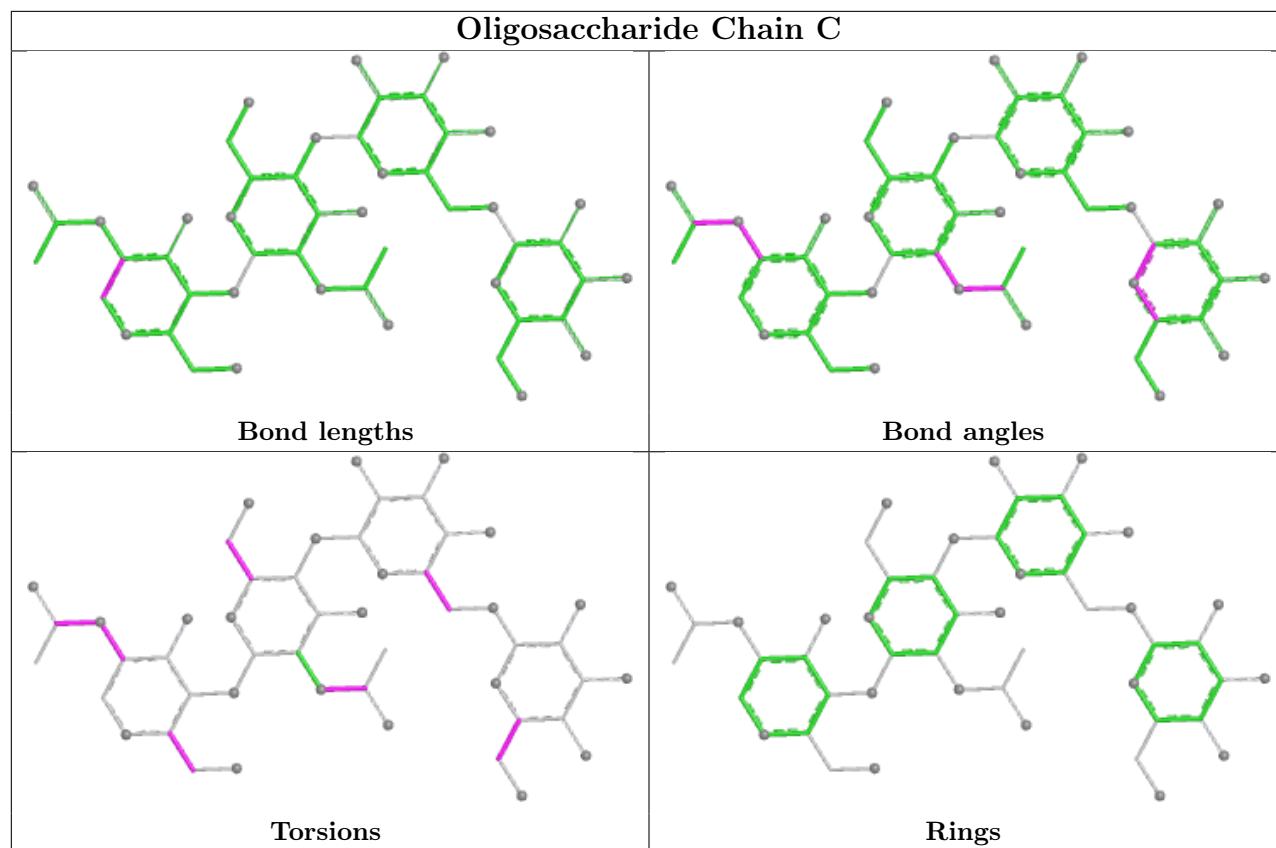
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | C     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | C     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | D     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1   | NAG  | C3-C2-N2-C7 |
| 5   | E     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | C     | 3   | BMA  | C4-C5-C6-O6 |
| 4   | D     | 1   | NAG  | C3-C2-N2-C7 |
| 4   | D     | 1   | NAG  | C1-C2-N2-C7 |
| 5   | E     | 5   | MAN  | O5-C5-C6-O6 |
| 5   | E     | 6   | MAN  | O5-C5-C6-O6 |

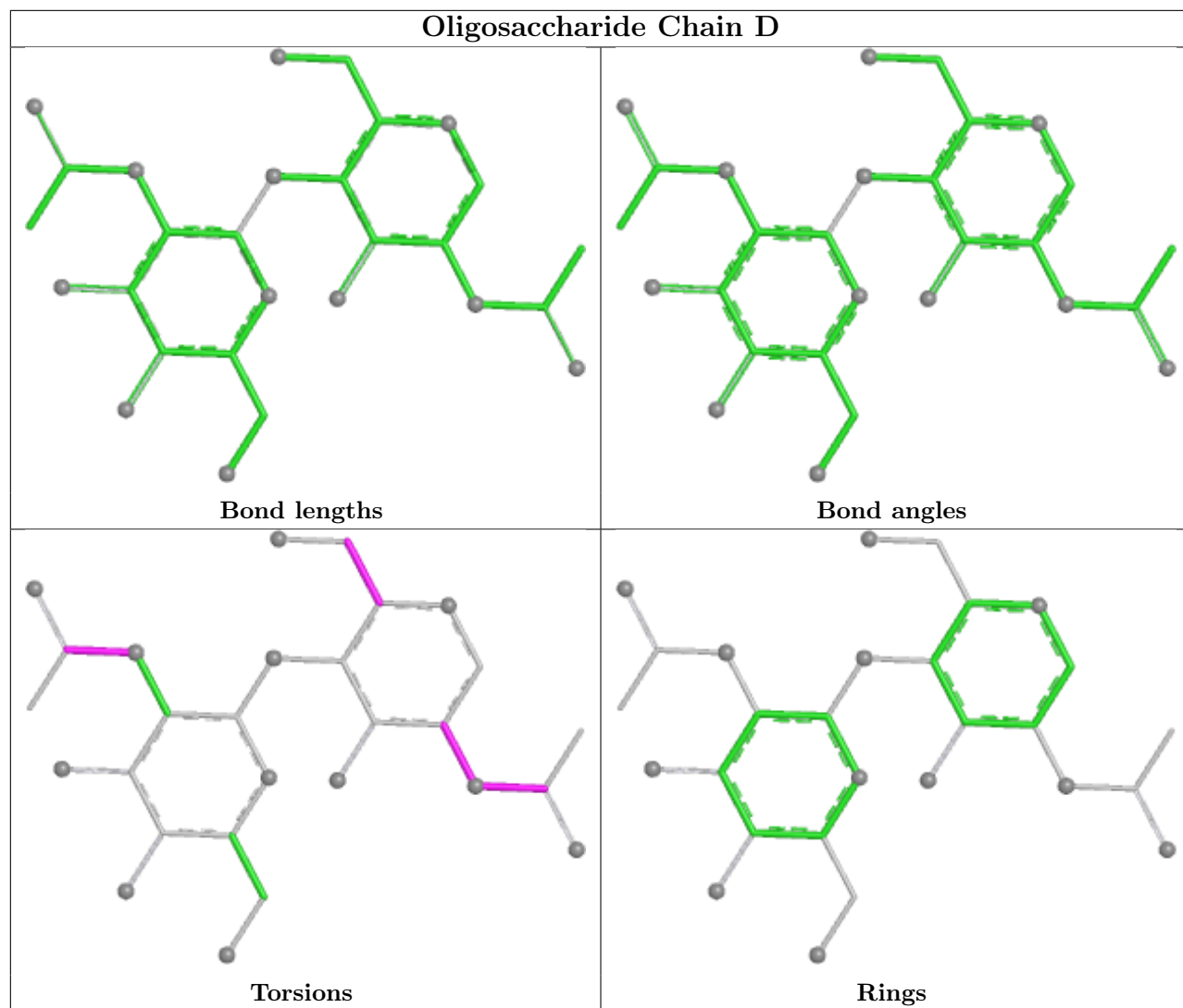
There are no ring outliers.

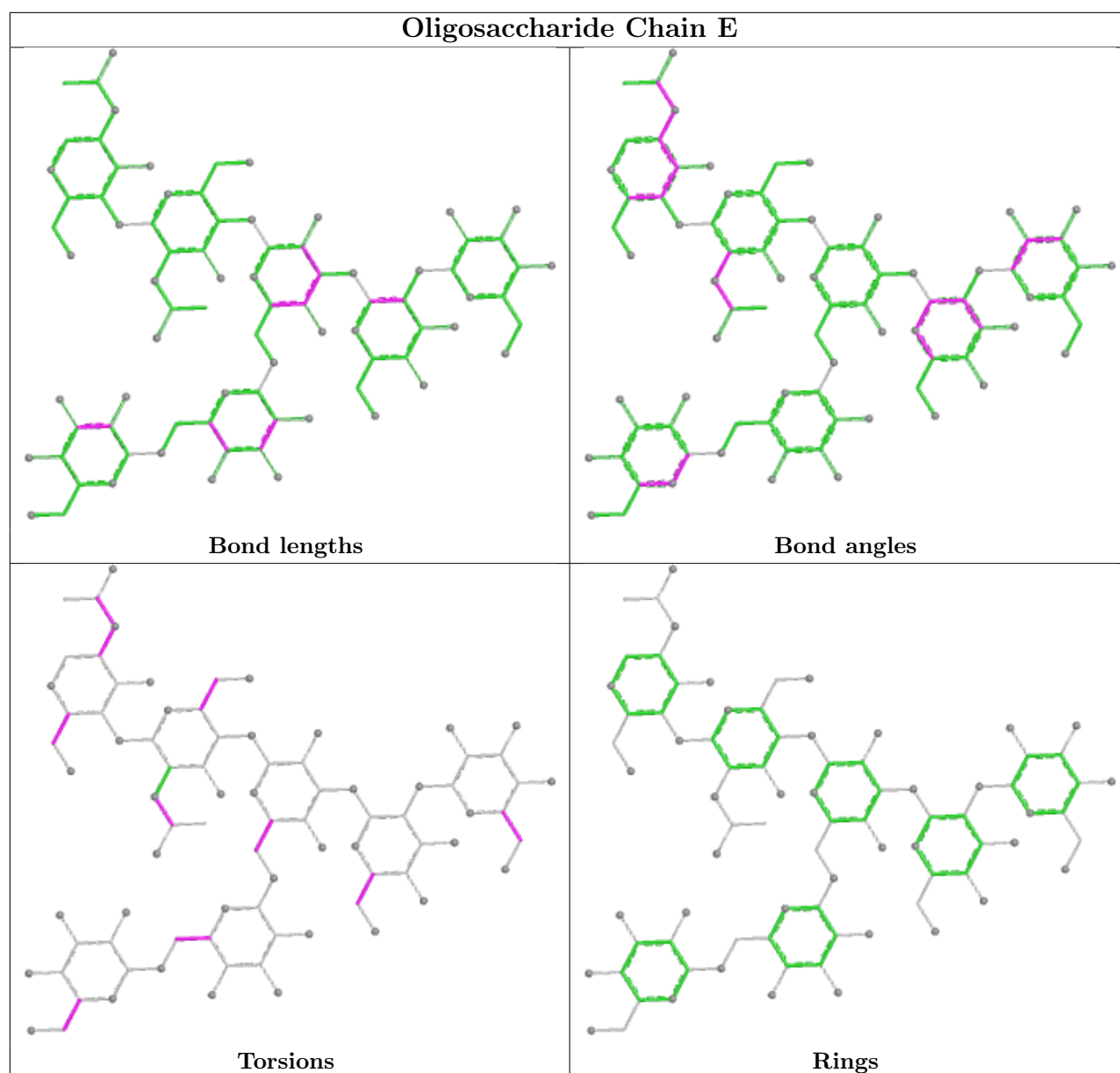
7 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 1   | NAG  | 3       | 0            |
| 5   | E     | 4   | BMA  | 1       | 0            |
| 5   | E     | 1   | NAG  | 2       | 0            |
| 5   | E     | 5   | MAN  | 1       | 0            |
| 3   | C     | 2   | NAG  | 2       | 0            |
| 5   | E     | 2   | NAG  | 1       | 0            |
| 5   | E     | 3   | BMA  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 693/742 (93%)   | 0.07   | 13 (1%) 66 42 | 75, 170, 206, 206     | 0     |
| 2   | B     | 644/770 (83%)   | -0.09  | 6 (0%) 81 58  | 89, 169, 206, 206     | 0     |
| All | All   | 1337/1512 (88%) | -0.01  | 19 (1%) 73 48 | 75, 170, 206, 206     | 0     |

All (19) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 225  | ALA  | 3.9  |
| 2   | B     | 2252 | LEU  | 3.5  |
| 1   | A     | 139  | GLN  | 3.1  |
| 1   | A     | 725  | ASP  | 3.0  |
| 1   | A     | 37   | SER  | 2.7  |
| 2   | B     | 1852 | ILE  | 2.6  |
| 1   | A     | 539  | MET  | 2.6  |
| 1   | A     | 526  | PRO  | 2.5  |
| 1   | A     | 678  | VAL  | 2.5  |
| 1   | A     | 137  | VAL  | 2.5  |
| 2   | B     | 1887 | LYS  | 2.4  |
| 1   | A     | 138  | TRP  | 2.4  |
| 2   | B     | 1796 | GLN  | 2.3  |
| 1   | A     | 324  | VAL  | 2.2  |
| 2   | B     | 2015 | LEU  | 2.2  |
| 2   | B     | 1798 | GLN  | 2.1  |
| 1   | A     | 272  | GLU  | 2.1  |
| 1   | A     | 391  | GLU  | 2.1  |
| 1   | A     | 255  | TRP  | 2.0  |

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

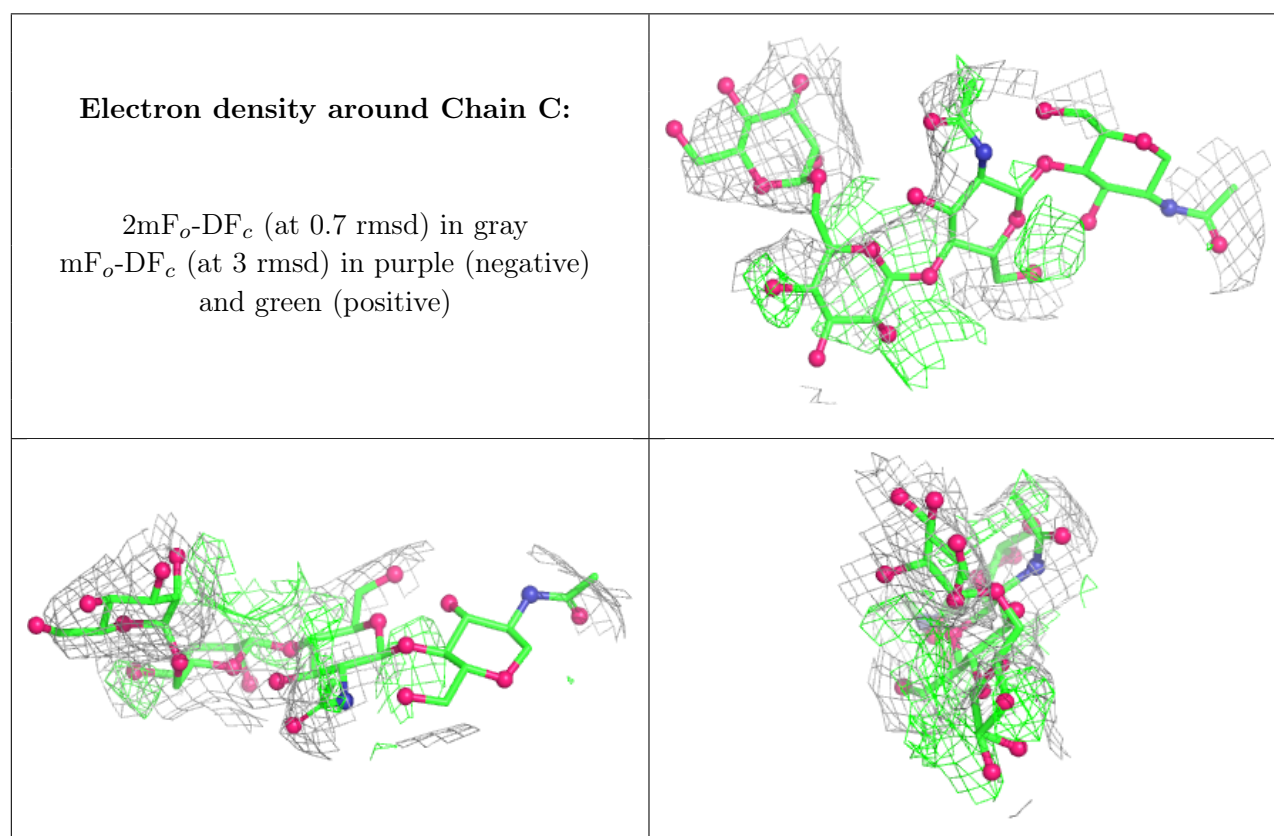
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

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

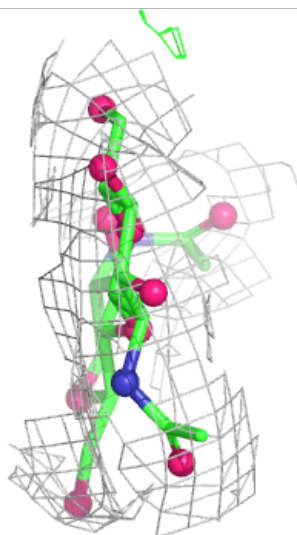
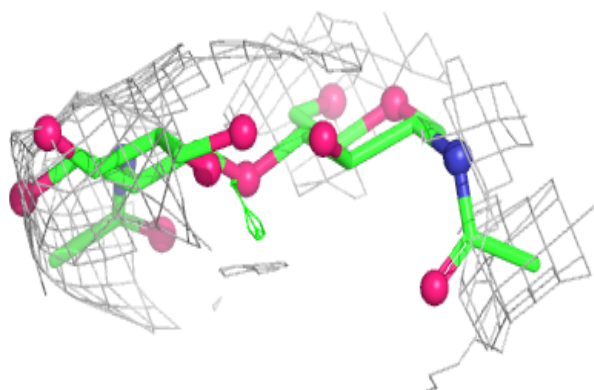
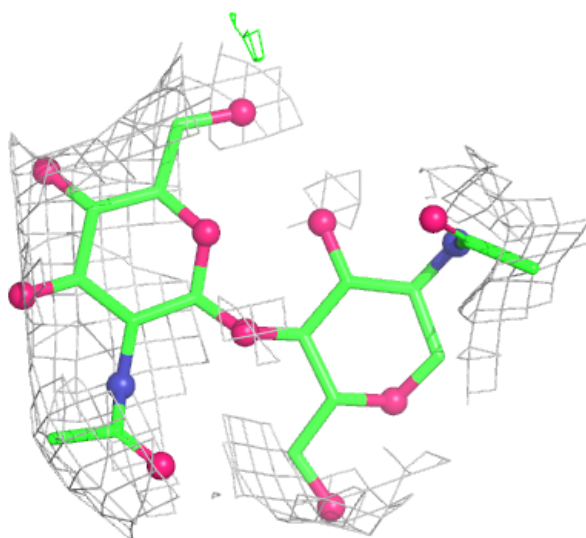
| Mol | Type | Chain | Res | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|-------|------|----------------------------|-------|
| 5   | BMA  | E     | 4   | 11/12 | -0.44 | 0.35 | 145,145,145,145            | 11    |
| 5   | MAN  | E     | 5   | 11/12 | 0.32  | 0.20 | 104,104,104,104            | 11    |
| 4   | NAG  | D     | 1   | 14/15 | 0.37  | 0.11 | 205,205,205,205            | 0     |
| 5   | BMA  | E     | 3   | 11/12 | 0.45  | 0.11 | 203,203,203,203            | 0     |
| 4   | NAG  | D     | 2   | 14/15 | 0.51  | 0.12 | 180,180,180,180            | 0     |
| 5   | MAN  | E     | 6   | 11/12 | 0.62  | 0.11 | 187,187,187,187            | 0     |
| 3   | MAN  | C     | 4   | 11/12 | 0.66  | 0.16 | 115,115,115,115            | 11    |
| 3   | BMA  | C     | 3   | 11/12 | 0.71  | 0.17 | 148,148,148,148            | 11    |
| 5   | NAG  | E     | 2   | 14/15 | 0.77  | 0.13 | 202,205,205,205            | 0     |
| 3   | NAG  | C     | 2   | 14/15 | 0.83  | 0.14 | 122,122,122,122            | 14    |
| 5   | MAN  | E     | 7   | 11/12 | 0.87  | 0.07 | 190,190,190,190            | 0     |
| 3   | NAG  | C     | 1   | 14/15 | 0.88  | 0.10 | 205,205,205,205            | 0     |
| 5   | NAG  | E     | 1   | 14/15 | 0.91  | 0.11 | 150,153,155,156            | 0     |

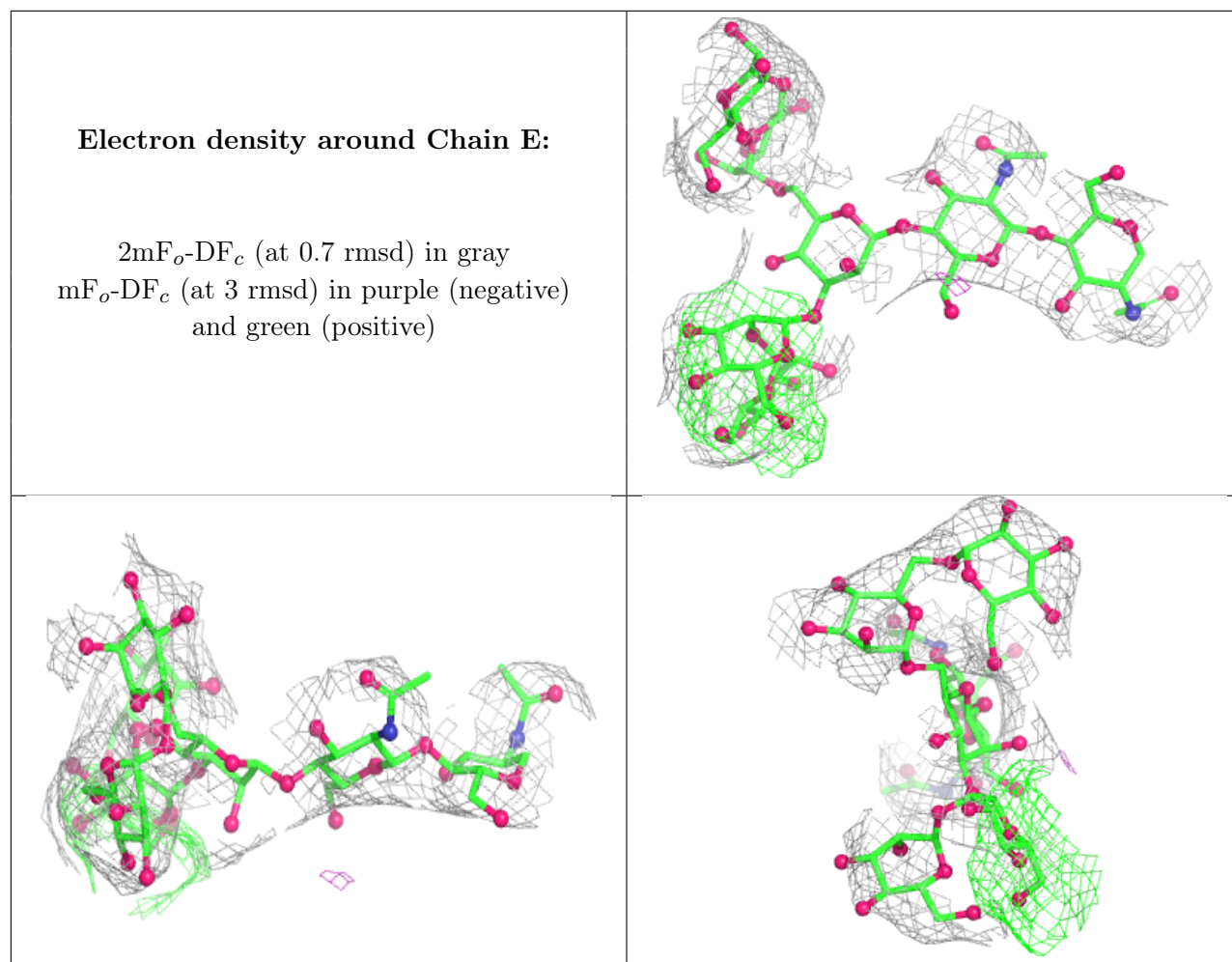
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain D:**

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





## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 6   | CA   | A     | 2400 | 1/1   | 0.42 | 0.30 | 341,341,341,341             | 0     |
| 6   | CA   | A     | 2402 | 1/1   | 0.87 | 0.08 | 352,352,352,352             | 0     |
| 6   | CA   | A     | 2401 | 1/1   | 0.87 | 0.16 | 275,275,275,275             | 0     |
| 7   | CU   | B     | 2404 | 1/1   | 0.98 | 0.08 | 349,349,349,349             | 0     |
| 7   | CU   | A     | 2403 | 1/1   | 0.99 | 0.07 | 359,359,359,359             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.