



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:42 am GMT

PDB ID : 4RUB  
Title : A CRYSTAL FORM OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE FROM NICOTIANA TABACUM IN THE ACTIVATED STATE  
Authors : Schreuder, H.; Cascio, D.; Curmi, P.M.G.; Eisenberg, D.  
Deposited on : 1990-05-25  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

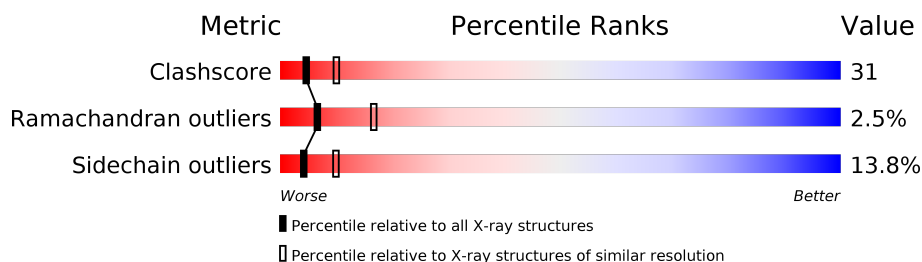
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 112137                      | 2590 (2.70-2.70)                                      |
| Ramachandran outliers | 110173                      | 2550 (2.70-2.70)                                      |
| Sidechain outliers    | 110143                      | 2550 (2.70-2.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 477    |                  |
| 1   | B     | 477    |                  |
| 1   | C     | 477    |                  |
| 1   | D     | 477    |                  |
| 2   | S     | 123    |                  |
| 2   | T     | 123    |                  |
| 2   | U     | 123    |                  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | V     | 123    | <div><div></div><div>27%</div><div>41%</div><div>25%</div><div>7%</div></div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18708 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 RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 3628  | 2307 | 641 | 664 | 16 |         |         |       |
| 1   | B     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 3628  | 2307 | 641 | 664 | 16 |         |         |       |
| 1   | C     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 3628  | 2307 | 641 | 664 | 16 |         |         |       |
| 1   | D     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 3628  | 2307 | 641 | 664 | 16 |         |         |       |

- Molecule 2 is a protein called RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | S     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1024  | 669 | 163 | 186 | 6 |         |         |       |
| 2   | T     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1024  | 669 | 163 | 186 | 6 |         |         |       |
| 2   | U     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1024  | 669 | 163 | 186 | 6 |         |         |       |
| 2   | V     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1024  | 669 | 163 | 186 | 6 |         |         |       |

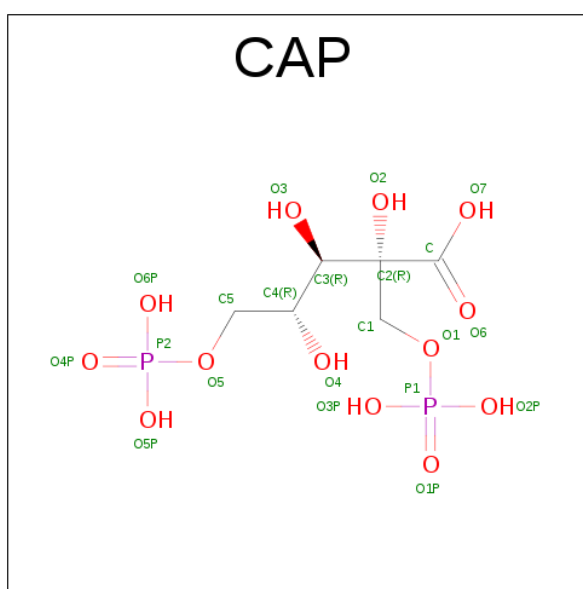
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| S     | 88      | GLY      | GLU    | CONFLICT | UNP P69249 |
| T     | 88      | GLY      | GLU    | CONFLICT | UNP P69249 |
| U     | 88      | GLY      | GLU    | CONFLICT | UNP P69249 |
| V     | 88      | GLY      | GLU    | CONFLICT | UNP P69249 |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula:  $C_6H_{14}O_{13}P_2$ ).



| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 4   | A     | 1        | Total C O P<br>21 6 13 2 | 0       | 0       |
| 4   | B     | 1        | Total C O P<br>21 6 13 2 | 0       | 0       |
| 4   | C     | 1        | Total C O P<br>21 6 13 2 | 0       | 0       |
| 4   | D     | 1        | Total C O P<br>21 6 13 2 | 0       | 0       |

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).

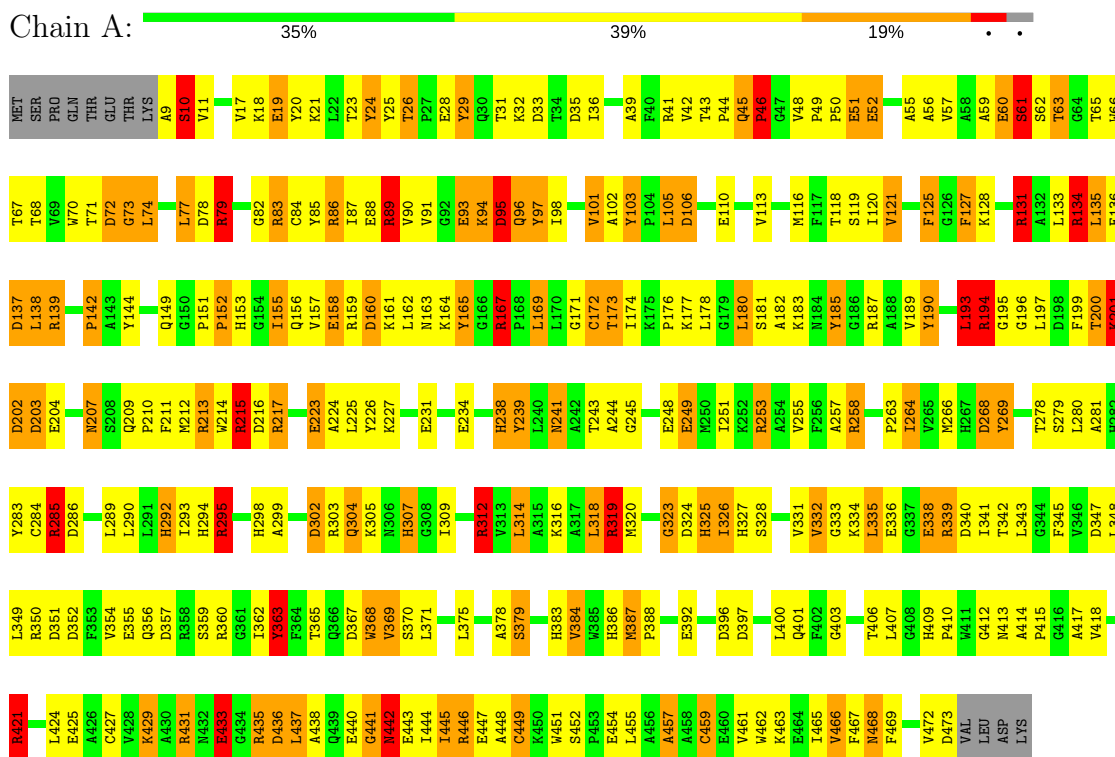


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 5   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 5   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 5   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |

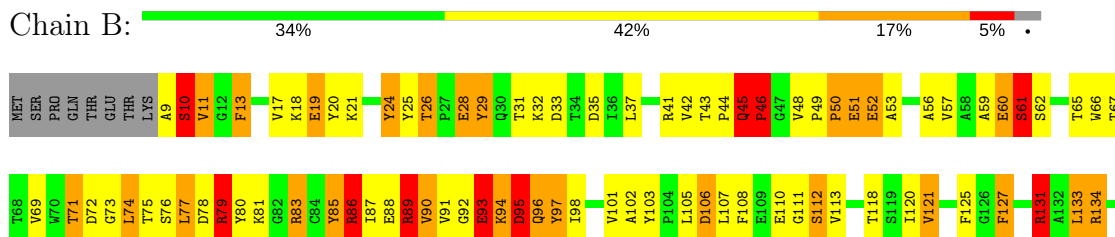
i

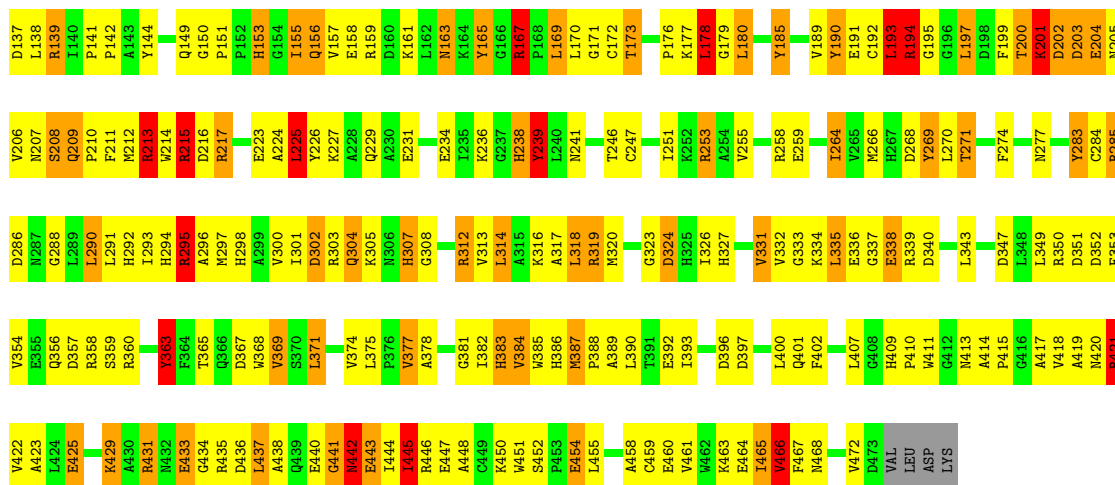
Note EDS was not executed.

- Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)



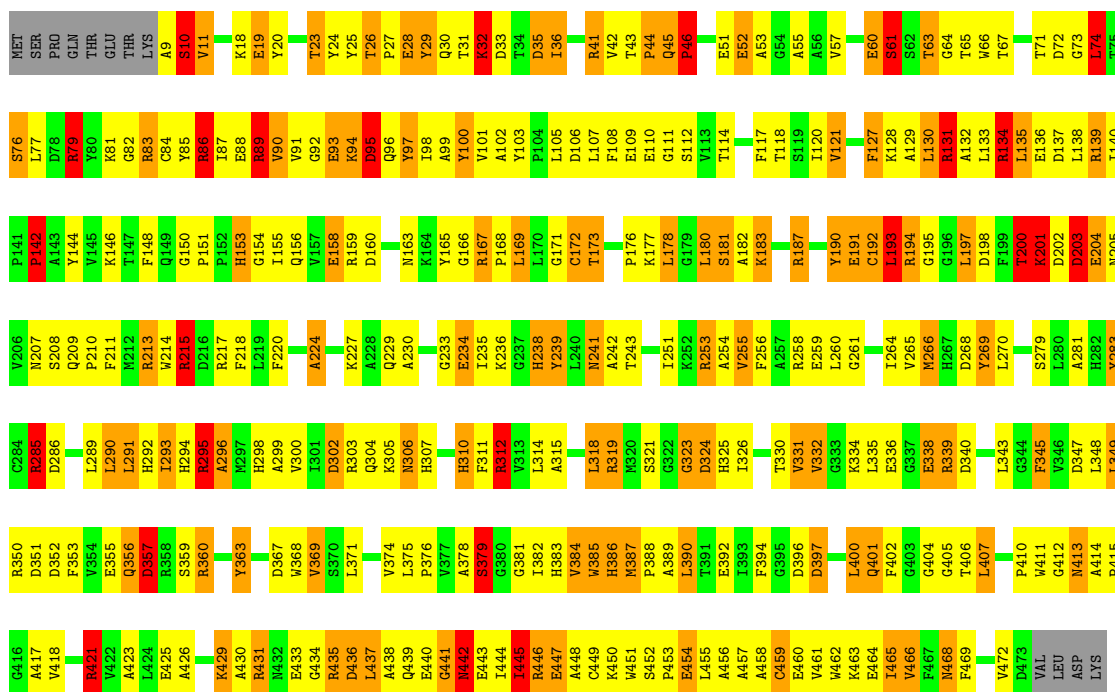
- Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)





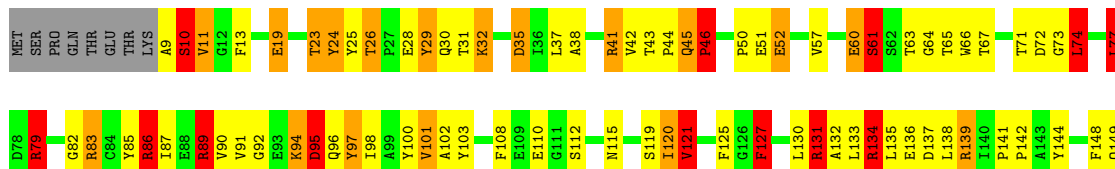
• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain C: 31% 41% 21% 5%

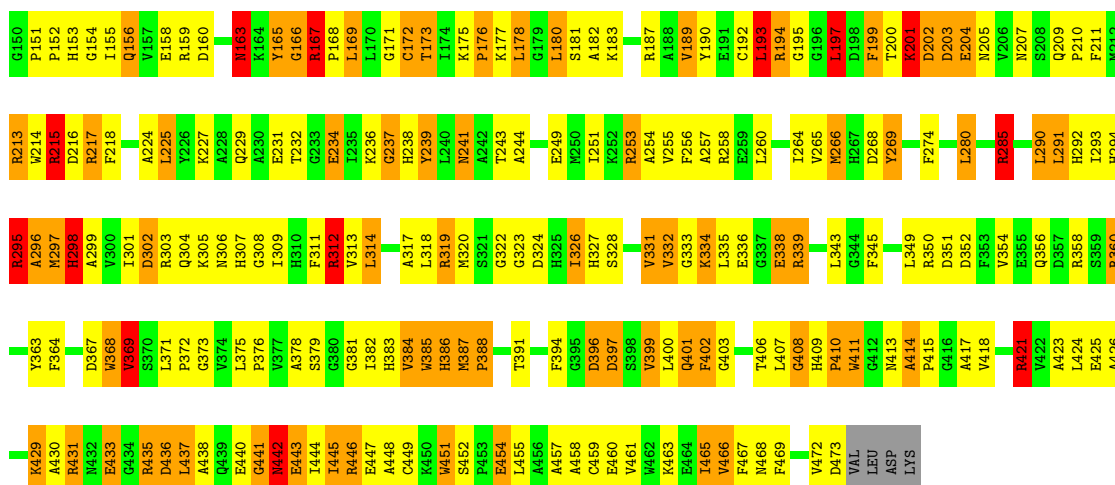


• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

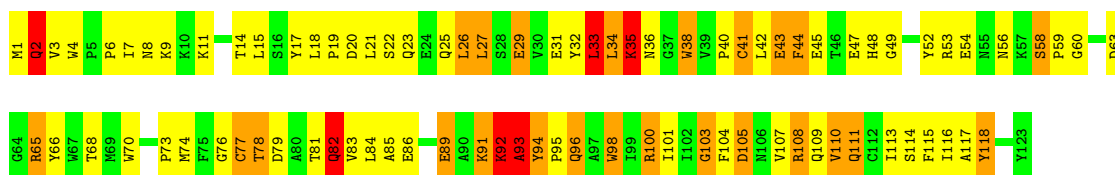
Chain D: 36% 38% 18% 5%



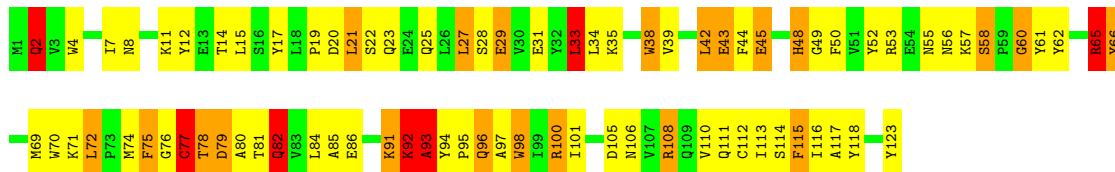
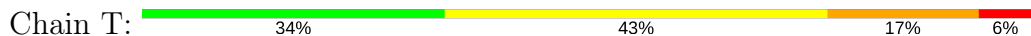




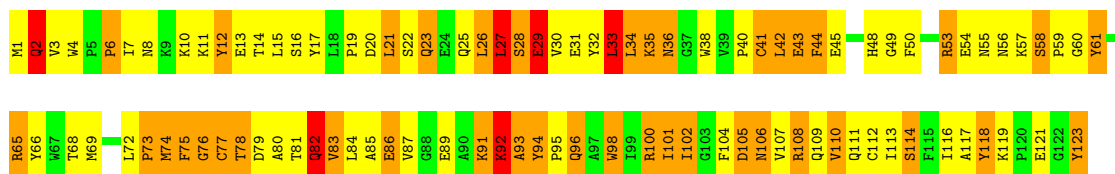
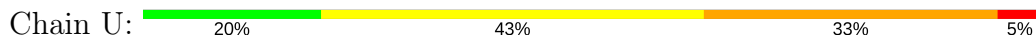
- Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)



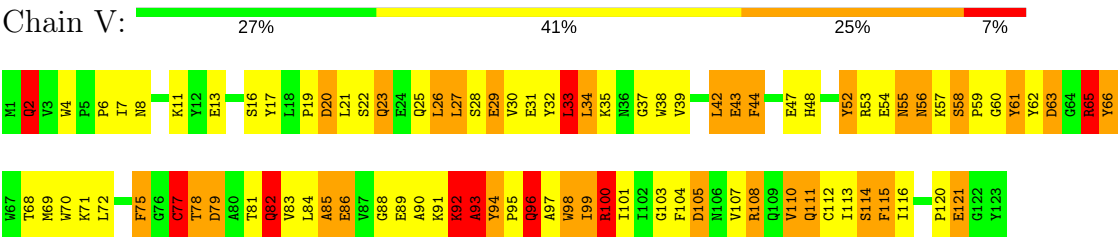
- Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)



- Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)



- Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)



## 4 Data and refinement statistics

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

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | P 31 2 1   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 204.60Å 204.60Å 117.40Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å)   | (Not available) – 2.70                           | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-2.70)           | Depositor |
| $R_{merge}$  | (Not available)                                  | Depositor |
| $R_{sym}$  | (Not available)                                  | Depositor |
| Refinement program                                       | PROFFT   | Depositor |
| R, $R_{free}$  | 0.202 , (Not available)                          | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 18708  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 21.0   | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 1   | A     | 1.69         | 30/3716 (0.8%)   | 2.59        | 253/5038 (5.0%)   |
| 1   | B     | 1.66         | 24/3716 (0.6%)   | 2.57        | 227/5038 (4.5%)   |
| 1   | C     | 1.75         | 46/3716 (1.2%)   | 2.66        | 253/5038 (5.0%)   |
| 1   | D     | 1.69         | 39/3716 (1.0%)   | 2.60        | 235/5038 (4.7%)   |
| 2   | S     | 1.57         | 8/1057 (0.8%)    | 2.51        | 71/1435 (4.9%)    |
| 2   | T     | 1.48         | 3/1057 (0.3%)    | 2.25        | 56/1435 (3.9%)    |
| 2   | U     | 1.79         | 13/1057 (1.2%)   | 2.53        | 70/1435 (4.9%)    |
| 2   | V     | 1.70         | 14/1057 (1.3%)   | 2.50        | 80/1435 (5.6%)    |
| All | All   | 1.68         | 177/19092 (0.9%) | 2.57        | 1245/25892 (4.8%) |

All (177) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | S     | 58  | SER  | CB-OG  | -9.13 | 1.30        | 1.42     |
| 1   | C     | 181 | SER  | CB-OG  | 8.99  | 1.53        | 1.42     |
| 1   | C     | 323 | GLY  | N-CA   | 8.87  | 1.59        | 1.46     |
| 1   | A     | 459 | CYS  | CB-SG  | -8.49 | 1.67        | 1.82     |
| 1   | A     | 134 | ARG  | CZ-NH1 | 8.02  | 1.43        | 1.33     |
| 1   | A     | 234 | GLU  | CD-OE2 | -7.93 | 1.17        | 1.25     |
| 1   | C     | 110 | GLU  | CB-CG  | -7.78 | 1.37        | 1.52     |
| 1   | C     | 201 | LYS  | CA-CB  | 7.77  | 1.71        | 1.53     |
| 2   | V     | 7   | ILE  | C-O    | 7.74  | 1.38        | 1.23     |
| 1   | C     | 405 | GLY  | C-O    | 7.74  | 1.36        | 1.23     |
| 1   | C     | 266 | MET  | C-O    | 7.70  | 1.38        | 1.23     |
| 1   | C     | 319 | ARG  | CD-NE  | -7.69 | 1.33        | 1.46     |
| 1   | D     | 201 | LYS  | CA-CB  | 7.43  | 1.70        | 1.53     |
| 2   | U     | 7   | ILE  | C-O    | 7.42  | 1.37        | 1.23     |
| 1   | D     | 403 | GLY  | N-CA   | 7.41  | 1.57        | 1.46     |
| 1   | C     | 243 | THR  | CB-OG1 | 7.37  | 1.57        | 1.43     |
| 1   | C     | 285 | ARG  | CZ-NH1 | 7.25  | 1.42        | 1.33     |
| 1   | D     | 158 | GLU  | CD-OE1 | 7.25  | 1.33        | 1.25     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 279 | SER  | CB-OG  | 7.17  | 1.51        | 1.42     |
| 1   | C     | 454 | GLU  | CD-OE2 | 7.13  | 1.33        | 1.25     |
| 1   | A     | 319 | ARG  | NE-CZ  | -7.02 | 1.24        | 1.33     |
| 2   | V     | 82  | GLN  | C-O    | 7.02  | 1.36        | 1.23     |
| 1   | B     | 459 | CYS  | CB-SG  | -6.98 | 1.70        | 1.82     |
| 1   | D     | 258 | ARG  | NE-CZ  | 6.97  | 1.42        | 1.33     |
| 1   | D     | 231 | GLU  | CD-OE1 | 6.97  | 1.33        | 1.25     |
| 1   | A     | 201 | LYS  | CA-CB  | 6.89  | 1.69        | 1.53     |
| 1   | B     | 223 | GLU  | CD-OE1 | -6.88 | 1.18        | 1.25     |
| 1   | A     | 319 | ARG  | CD-NE  | -6.77 | 1.34        | 1.46     |
| 1   | A     | 427 | CYS  | CB-SG  | -6.74 | 1.70        | 1.82     |
| 1   | C     | 259 | GLU  | CD-OE2 | 6.73  | 1.33        | 1.25     |
| 1   | B     | 201 | LYS  | CA-CB  | 6.66  | 1.68        | 1.53     |
| 1   | C     | 156 | GLN  | CD-NE2 | 6.59  | 1.49        | 1.32     |
| 1   | C     | 253 | ARG  | CZ-NH1 | 6.58  | 1.41        | 1.33     |
| 1   | B     | 110 | GLU  | CD-OE2 | -6.56 | 1.18        | 1.25     |
| 1   | D     | 290 | LEU  | C-O    | 6.55  | 1.35        | 1.23     |
| 2   | S     | 7   | ILE  | C-O    | 6.55  | 1.35        | 1.23     |
| 1   | C     | 310 | HIS  | C-O    | 6.53  | 1.35        | 1.23     |
| 2   | T     | 62  | TYR  | CE2-CZ | -6.50 | 1.30        | 1.38     |
| 1   | B     | 52  | GLU  | CD-OE1 | -6.48 | 1.18        | 1.25     |
| 1   | A     | 279 | SER  | CA-CB  | -6.47 | 1.43        | 1.52     |
| 2   | U     | 65  | ARG  | NE-CZ  | 6.45  | 1.41        | 1.33     |
| 1   | A     | 72  | ASP  | C-O    | 6.42  | 1.35        | 1.23     |
| 1   | D     | 201 | LYS  | CE-NZ  | -6.38 | 1.33        | 1.49     |
| 1   | D     | 388 | PRO  | N-CD   | 6.36  | 1.56        | 1.47     |
| 1   | D     | 364 | PHE  | CE2-CZ | 6.35  | 1.49        | 1.37     |
| 1   | D     | 172 | CYS  | CB-SG  | -6.29 | 1.71        | 1.82     |
| 1   | A     | 449 | CYS  | CB-SG  | -6.20 | 1.71        | 1.82     |
| 1   | B     | 425 | GLU  | CD-OE1 | -6.19 | 1.18        | 1.25     |
| 1   | C     | 153 | HIS  | C-O    | 6.15  | 1.35        | 1.23     |
| 1   | D     | 217 | ARG  | CZ-NH2 | 6.14  | 1.41        | 1.33     |
| 1   | A     | 61  | SER  | CA-CB  | 6.09  | 1.62        | 1.52     |
| 1   | C     | 127 | PHE  | C-O    | 6.04  | 1.34        | 1.23     |
| 1   | D     | 60  | GLU  | CD-OE2 | -6.02 | 1.19        | 1.25     |
| 2   | V     | 65  | ARG  | NE-CZ  | 6.01  | 1.40        | 1.33     |
| 1   | A     | 201 | LYS  | CE-NZ  | -6.00 | 1.34        | 1.49     |
| 1   | D     | 328 | SER  | CB-OG  | 5.97  | 1.50        | 1.42     |
| 1   | A     | 370 | SER  | C-O    | 5.94  | 1.34        | 1.23     |
| 1   | A     | 24  | TYR  | C-O    | 5.93  | 1.34        | 1.23     |
| 1   | C     | 215 | ARG  | CZ-NH1 | 5.92  | 1.40        | 1.33     |
| 2   | V     | 13  | GLU  | CD-OE2 | 5.90  | 1.32        | 1.25     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 112 | SER  | CB-OG  | -5.86 | 1.34        | 1.42     |
| 1   | A     | 350 | ARG  | CD-NE  | -5.85 | 1.36        | 1.46     |
| 2   | S     | 8   | ASN  | N-CA   | 5.83  | 1.58        | 1.46     |
| 1   | B     | 284 | CYS  | CB-SG  | -5.82 | 1.72        | 1.81     |
| 1   | D     | 319 | ARG  | NE-CZ  | -5.81 | 1.25        | 1.33     |
| 2   | U     | 8   | ASN  | N-CA   | 5.80  | 1.57        | 1.46     |
| 1   | D     | 61  | SER  | CB-OG  | -5.79 | 1.34        | 1.42     |
| 2   | V     | 69  | MET  | CG-SD  | 5.79  | 1.96        | 1.81     |
| 2   | V     | 43  | GLU  | CD-OE1 | -5.77 | 1.19        | 1.25     |
| 1   | C     | 111 | GLY  | C-O    | 5.77  | 1.32        | 1.23     |
| 1   | B     | 83  | ARG  | CZ-NH2 | 5.76  | 1.40        | 1.33     |
| 2   | S     | 47  | GLU  | CD-OE2 | 5.75  | 1.31        | 1.25     |
| 1   | C     | 431 | ARG  | NE-CZ  | 5.74  | 1.40        | 1.33     |
| 1   | A     | 119 | SER  | C-O    | 5.73  | 1.34        | 1.23     |
| 1   | B     | 223 | GLU  | CG-CD  | -5.70 | 1.43        | 1.51     |
| 1   | A     | 217 | ARG  | CD-NE  | -5.68 | 1.36        | 1.46     |
| 1   | D     | 368 | TRP  | CG-CD1 | 5.68  | 1.44        | 1.36     |
| 2   | V     | 53  | ARG  | CZ-NH1 | 5.66  | 1.40        | 1.33     |
| 1   | A     | 238 | HIS  | CG-CD2 | -5.66 | 1.26        | 1.35     |
| 1   | C     | 319 | ARG  | CZ-NH1 | 5.66  | 1.40        | 1.33     |
| 1   | D     | 306 | ASN  | C-O    | 5.65  | 1.34        | 1.23     |
| 1   | C     | 256 | PHE  | C-O    | 5.64  | 1.34        | 1.23     |
| 1   | D     | 285 | ARG  | NE-CZ  | 5.62  | 1.40        | 1.33     |
| 2   | U     | 49  | GLY  | C-O    | 5.60  | 1.32        | 1.23     |
| 1   | D     | 148 | PHE  | CG-CD1 | -5.60 | 1.30        | 1.38     |
| 1   | B     | 201 | LYS  | N-CA   | -5.59 | 1.35        | 1.46     |
| 1   | C     | 238 | HIS  | C-O    | 5.58  | 1.33        | 1.23     |
| 1   | B     | 433 | GLU  | CB-CG  | -5.57 | 1.41        | 1.52     |
| 2   | T     | 92  | LYS  | C-O    | 5.57  | 1.33        | 1.23     |
| 2   | V     | 8   | ASN  | N-CA   | 5.56  | 1.57        | 1.46     |
| 1   | B     | 350 | ARG  | CD-NE  | -5.56 | 1.36        | 1.46     |
| 1   | D     | 411 | TRP  | C-O    | 5.55  | 1.33        | 1.23     |
| 2   | V     | 88  | GLY  | N-CA   | 5.55  | 1.54        | 1.46     |
| 1   | D     | 258 | ARG  | CG-CD  | -5.55 | 1.38        | 1.51     |
| 2   | S     | 73  | PRO  | N-CD   | -5.51 | 1.40        | 1.47     |
| 1   | C     | 306 | ASN  | C-O    | 5.50  | 1.33        | 1.23     |
| 1   | B     | 365 | THR  | C-O    | 5.49  | 1.33        | 1.23     |
| 1   | C     | 177 | LYS  | C-O    | 5.49  | 1.33        | 1.23     |
| 2   | U     | 76  | GLY  | C-O    | 5.44  | 1.32        | 1.23     |
| 1   | D     | 291 | LEU  | C-O    | 5.42  | 1.33        | 1.23     |
| 1   | C     | 36  | ILE  | C-O    | 5.42  | 1.33        | 1.23     |
| 2   | S     | 53  | ARG  | CZ-NH2 | -5.42 | 1.26        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 295 | ARG  | C-O    | 5.40  | 1.33        | 1.23     |
| 1   | A     | 359 | SER  | CA-CB  | -5.40 | 1.44        | 1.52     |
| 1   | A     | 284 | CYS  | CB-SG  | -5.40 | 1.73        | 1.81     |
| 2   | S     | 65  | ARG  | CG-CD  | -5.40 | 1.38        | 1.51     |
| 1   | D     | 237 | GLY  | C-O    | 5.39  | 1.32        | 1.23     |
| 2   | V     | 37  | GLY  | C-O    | 5.39  | 1.32        | 1.23     |
| 1   | D     | 408 | GLY  | C-O    | 5.37  | 1.32        | 1.23     |
| 1   | D     | 112 | SER  | CB-OG  | -5.36 | 1.35        | 1.42     |
| 1   | C     | 445 | ILE  | N-CA   | 5.34  | 1.57        | 1.46     |
| 1   | A     | 362 | ILE  | C-O    | 5.32  | 1.33        | 1.23     |
| 1   | C     | 379 | SER  | CB-OG  | 5.32  | 1.49        | 1.42     |
| 1   | B     | 259 | GLU  | CD-OE1 | 5.31  | 1.31        | 1.25     |
| 1   | D     | 339 | ARG  | CZ-NH1 | 5.31  | 1.40        | 1.33     |
| 1   | A     | 433 | GLU  | CB-CG  | -5.30 | 1.42        | 1.52     |
| 1   | C     | 321 | SER  | CA-CB  | -5.30 | 1.45        | 1.52     |
| 2   | U     | 102 | ILE  | C-O    | 5.30  | 1.33        | 1.23     |
| 1   | A     | 103 | TYR  | C-O    | 5.29  | 1.33        | 1.23     |
| 1   | C     | 261 | GLY  | C-O    | 5.29  | 1.32        | 1.23     |
| 1   | D     | 443 | GLU  | CB-CG  | 5.29  | 1.62        | 1.52     |
| 1   | A     | 379 | SER  | CB-OG  | -5.28 | 1.35        | 1.42     |
| 1   | C     | 201 | LYS  | CE-NZ  | -5.28 | 1.35        | 1.49     |
| 1   | C     | 406 | THR  | CB-OG1 | 5.27  | 1.53        | 1.43     |
| 2   | V     | 93  | ALA  | N-CA   | 5.27  | 1.56        | 1.46     |
| 1   | D     | 460 | GLU  | CD-OE1 | 5.27  | 1.31        | 1.25     |
| 1   | D     | 176 | PRO  | C-O    | 5.27  | 1.33        | 1.23     |
| 1   | D     | 385 | TRP  | CA-CB  | 5.26  | 1.65        | 1.53     |
| 1   | D     | 421 | ARG  | C-O    | 5.25  | 1.33        | 1.23     |
| 1   | B     | 206 | VAL  | C-O    | -5.25 | 1.13        | 1.23     |
| 2   | U     | 86  | GLU  | CB-CG  | 5.25  | 1.62        | 1.52     |
| 2   | S     | 100 | ARG  | CG-CD  | -5.25 | 1.38        | 1.51     |
| 1   | C     | 233 | GLY  | C-O    | 5.24  | 1.32        | 1.23     |
| 1   | B     | 179 | GLY  | N-CA   | -5.22 | 1.38        | 1.46     |
| 1   | C     | 201 | LYS  | N-CA   | -5.22 | 1.35        | 1.46     |
| 1   | C     | 435 | ARG  | N-CA   | 5.21  | 1.56        | 1.46     |
| 1   | C     | 114 | THR  | CB-OG1 | 5.21  | 1.53        | 1.43     |
| 1   | C     | 421 | ARG  | C-O    | 5.21  | 1.33        | 1.23     |
| 2   | U     | 54  | GLU  | C-O    | 5.21  | 1.33        | 1.23     |
| 1   | B     | 204 | GLU  | CD-OE1 | -5.21 | 1.20        | 1.25     |
| 2   | V     | 77  | CYS  | CB-SG  | 5.17  | 1.91        | 1.82     |
| 1   | D     | 332 | VAL  | C-O    | 5.17  | 1.33        | 1.23     |
| 2   | U     | 41  | CYS  | CB-SG  | 5.17  | 1.91        | 1.82     |
| 1   | C     | 293 | ILE  | C-N    | -5.16 | 1.22        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 211 | PHE  | CE1-CZ  | 5.15  | 1.47        | 1.37     |
| 1   | D     | 290 | LEU  | N-CA    | 5.15  | 1.56        | 1.46     |
| 1   | C     | 204 | GLU  | CD-OE1  | -5.14 | 1.20        | 1.25     |
| 2   | U     | 74  | MET  | CG-SD   | 5.13  | 1.94        | 1.81     |
| 2   | V     | 62  | TYR  | CD2-CE2 | 5.13  | 1.47        | 1.39     |
| 2   | U     | 98  | TRP  | C-O     | 5.12  | 1.33        | 1.23     |
| 1   | D     | 232 | THR  | CB-OG1  | 5.11  | 1.53        | 1.43     |
| 1   | C     | 217 | ARG  | CZ-NH2  | 5.11  | 1.39        | 1.33     |
| 1   | C     | 459 | CYS  | CB-SG   | -5.11 | 1.73        | 1.81     |
| 1   | C     | 404 | GLY  | N-CA    | 5.10  | 1.53        | 1.46     |
| 1   | A     | 285 | ARG  | CD-NE   | 5.10  | 1.55        | 1.46     |
| 1   | D     | 167 | ARG  | CZ-NH1  | 5.10  | 1.39        | 1.33     |
| 1   | B     | 201 | LYS  | CE-NZ   | -5.09 | 1.36        | 1.49     |
| 1   | B     | 247 | CYS  | CB-SG   | -5.09 | 1.73        | 1.81     |
| 1   | C     | 158 | GLU  | CB-CG   | 5.09  | 1.61        | 1.52     |
| 1   | C     | 110 | GLU  | CG-CD   | -5.09 | 1.44        | 1.51     |
| 1   | D     | 322 | GLY  | N-CA    | -5.08 | 1.38        | 1.46     |
| 1   | B     | 190 | TYR  | CG-CD2  | -5.07 | 1.32        | 1.39     |
| 1   | D     | 197 | LEU  | C-O     | 5.07  | 1.32        | 1.23     |
| 1   | C     | 173 | THR  | CB-OG1  | 5.05  | 1.53        | 1.43     |
| 1   | A     | 368 | TRP  | C-N     | -5.05 | 1.22        | 1.34     |
| 1   | A     | 342 | THR  | CB-OG1  | 5.04  | 1.53        | 1.43     |
| 2   | U     | 114 | SER  | CA-CB   | -5.04 | 1.45        | 1.52     |
| 1   | A     | 73  | GLY  | N-CA    | 5.04  | 1.53        | 1.46     |
| 1   | A     | 172 | CYS  | CB-SG   | -5.04 | 1.73        | 1.81     |
| 1   | B     | 367 | ASP  | N-CA    | 5.04  | 1.56        | 1.46     |
| 1   | B     | 61  | SER  | CA-CB   | 5.02  | 1.60        | 1.52     |
| 2   | T     | 106 | ASN  | C-O     | 5.02  | 1.32        | 1.23     |
| 2   | V     | 62  | TYR  | N-CA    | 5.02  | 1.56        | 1.46     |
| 1   | A     | 253 | ARG  | CZ-NH1  | 5.01  | 1.39        | 1.33     |
| 2   | U     | 59  | PRO  | C-O     | 5.01  | 1.33        | 1.23     |
| 1   | D     | 144 | TYR  | CG-CD1  | -5.01 | 1.32        | 1.39     |
| 1   | B     | 208 | SER  | CA-CB   | -5.00 | 1.45        | 1.52     |

All (1245) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | C     | 350 | ARG  | NE-CZ-NH2 | -35.79 | 102.40      | 120.30   |
| 1   | A     | 319 | ARG  | CD-NE-CZ  | 25.36  | 159.11      | 123.60   |
| 1   | C     | 319 | ARG  | CD-NE-CZ  | 23.95  | 157.13      | 123.60   |
| 1   | D     | 139 | ARG  | NE-CZ-NH1 | -23.24 | 108.68      | 120.30   |
| 1   | A     | 139 | ARG  | NE-CZ-NH2 | 23.20  | 131.90      | 120.30   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | C     | 217 | ARG  | NE-CZ-NH2 | -21.79 | 109.41      | 120.30   |
| 2   | U     | 65  | ARG  | NE-CZ-NH2 | -20.93 | 109.83      | 120.30   |
| 1   | D     | 139 | ARG  | NE-CZ-NH2 | 20.81  | 130.71      | 120.30   |
| 1   | B     | 350 | ARG  | NE-CZ-NH2 | -20.56 | 110.02      | 120.30   |
| 1   | D     | 350 | ARG  | NE-CZ-NH2 | -20.44 | 110.08      | 120.30   |
| 1   | C     | 215 | ARG  | NE-CZ-NH1 | -19.88 | 110.36      | 120.30   |
| 1   | D     | 215 | ARG  | NE-CZ-NH2 | 19.77  | 130.19      | 120.30   |
| 1   | B     | 215 | ARG  | NE-CZ-NH1 | -19.20 | 110.70      | 120.30   |
| 1   | A     | 134 | ARG  | NE-CZ-NH1 | -18.79 | 110.90      | 120.30   |
| 1   | B     | 139 | ARG  | NE-CZ-NH2 | 18.71  | 129.65      | 120.30   |
| 2   | S     | 65  | ARG  | NE-CZ-NH2 | -18.54 | 111.03      | 120.30   |
| 1   | C     | 217 | ARG  | NE-CZ-NH1 | 18.11  | 129.35      | 120.30   |
| 1   | D     | 319 | ARG  | CD-NE-CZ  | 18.00  | 148.80      | 123.60   |
| 2   | S     | 53  | ARG  | NE-CZ-NH2 | 17.98  | 129.29      | 120.30   |
| 1   | B     | 319 | ARG  | CD-NE-CZ  | 17.68  | 148.35      | 123.60   |
| 1   | D     | 194 | ARG  | NE-CZ-NH1 | 17.60  | 129.10      | 120.30   |
| 1   | B     | 139 | ARG  | NE-CZ-NH1 | -17.49 | 111.56      | 120.30   |
| 1   | B     | 217 | ARG  | NE-CZ-NH1 | 17.46  | 129.03      | 120.30   |
| 1   | C     | 79  | ARG  | NE-CZ-NH1 | -16.98 | 111.81      | 120.30   |
| 1   | B     | 215 | ARG  | NE-CZ-NH2 | 16.97  | 128.78      | 120.30   |
| 2   | S     | 66  | TYR  | CB-CG-CD2 | 16.71  | 131.03      | 121.00   |
| 1   | A     | 217 | ARG  | CD-NE-CZ  | 16.66  | 146.93      | 123.60   |
| 1   | A     | 295 | ARG  | NE-CZ-NH1 | 16.55  | 128.58      | 120.30   |
| 1   | A     | 350 | ARG  | CD-NE-CZ  | 16.47  | 146.65      | 123.60   |
| 1   | D     | 79  | ARG  | NE-CZ-NH1 | -16.43 | 112.08      | 120.30   |
| 1   | C     | 360 | ARG  | NE-CZ-NH1 | -16.38 | 112.11      | 120.30   |
| 1   | C     | 258 | ARG  | NE-CZ-NH1 | 16.18  | 128.39      | 120.30   |
| 1   | D     | 421 | ARG  | NE-CZ-NH1 | -16.15 | 112.22      | 120.30   |
| 1   | A     | 258 | ARG  | NE-CZ-NH1 | 16.12  | 128.36      | 120.30   |
| 1   | A     | 213 | ARG  | NE-CZ-NH2 | 16.12  | 128.36      | 120.30   |
| 1   | B     | 217 | ARG  | CD-NE-CZ  | 15.98  | 145.97      | 123.60   |
| 1   | A     | 89  | ARG  | CD-NE-CZ  | 15.91  | 145.87      | 123.60   |
| 1   | A     | 139 | ARG  | NE-CZ-NH1 | -15.73 | 112.44      | 120.30   |
| 1   | B     | 319 | ARG  | NE-CZ-NH1 | 15.70  | 128.15      | 120.30   |
| 1   | C     | 350 | ARG  | NE-CZ-NH1 | 15.65  | 128.12      | 120.30   |
| 1   | C     | 89  | ARG  | NE-CZ-NH1 | 14.89  | 127.75      | 120.30   |
| 1   | D     | 86  | ARG  | NE-CZ-NH2 | 14.80  | 127.70      | 120.30   |
| 1   | D     | 350 | ARG  | NE-CZ-NH1 | 14.63  | 127.62      | 120.30   |
| 1   | B     | 201 | LYS  | CA-CB-CG  | 14.62  | 145.55      | 113.40   |
| 1   | C     | 41  | ARG  | NE-CZ-NH2 | 14.56  | 127.58      | 120.30   |
| 2   | U     | 105 | ASP  | CB-CG-OD1 | 14.52  | 131.37      | 118.30   |
| 1   | B     | 283 | TYR  | CB-CG-CD1 | 14.50  | 129.70      | 121.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | D     | 431 | ARG  | NE-CZ-NH2 | -14.35 | 113.12      | 120.30   |
| 2   | S     | 53  | ARG  | NE-CZ-NH1 | -14.05 | 113.28      | 120.30   |
| 1   | D     | 367 | ASP  | CB-CG-OD1 | 13.75  | 130.68      | 118.30   |
| 1   | B     | 360 | ARG  | NE-CZ-NH1 | -13.56 | 113.52      | 120.30   |
| 1   | C     | 269 | TYR  | CB-CG-CD1 | 13.47  | 129.08      | 121.00   |
| 1   | C     | 41  | ARG  | NE-CZ-NH1 | -13.45 | 113.57      | 120.30   |
| 1   | D     | 217 | ARG  | CD-NE-CZ  | 13.23  | 142.12      | 123.60   |
| 1   | B     | 89  | ARG  | CD-NE-CZ  | 13.21  | 142.09      | 123.60   |
| 1   | C     | 253 | ARG  | NE-CZ-NH2 | -13.14 | 113.73      | 120.30   |
| 1   | D     | 83  | ARG  | NE-CZ-NH1 | -13.10 | 113.75      | 120.30   |
| 1   | C     | 89  | ARG  | CD-NE-CZ  | 13.06  | 141.89      | 123.60   |
| 1   | A     | 367 | ASP  | CB-CG-OD1 | 13.06  | 130.05      | 118.30   |
| 1   | C     | 134 | ARG  | NE-CZ-NH1 | -13.01 | 113.80      | 120.30   |
| 1   | D     | 89  | ARG  | CD-NE-CZ  | 13.00  | 141.79      | 123.60   |
| 1   | A     | 312 | ARG  | NE-CZ-NH1 | -12.97 | 113.82      | 120.30   |
| 1   | A     | 215 | ARG  | NE-CZ-NH1 | -12.84 | 113.88      | 120.30   |
| 1   | C     | 160 | ASP  | CB-CG-OD1 | -12.80 | 106.78      | 118.30   |
| 1   | B     | 351 | ASP  | CB-CG-OD2 | -12.62 | 106.94      | 118.30   |
| 1   | A     | 367 | ASP  | CB-CG-OD2 | -12.61 | 106.95      | 118.30   |
| 1   | A     | 167 | ARG  | NE-CZ-NH1 | -12.54 | 114.03      | 120.30   |
| 1   | C     | 367 | ASP  | CB-CG-OD1 | 12.34  | 129.41      | 118.30   |
| 1   | C     | 339 | ARG  | NE-CZ-NH2 | -12.14 | 114.23      | 120.30   |
| 1   | A     | 324 | ASP  | CB-CG-OD1 | 12.03  | 129.12      | 118.30   |
| 1   | A     | 347 | ASP  | CB-CG-OD1 | 11.99  | 129.09      | 118.30   |
| 1   | B     | 167 | ARG  | NE-CZ-NH2 | 11.85  | 126.23      | 120.30   |
| 1   | C     | 72  | ASP  | CB-CG-OD1 | 11.84  | 128.95      | 118.30   |
| 1   | A     | 33  | ASP  | CB-CG-OD2 | -11.66 | 107.81      | 118.30   |
| 1   | D     | 253 | ARG  | NE-CZ-NH2 | -11.65 | 114.47      | 120.30   |
| 1   | B     | 25  | TYR  | CB-CG-CD1 | -11.63 | 114.02      | 121.00   |
| 2   | T     | 20  | ASP  | CB-CG-OD2 | -11.57 | 107.89      | 118.30   |
| 1   | D     | 41  | ARG  | NE-CZ-NH1 | -11.52 | 114.54      | 120.30   |
| 1   | C     | 217 | ARG  | CD-NE-CZ  | 11.46  | 139.65      | 123.60   |
| 1   | C     | 295 | ARG  | NE-CZ-NH1 | 11.38  | 125.99      | 120.30   |
| 1   | A     | 285 | ARG  | NE-CZ-NH2 | -11.35 | 114.63      | 120.30   |
| 1   | C     | 285 | ARG  | NE-CZ-NH2 | 11.32  | 125.96      | 120.30   |
| 1   | C     | 431 | ARG  | NE-CZ-NH1 | 11.25  | 125.93      | 120.30   |
| 1   | A     | 319 | ARG  | NE-CZ-NH1 | 11.21  | 125.91      | 120.30   |
| 1   | D     | 352 | ASP  | CB-CG-OD2 | 11.18  | 128.36      | 118.30   |
| 1   | A     | 433 | GLU  | CA-CB-CG  | 11.16  | 137.95      | 113.40   |
| 2   | V     | 105 | ASP  | CB-CG-OD1 | 11.09  | 128.28      | 118.30   |
| 1   | C     | 295 | ARG  | NE-CZ-NH2 | -11.06 | 114.77      | 120.30   |
| 1   | D     | 360 | ARG  | NE-CZ-NH1 | -11.00 | 114.80      | 120.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 25  | TYR  | CB-CG-CD1  | -10.90 | 114.46      | 121.00   |
| 1   | D     | 160 | ASP  | CB-CG-OD2  | 10.78  | 128.00      | 118.30   |
| 2   | V     | 62  | TYR  | CB-CG-CD1  | -10.75 | 114.55      | 121.00   |
| 1   | A     | 25  | TYR  | CB-CG-CD2  | 10.72  | 127.43      | 121.00   |
| 1   | A     | 190 | TYR  | CB-CG-CD2  | 10.69  | 127.42      | 121.00   |
| 1   | C     | 46  | PRO  | N-CA-CB    | -10.68 | 90.49       | 103.30   |
| 1   | D     | 396 | ASP  | CB-CG-OD1  | -10.68 | 108.69      | 118.30   |
| 2   | V     | 62  | TYR  | CB-CG-CD2  | 10.66  | 127.39      | 121.00   |
| 1   | B     | 89  | ARG  | NE-CZ-NH1  | 10.62  | 125.61      | 120.30   |
| 1   | A     | 216 | ASP  | CB-CG-OD2  | 10.58  | 127.82      | 118.30   |
| 1   | D     | 319 | ARG  | NE-CZ-NH1  | -10.56 | 115.02      | 120.30   |
| 1   | A     | 25  | TYR  | CB-CG-CD1  | -10.54 | 114.68      | 121.00   |
| 1   | D     | 324 | ASP  | CB-CG-OD1  | 10.54  | 127.78      | 118.30   |
| 2   | U     | 66  | TYR  | CB-CG-CD2  | 10.52  | 127.31      | 121.00   |
| 1   | B     | 79  | ARG  | NE-CZ-NH2  | -10.51 | 115.05      | 120.30   |
| 1   | B     | 41  | ARG  | NE-CZ-NH2  | 10.50  | 125.55      | 120.30   |
| 1   | A     | 286 | ASP  | CB-CG-OD2  | -10.49 | 108.86      | 118.30   |
| 1   | B     | 350 | ARG  | NE-CZ-NH1  | 10.49  | 125.55      | 120.30   |
| 1   | B     | 131 | ARG  | NE-CZ-NH1  | 10.46  | 125.53      | 120.30   |
| 1   | A     | 72  | ASP  | CA-CB-CG   | 10.44  | 136.36      | 113.40   |
| 1   | A     | 169 | LEU  | CA-CB-CG   | 10.44  | 139.30      | 115.30   |
| 1   | A     | 217 | ARG  | NE-CZ-NH1  | 10.42  | 125.51      | 120.30   |
| 1   | B     | 421 | ARG  | NE-CZ-NH1  | -10.37 | 115.11      | 120.30   |
| 1   | B     | 312 | ARG  | NE-CZ-NH2  | -10.35 | 115.13      | 120.30   |
| 1   | D     | 446 | ARG  | NE-CZ-NH2  | 10.34  | 125.47      | 120.30   |
| 1   | D     | 433 | GLU  | CA-CB-CG   | 10.33  | 136.12      | 113.40   |
| 1   | B     | 269 | TYR  | CB-CG-CD1  | 10.32  | 127.19      | 121.00   |
| 1   | B     | 156 | GLN  | CG-CD-OE1  | 10.31  | 142.23      | 121.60   |
| 1   | C     | 79  | ARG  | NH1-CZ-NH2 | 10.28  | 130.71      | 119.40   |
| 2   | S     | 43  | GLU  | OE1-CD-OE2 | -10.20 | 111.06      | 123.30   |
| 1   | D     | 397 | ASP  | O-C-N      | 10.20  | 139.03      | 122.70   |
| 1   | C     | 110 | GLU  | OE1-CD-OE2 | -10.13 | 111.15      | 123.30   |
| 1   | B     | 433 | GLU  | CA-CB-CG   | 10.09  | 135.60      | 113.40   |
| 1   | D     | 167 | ARG  | NE-CZ-NH2  | 10.07  | 125.34      | 120.30   |
| 1   | D     | 25  | TYR  | CB-CG-CD1  | -10.06 | 114.96      | 121.00   |
| 1   | B     | 217 | ARG  | NH1-CZ-NH2 | -10.02 | 108.38      | 119.40   |
| 1   | A     | 83  | ARG  | NE-CZ-NH1  | -10.00 | 115.30      | 120.30   |
| 1   | A     | 83  | ARG  | NE-CZ-NH2  | 10.00  | 125.30      | 120.30   |
| 2   | S     | 66  | TYR  | CB-CG-CD1  | -9.98  | 115.01      | 121.00   |
| 1   | D     | 165 | TYR  | CB-CG-CD1  | -9.98  | 115.01      | 121.00   |
| 1   | B     | 283 | TYR  | CB-CG-CD2  | -9.94  | 115.04      | 121.00   |
| 1   | A     | 216 | ASP  | CB-CG-OD1  | -9.90  | 109.39      | 118.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 347 | ASP  | CB-CG-OD1  | 9.89  | 127.20      | 118.30   |
| 1   | D     | 350 | ARG  | CD-NE-CZ   | 9.86  | 137.41      | 123.60   |
| 1   | D     | 258 | ARG  | NE-CZ-NH1  | 9.85  | 125.22      | 120.30   |
| 1   | D     | 360 | ARG  | CD-NE-CZ   | -9.84 | 109.83      | 123.60   |
| 1   | A     | 421 | ARG  | NE-CZ-NH1  | -9.83 | 115.39      | 120.30   |
| 1   | B     | 72  | ASP  | CB-CG-OD1  | 9.79  | 127.11      | 118.30   |
| 1   | B     | 33  | ASP  | CB-CG-OD2  | -9.79 | 109.49      | 118.30   |
| 1   | D     | 79  | ARG  | NH1-CZ-NH2 | 9.75  | 130.13      | 119.40   |
| 1   | D     | 358 | ARG  | NE-CZ-NH1  | -9.72 | 115.44      | 120.30   |
| 2   | S     | 7   | ILE  | CA-C-O     | -9.67 | 99.79       | 120.10   |
| 2   | V     | 65  | ARG  | NE-CZ-NH1  | 9.65  | 125.12      | 120.30   |
| 1   | D     | 446 | ARG  | NE-CZ-NH1  | -9.60 | 115.50      | 120.30   |
| 1   | D     | 202 | ASP  | CB-CG-OD1  | 9.60  | 126.94      | 118.30   |
| 1   | D     | 134 | ARG  | NE-CZ-NH1  | -9.59 | 115.50      | 120.30   |
| 1   | B     | 88  | GLU  | CA-CB-CG   | 9.58  | 134.48      | 113.40   |
| 1   | C     | 367 | ASP  | CB-CG-OD2  | -9.54 | 109.71      | 118.30   |
| 2   | U     | 66  | TYR  | CB-CG-CD1  | -9.54 | 115.27      | 121.00   |
| 1   | D     | 72  | ASP  | CA-CB-CG   | 9.52  | 134.35      | 113.40   |
| 1   | B     | 46  | PRO  | N-CA-CB    | -9.52 | 91.88       | 103.30   |
| 1   | C     | 218 | PHE  | CB-CG-CD2  | -9.52 | 114.14      | 120.80   |
| 2   | S     | 82  | GLN  | CB-CG-CD   | 9.50  | 136.31      | 111.60   |
| 2   | T     | 110 | VAL  | CA-CB-CG1  | 9.50  | 125.15      | 110.90   |
| 1   | B     | 86  | ARG  | NE-CZ-NH1  | -9.48 | 115.56      | 120.30   |
| 1   | D     | 352 | ASP  | CB-CG-OD1  | -9.47 | 109.77      | 118.30   |
| 1   | C     | 131 | ARG  | NE-CZ-NH1  | 9.47  | 125.04      | 120.30   |
| 1   | B     | 25  | TYR  | CB-CG-CD2  | 9.44  | 126.66      | 121.00   |
| 1   | B     | 139 | ARG  | CD-NE-CZ   | -9.43 | 110.40      | 123.60   |
| 1   | B     | 72  | ASP  | CA-CB-CG   | 9.42  | 134.13      | 113.40   |
| 1   | C     | 85  | TYR  | CB-CG-CD1  | 9.42  | 126.65      | 121.00   |
| 1   | A     | 339 | ARG  | NE-CZ-NH2  | -9.42 | 115.59      | 120.30   |
| 1   | A     | 185 | TYR  | CB-CG-CD2  | 9.31  | 126.59      | 121.00   |
| 2   | S     | 100 | ARG  | N-CA-CB    | -9.30 | 93.86       | 110.60   |
| 1   | C     | 110 | GLU  | CG-CD-OE2  | 9.30  | 136.89      | 118.30   |
| 1   | D     | 285 | ARG  | NE-CZ-NH1  | -9.30 | 115.65      | 120.30   |
| 1   | D     | 72  | ASP  | CB-CG-OD1  | 9.29  | 126.66      | 118.30   |
| 2   | U     | 105 | ASP  | CB-CG-OD2  | -9.27 | 109.96      | 118.30   |
| 1   | C     | 433 | GLU  | CA-CB-CG   | 9.27  | 133.79      | 113.40   |
| 2   | T     | 53  | ARG  | NE-CZ-NH1  | -9.25 | 115.67      | 120.30   |
| 1   | C     | 269 | TYR  | CB-CG-CD2  | -9.22 | 115.47      | 121.00   |
| 1   | B     | 33  | ASP  | CB-CG-OD1  | 9.19  | 126.57      | 118.30   |
| 1   | B     | 24  | TYR  | CB-CG-CD1  | 9.17  | 126.50      | 121.00   |
| 1   | C     | 350 | ARG  | NH1-CZ-NH2 | 9.15  | 129.47      | 119.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | U     | 108 | ARG  | NE-CZ-NH1  | -9.15 | 115.72      | 120.30   |
| 1   | A     | 312 | ARG  | NH1-CZ-NH2 | 9.15  | 129.46      | 119.40   |
| 1   | C     | 72  | ASP  | CA-CB-CG   | 9.15  | 133.53      | 113.40   |
| 1   | A     | 79  | ARG  | NE-CZ-NH1  | -9.13 | 115.73      | 120.30   |
| 1   | D     | 201 | LYS  | CG-CD-CE   | -9.13 | 84.52       | 111.90   |
| 1   | A     | 33  | ASP  | CB-CG-OD1  | 9.12  | 126.51      | 118.30   |
| 1   | A     | 193 | LEU  | CA-CB-CG   | 9.09  | 136.21      | 115.30   |
| 1   | D     | 86  | ARG  | NE-CZ-NH1  | -9.07 | 115.76      | 120.30   |
| 1   | D     | 386 | HIS  | CA-CB-CG   | 9.07  | 129.01      | 113.60   |
| 1   | B     | 347 | ASP  | CB-CG-OD1  | 9.06  | 126.45      | 118.30   |
| 1   | D     | 83  | ARG  | CD-NE-CZ   | 9.03  | 136.24      | 123.60   |
| 1   | A     | 258 | ARG  | NH1-CZ-NH2 | -9.01 | 109.49      | 119.40   |
| 1   | A     | 144 | TYR  | CB-CG-CD1  | -9.00 | 115.60      | 121.00   |
| 1   | C     | 243 | THR  | O-C-N      | 8.98  | 137.07      | 122.70   |
| 1   | D     | 213 | ARG  | NE-CZ-NH2  | 8.98  | 124.79      | 120.30   |
| 1   | B     | 295 | ARG  | NE-CZ-NH2  | -8.96 | 115.82      | 120.30   |
| 1   | C     | 86  | ARG  | NE-CZ-NH2  | 8.95  | 124.77      | 120.30   |
| 1   | D     | 89  | ARG  | CA-CB-CG   | 8.93  | 133.04      | 113.40   |
| 1   | C     | 266 | MET  | N-CA-CB    | -8.92 | 94.55       | 110.60   |
| 1   | D     | 201 | LYS  | CA-CB-CG   | 8.90  | 132.98      | 113.40   |
| 1   | A     | 156 | GLN  | CG-CD-OE1  | 8.86  | 139.33      | 121.60   |
| 1   | D     | 19  | GLU  | CA-CB-CG   | 8.85  | 132.87      | 113.40   |
| 1   | C     | 187 | ARG  | NE-CZ-NH1  | 8.84  | 124.72      | 120.30   |
| 2   | T     | 7   | ILE  | CA-C-O     | -8.80 | 101.63      | 120.10   |
| 1   | C     | 397 | ASP  | CB-CG-OD2  | -8.79 | 110.39      | 118.30   |
| 1   | C     | 190 | TYR  | CB-CG-CD1  | -8.77 | 115.74      | 121.00   |
| 2   | U     | 65  | ARG  | CD-NE-CZ   | -8.76 | 111.34      | 123.60   |
| 1   | D     | 41  | ARG  | NH1-CZ-NH2 | 8.76  | 129.04      | 119.40   |
| 1   | D     | 266 | MET  | N-CA-CB    | -8.76 | 94.84       | 110.60   |
| 1   | C     | 83  | ARG  | NE-CZ-NH1  | -8.75 | 115.93      | 120.30   |
| 1   | B     | 350 | ARG  | CD-NE-CZ   | 8.74  | 135.84      | 123.60   |
| 1   | C     | 156 | GLN  | CG-CD-OE1  | 8.71  | 139.03      | 121.60   |
| 1   | C     | 347 | ASP  | CB-CG-OD2  | -8.70 | 110.47      | 118.30   |
| 1   | D     | 156 | GLN  | CG-CD-OE1  | 8.69  | 138.97      | 121.60   |
| 1   | B     | 97  | TYR  | CB-CG-CD1  | -8.67 | 115.80      | 121.00   |
| 1   | D     | 225 | LEU  | CB-CG-CD2  | -8.66 | 96.28       | 111.00   |
| 1   | A     | 46  | PRO  | N-CA-CB    | -8.59 | 93.00       | 103.30   |
| 1   | C     | 387 | MET  | CA-CB-CG   | -8.59 | 98.71       | 113.30   |
| 1   | D     | 46  | PRO  | N-CA-CB    | -8.58 | 93.01       | 103.30   |
| 1   | C     | 435 | ARG  | NE-CZ-NH1  | 8.56  | 124.58      | 120.30   |
| 1   | C     | 258 | ARG  | NH1-CZ-NH2 | -8.51 | 110.04      | 119.40   |
| 1   | D     | 231 | GLU  | OE1-CD-OE2 | 8.50  | 133.50      | 123.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 194 | ARG  | NE-CZ-NH1  | 8.50  | 124.55      | 120.30   |
| 1   | A     | 360 | ARG  | NE-CZ-NH2  | -8.50 | 116.05      | 120.30   |
| 1   | B     | 201 | LYS  | CB-CA-C    | -8.48 | 93.44       | 110.40   |
| 1   | C     | 173 | THR  | CA-CB-CG2  | 8.48  | 124.27      | 112.40   |
| 1   | B     | 203 | ASP  | CB-CG-OD2  | -8.47 | 110.67      | 118.30   |
| 1   | A     | 187 | ARG  | NE-CZ-NH1  | -8.46 | 116.07      | 120.30   |
| 1   | D     | 302 | ASP  | CB-CG-OD2  | 8.42  | 125.88      | 118.30   |
| 2   | U     | 20  | ASP  | CB-CG-OD2  | -8.41 | 110.73      | 118.30   |
| 1   | B     | 216 | ASP  | CB-CG-OD1  | -8.38 | 110.76      | 118.30   |
| 2   | V     | 66  | TYR  | CB-CG-CD1  | -8.38 | 115.97      | 121.00   |
| 1   | D     | 338 | GLU  | OE1-CD-OE2 | -8.37 | 113.26      | 123.30   |
| 1   | A     | 190 | TYR  | CB-CG-CD1  | -8.35 | 115.99      | 121.00   |
| 1   | A     | 121 | VAL  | N-CA-CB    | -8.33 | 93.17       | 111.50   |
| 1   | B     | 83  | ARG  | NE-CZ-NH1  | -8.33 | 116.13      | 120.30   |
| 1   | A     | 435 | ARG  | NE-CZ-NH1  | 8.32  | 124.46      | 120.30   |
| 1   | C     | 160 | ASP  | CB-CG-OD2  | 8.31  | 125.78      | 118.30   |
| 1   | A     | 435 | ARG  | NE-CZ-NH2  | -8.28 | 116.16      | 120.30   |
| 1   | A     | 215 | ARG  | CD-NE-CZ   | -8.28 | 112.01      | 123.60   |
| 1   | A     | 201 | LYS  | CA-CB-CG   | 8.26  | 131.57      | 113.40   |
| 1   | C     | 311 | PHE  | CB-CG-CD2  | 8.26  | 126.58      | 120.80   |
| 1   | C     | 60  | GLU  | CG-CD-OE2  | 8.26  | 134.82      | 118.30   |
| 2   | U     | 12  | TYR  | CB-CG-CD1  | 8.22  | 125.93      | 121.00   |
| 2   | U     | 65  | ARG  | NE-CZ-NH1  | 8.21  | 124.41      | 120.30   |
| 2   | T     | 7   | ILE  | CA-C-N     | 8.21  | 135.27      | 117.20   |
| 1   | C     | 138 | LEU  | CA-CB-CG   | 8.19  | 134.13      | 115.30   |
| 1   | A     | 156 | GLN  | CB-CG-CD   | 8.18  | 132.85      | 111.60   |
| 2   | U     | 61  | TYR  | CB-CG-CD2  | -8.17 | 116.09      | 121.00   |
| 1   | A     | 302 | ASP  | CB-CG-OD2  | 8.14  | 125.63      | 118.30   |
| 1   | C     | 312 | ARG  | NE-CZ-NH1  | -8.12 | 116.24      | 120.30   |
| 2   | V     | 7   | ILE  | CA-C-O     | -8.12 | 103.05      | 120.10   |
| 1   | C     | 253 | ARG  | NH1-CZ-NH2 | 8.12  | 128.33      | 119.40   |
| 2   | V     | 66  | TYR  | CB-CG-CD2  | 8.10  | 125.86      | 121.00   |
| 2   | V     | 61  | TYR  | CG-CD2-CE2 | -8.10 | 114.82      | 121.30   |
| 1   | A     | 360 | ARG  | CD-NE-CZ   | -8.07 | 112.30      | 123.60   |
| 1   | C     | 340 | ASP  | CB-CG-OD2  | -8.06 | 111.05      | 118.30   |
| 1   | D     | 312 | ARG  | NE-CZ-NH2  | -8.04 | 116.28      | 120.30   |
| 2   | U     | 100 | ARG  | N-CA-CB    | -8.03 | 96.14       | 110.60   |
| 1   | B     | 91  | VAL  | CA-C-N     | -8.00 | 100.20      | 116.20   |
| 1   | B     | 41  | ARG  | NE-CZ-NH1  | -7.99 | 116.30      | 120.30   |
| 2   | V     | 52  | TYR  | CB-CG-CD2  | -7.98 | 116.21      | 121.00   |
| 1   | C     | 10  | SER  | N-CA-CB    | 7.98  | 122.47      | 110.50   |
| 2   | U     | 2   | GLN  | N-CA-CB    | 7.97  | 124.95      | 110.60   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | V     | 108 | ARG  | NE-CZ-NH2  | 7.95  | 124.28      | 120.30   |
| 1   | B     | 269 | TYR  | CA-CB-CG   | 7.94  | 128.49      | 113.40   |
| 1   | C     | 295 | ARG  | CD-NE-CZ   | -7.91 | 112.52      | 123.60   |
| 2   | S     | 21  | LEU  | CA-CB-CG   | 7.90  | 133.47      | 115.30   |
| 1   | A     | 324 | ASP  | CB-CG-OD2  | -7.90 | 111.19      | 118.30   |
| 2   | V     | 98  | TRP  | N-CA-CB    | 7.89  | 124.80      | 110.60   |
| 1   | B     | 358 | ARG  | NE-CZ-NH1  | -7.88 | 116.36      | 120.30   |
| 1   | C     | 386 | HIS  | CA-CB-CG   | 7.87  | 126.97      | 113.60   |
| 1   | B     | 26  | THR  | N-CA-CB    | -7.83 | 95.41       | 110.30   |
| 1   | B     | 216 | ASP  | CB-CG-OD2  | 7.83  | 125.35      | 118.30   |
| 2   | U     | 58  | SER  | CB-CA-C    | 7.83  | 124.98      | 110.10   |
| 1   | B     | 137 | ASP  | CB-CG-OD1  | -7.82 | 111.26      | 118.30   |
| 1   | D     | 256 | PHE  | CB-CG-CD2  | -7.81 | 115.33      | 120.80   |
| 1   | B     | 144 | TYR  | CB-CG-CD2  | 7.81  | 125.68      | 121.00   |
| 2   | V     | 2   | GLN  | N-CA-CB    | 7.80  | 124.64      | 110.60   |
| 1   | C     | 90  | VAL  | O-C-N      | 7.80  | 135.18      | 122.70   |
| 1   | C     | 213 | ARG  | NE-CZ-NH1  | 7.79  | 124.20      | 120.30   |
| 1   | A     | 185 | TYR  | CB-CG-CD1  | -7.79 | 116.33      | 121.00   |
| 2   | S     | 65  | ARG  | CG-CD-NE   | 7.78  | 128.15      | 111.80   |
| 1   | D     | 41  | ARG  | NE-CZ-NH2  | -7.77 | 116.42      | 120.30   |
| 1   | B     | 201 | LYS  | CG-CD-CE   | -7.76 | 88.60       | 111.90   |
| 1   | C     | 351 | ASP  | CB-CG-OD2  | -7.76 | 111.31      | 118.30   |
| 1   | C     | 33  | ASP  | CB-CG-OD2  | -7.75 | 111.32      | 118.30   |
| 1   | A     | 253 | ARG  | NE-CZ-NH1  | -7.75 | 116.42      | 120.30   |
| 1   | D     | 303 | ARG  | NE-CZ-NH2  | -7.74 | 116.43      | 120.30   |
| 1   | A     | 216 | ASP  | O-C-N      | 7.72  | 135.06      | 122.70   |
| 1   | D     | 435 | ARG  | NE-CZ-NH1  | 7.71  | 124.15      | 120.30   |
| 1   | C     | 201 | LYS  | CA-CB-CG   | 7.69  | 130.33      | 113.40   |
| 1   | C     | 91  | VAL  | CA-C-N     | -7.69 | 100.82      | 116.20   |
| 1   | B     | 302 | ASP  | CB-CG-OD2  | 7.67  | 125.20      | 118.30   |
| 1   | A     | 339 | ARG  | NH1-CZ-NH2 | 7.66  | 127.82      | 119.40   |
| 1   | B     | 45  | GLN  | CA-CB-CG   | 7.65  | 130.23      | 113.40   |
| 1   | A     | 436 | ASP  | O-C-N      | 7.65  | 134.94      | 122.70   |
| 1   | B     | 156 | GLN  | CB-CG-CD   | 7.64  | 131.47      | 111.60   |
| 2   | T     | 53  | ARG  | NE-CZ-NH2  | 7.64  | 124.12      | 120.30   |
| 1   | C     | 79  | ARG  | O-C-N      | 7.63  | 134.90      | 122.70   |
| 1   | D     | 258 | ARG  | CB-CG-CD   | 7.62  | 131.42      | 111.60   |
| 2   | U     | 33  | LEU  | CB-CA-C    | 7.61  | 124.66      | 110.20   |
| 1   | A     | 149 | GLN  | O-C-N      | 7.61  | 136.13      | 123.20   |
| 2   | S     | 100 | ARG  | CG-CD-NE   | 7.60  | 127.75      | 111.80   |
| 1   | A     | 269 | TYR  | CB-CG-CD1  | 7.59  | 125.56      | 121.00   |
| 1   | D     | 110 | GLU  | OE1-CD-OE2 | -7.59 | 114.19      | 123.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 96  | GLN  | CA-CB-CG   | 7.56  | 130.03      | 113.40   |
| 1   | B     | 180 | LEU  | N-CA-CB    | -7.55 | 95.29       | 110.40   |
| 1   | D     | 269 | TYR  | CB-CG-CD2  | -7.54 | 116.47      | 121.00   |
| 1   | C     | 169 | LEU  | CA-CB-CG   | 7.52  | 132.59      | 115.30   |
| 1   | C     | 72  | ASP  | OD1-CG-OD2 | -7.51 | 109.03      | 123.30   |
| 1   | D     | 431 | ARG  | NE-CZ-NH1  | 7.51  | 124.06      | 120.30   |
| 1   | A     | 226 | TYR  | CG-CD1-CE1 | -7.51 | 115.29      | 121.30   |
| 2   | V     | 26  | LEU  | CB-CA-C    | 7.51  | 124.47      | 110.20   |
| 1   | C     | 201 | LYS  | N-CA-CB    | -7.50 | 97.09       | 110.60   |
| 1   | A     | 35  | ASP  | CB-CG-OD1  | -7.50 | 111.55      | 118.30   |
| 1   | A     | 339 | ARG  | NE-CZ-NH1  | -7.50 | 116.55      | 120.30   |
| 1   | D     | 28  | GLU  | CG-CD-OE2  | -7.49 | 103.32      | 118.30   |
| 1   | D     | 351 | ASP  | CB-CG-OD2  | -7.49 | 111.56      | 118.30   |
| 1   | A     | 110 | GLU  | CA-CB-CG   | 7.49  | 129.87      | 113.40   |
| 1   | D     | 290 | LEU  | CB-CG-CD1  | -7.48 | 98.29       | 111.00   |
| 1   | A     | 134 | ARG  | NH1-CZ-NH2 | 7.47  | 127.62      | 119.40   |
| 1   | D     | 339 | ARG  | NE-CZ-NH2  | -7.47 | 116.56      | 120.30   |
| 1   | D     | 121 | VAL  | N-CA-CB    | -7.47 | 95.07       | 111.50   |
| 1   | D     | 201 | LYS  | CB-CA-C    | -7.47 | 95.47       | 110.40   |
| 1   | A     | 61  | SER  | CB-CA-C    | -7.46 | 95.93       | 110.10   |
| 1   | C     | 319 | ARG  | CA-CB-CG   | 7.46  | 129.80      | 113.40   |
| 1   | A     | 245 | GLY  | CA-C-O     | -7.45 | 107.19      | 120.60   |
| 1   | B     | 352 | ASP  | CB-CG-OD1  | -7.45 | 111.59      | 118.30   |
| 1   | A     | 159 | ARG  | NE-CZ-NH1  | -7.44 | 116.58      | 120.30   |
| 1   | C     | 215 | ARG  | NE-CZ-NH2  | 7.44  | 124.02      | 120.30   |
| 2   | S     | 7   | ILE  | CA-C-N     | 7.44  | 133.57      | 117.20   |
| 1   | B     | 127 | PHE  | CA-CB-CG   | -7.44 | 96.05       | 113.90   |
| 1   | B     | 194 | ARG  | NE-CZ-NH1  | 7.43  | 124.02      | 120.30   |
| 1   | C     | 193 | LEU  | CB-CG-CD1  | 7.43  | 123.63      | 111.00   |
| 1   | C     | 360 | ARG  | CD-NE-CZ   | -7.43 | 113.20      | 123.60   |
| 2   | S     | 47  | GLU  | OE1-CD-OE2 | 7.43  | 132.21      | 123.30   |
| 2   | V     | 114 | SER  | CB-CA-C    | 7.43  | 124.21      | 110.10   |
| 1   | A     | 137 | ASP  | CB-CG-OD1  | -7.42 | 111.62      | 118.30   |
| 2   | V     | 47  | GLU  | OE1-CD-OE2 | 7.42  | 132.20      | 123.30   |
| 1   | A     | 312 | ARG  | NE-CZ-NH2  | -7.41 | 116.59      | 120.30   |
| 1   | D     | 108 | PHE  | O-C-N      | 7.40  | 134.55      | 122.70   |
| 1   | A     | 85  | TYR  | CB-CG-CD1  | 7.40  | 125.44      | 121.00   |
| 2   | U     | 121 | GLU  | CA-CB-CG   | 7.40  | 129.68      | 113.40   |
| 1   | A     | 10  | SER  | N-CA-CB    | 7.39  | 121.59      | 110.50   |
| 1   | D     | 131 | ARG  | NE-CZ-NH1  | 7.39  | 124.00      | 120.30   |
| 1   | A     | 225 | LEU  | CB-CG-CD1  | 7.38  | 123.55      | 111.00   |
| 1   | B     | 60  | GLU  | CG-CD-OE2  | 7.37  | 133.04      | 118.30   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 97  | TYR  | CB-CG-CD2  | -7.37 | 116.58      | 121.00   |
| 1   | D     | 217 | ARG  | NE-CZ-NH2  | -7.37 | 116.62      | 120.30   |
| 2   | S     | 63  | ASP  | CA-CB-CG   | 7.36  | 129.59      | 113.40   |
| 2   | S     | 89  | GLU  | OE1-CD-OE2 | 7.36  | 132.13      | 123.30   |
| 1   | D     | 213 | ARG  | CA-CB-CG   | -7.35 | 97.22       | 113.40   |
| 1   | B     | 85  | TYR  | CB-CG-CD1  | 7.34  | 125.40      | 121.00   |
| 2   | V     | 59  | PRO  | O-C-N      | 7.34  | 135.68      | 123.20   |
| 2   | U     | 21  | LEU  | CA-CB-CG   | 7.32  | 132.13      | 115.30   |
| 2   | V     | 7   | ILE  | CA-C-N     | 7.32  | 133.29      | 117.20   |
| 1   | D     | 215 | ARG  | NE-CZ-NH1  | -7.30 | 116.65      | 120.30   |
| 1   | C     | 200 | THR  | CA-CB-CG2  | -7.30 | 102.18      | 112.40   |
| 2   | V     | 104 | PHE  | CB-CG-CD1  | -7.30 | 115.69      | 120.80   |
| 1   | D     | 136 | GLU  | OE1-CD-OE2 | 7.29  | 132.05      | 123.30   |
| 1   | D     | 24  | TYR  | CB-CA-C    | 7.28  | 124.97      | 110.40   |
| 2   | V     | 53  | ARG  | NE-CZ-NH1  | 7.28  | 123.94      | 120.30   |
| 1   | C     | 291 | LEU  | CA-CB-CG   | 7.27  | 132.03      | 115.30   |
| 2   | V     | 99  | ILE  | O-C-N      | 7.26  | 134.32      | 122.70   |
| 1   | C     | 338 | GLU  | OE1-CD-OE2 | -7.26 | 114.59      | 123.30   |
| 1   | C     | 302 | ASP  | CB-CG-OD2  | 7.25  | 124.83      | 118.30   |
| 1   | A     | 60  | GLU  | CG-CD-OE2  | 7.25  | 132.79      | 118.30   |
| 1   | B     | 169 | LEU  | CA-CB-CG   | 7.25  | 131.97      | 115.30   |
| 1   | A     | 28  | GLU  | OE1-CD-OE2 | 7.24  | 131.98      | 123.30   |
| 1   | D     | 294 | HIS  | CA-C-O     | -7.24 | 104.91      | 120.10   |
| 1   | A     | 213 | ARG  | CB-CG-CD   | 7.23  | 130.40      | 111.60   |
| 1   | D     | 202 | ASP  | CB-CG-OD2  | -7.23 | 111.80      | 118.30   |
| 1   | A     | 204 | GLU  | CG-CD-OE1  | 7.22  | 132.74      | 118.30   |
| 2   | V     | 48  | HIS  | O-C-N      | 7.21  | 135.45      | 123.20   |
| 2   | V     | 82  | GLN  | CB-CA-C    | 7.21  | 124.81      | 110.40   |
| 1   | D     | 394 | PHE  | CB-CG-CD1  | -7.20 | 115.76      | 120.80   |
| 1   | B     | 363 | TYR  | CB-CG-CD1  | -7.20 | 116.68      | 121.00   |
| 2   | V     | 57  | LYS  | N-CA-CB    | 7.20  | 123.55      | 110.60   |
| 1   | D     | 127 | PHE  | CB-CG-CD1  | -7.19 | 115.77      | 120.80   |
| 2   | V     | 115 | PHE  | O-C-N      | 7.19  | 134.21      | 122.70   |
| 1   | B     | 215 | ARG  | CD-NE-CZ   | -7.19 | 113.53      | 123.60   |
| 1   | C     | 103 | TYR  | N-CA-CB    | -7.19 | 97.67       | 110.60   |
| 2   | U     | 53  | ARG  | CD-NE-CZ   | -7.18 | 113.55      | 123.60   |
| 1   | B     | 212 | MET  | O-C-N      | 7.18  | 134.19      | 122.70   |
| 1   | D     | 156 | GLN  | CB-CG-CD   | 7.17  | 130.24      | 111.60   |
| 1   | B     | 108 | PHE  | CB-CG-CD2  | 7.17  | 125.82      | 120.80   |
| 1   | A     | 95  | ASP  | CB-CG-OD1  | -7.16 | 111.86      | 118.30   |
| 1   | C     | 360 | ARG  | NH1-CZ-NH2 | 7.16  | 127.28      | 119.40   |
| 2   | T     | 65  | ARG  | CG-CD-NE   | 7.16  | 126.83      | 111.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 79  | ARG  | CB-CA-C    | -7.15 | 96.09       | 110.40   |
| 1   | A     | 396 | ASP  | CB-CG-OD1  | 7.15  | 124.74      | 118.30   |
| 2   | V     | 58  | SER  | CB-CA-C    | 7.15  | 123.68      | 110.10   |
| 2   | S     | 32  | TYR  | CB-CG-CD2  | 7.14  | 125.28      | 121.00   |
| 1   | A     | 249 | GLU  | N-CA-CB    | 7.14  | 123.45      | 110.60   |
| 1   | C     | 198 | ASP  | CB-CG-OD1  | -7.13 | 111.88      | 118.30   |
| 1   | B     | 110 | GLU  | OE1-CD-OE2 | 7.13  | 131.85      | 123.30   |
| 1   | D     | 194 | ARG  | CD-NE-CZ   | 7.13  | 133.58      | 123.60   |
| 1   | D     | 172 | CYS  | N-CA-CB    | -7.11 | 97.80       | 110.60   |
| 1   | A     | 89  | ARG  | CA-CB-CG   | 7.11  | 129.04      | 113.40   |
| 1   | D     | 91  | VAL  | CA-C-N     | -7.11 | 101.99      | 116.20   |
| 2   | S     | 43  | GLU  | CG-CD-OE2  | 7.09  | 132.49      | 118.30   |
| 1   | C     | 130 | LEU  | O-C-N      | 7.09  | 134.05      | 122.70   |
| 2   | S     | 118 | TYR  | CB-CG-CD1  | 7.09  | 125.25      | 121.00   |
| 1   | A     | 165 | TYR  | C-N-CA     | 7.07  | 137.16      | 122.30   |
| 2   | S     | 98  | TRP  | N-CA-C     | -7.07 | 91.91       | 111.00   |
| 1   | C     | 435 | ARG  | NE-CZ-NH2  | -7.07 | 116.77      | 120.30   |
| 1   | C     | 137 | ASP  | CB-CG-OD2  | 7.06  | 124.66      | 118.30   |
| 1   | A     | 19  | GLU  | N-CA-CB    | 7.06  | 123.30      | 110.60   |
| 1   | A     | 131 | ARG  | NE-CZ-NH1  | 7.06  | 123.83      | 120.30   |
| 1   | C     | 192 | CYS  | CA-CB-SG   | -7.06 | 101.30      | 114.00   |
| 1   | D     | 257 | ALA  | CB-CA-C    | 7.05  | 120.68      | 110.10   |
| 2   | S     | 34  | LEU  | CB-CA-C    | 7.05  | 123.60      | 110.20   |
| 1   | C     | 33  | ASP  | CB-CG-OD1  | 7.04  | 124.63      | 118.30   |
| 1   | D     | 79  | ARG  | CG-CD-NE   | 7.04  | 126.58      | 111.80   |
| 2   | S     | 100 | ARG  | CB-CG-CD   | 7.03  | 129.89      | 111.60   |
| 1   | B     | 95  | ASP  | CB-CG-OD1  | -7.03 | 111.97      | 118.30   |
| 2   | V     | 53  | ARG  | O-C-N      | 7.03  | 133.95      | 122.70   |
| 2   | U     | 7   | ILE  | N-CA-C     | 7.03  | 129.97      | 111.00   |
| 1   | B     | 149 | GLN  | O-C-N      | 7.02  | 135.14      | 123.20   |
| 1   | B     | 125 | PHE  | CB-CG-CD2  | -7.01 | 115.89      | 120.80   |
| 1   | D     | 324 | ASP  | CB-CA-C    | 7.00  | 124.40      | 110.40   |
| 1   | B     | 61  | SER  | CB-CA-C    | -6.99 | 96.81       | 110.10   |
| 1   | D     | 204 | GLU  | CG-CD-OE2  | -6.99 | 104.33      | 118.30   |
| 1   | D     | 194 | ARG  | NE-CZ-NH2  | -6.98 | 116.81      | 120.30   |
| 1   | A     | 295 | ARG  | NE-CZ-NH2  | -6.97 | 116.82      | 120.30   |
| 1   | A     | 180 | LEU  | CB-CA-C    | 6.96  | 123.43      | 110.20   |
| 2   | S     | 105 | ASP  | CB-CG-OD1  | 6.96  | 124.56      | 118.30   |
| 1   | B     | 226 | TYR  | CB-CG-CD2  | 6.95  | 125.17      | 121.00   |
| 1   | C     | 35  | ASP  | CB-CG-OD1  | -6.94 | 112.05      | 118.30   |
| 1   | B     | 270 | LEU  | CA-C-O     | -6.93 | 105.54      | 120.10   |
| 2   | U     | 75  | PHE  | CA-C-O     | -6.93 | 105.54      | 120.10   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 10  | SER  | N-CA-CB    | 6.91  | 120.87      | 110.50   |
| 1   | C     | 25  | TYR  | CB-CG-CD2  | 6.91  | 125.14      | 121.00   |
| 1   | A     | 204 | GLU  | CG-CD-OE2  | -6.91 | 104.49      | 118.30   |
| 1   | D     | 358 | ARG  | NE-CZ-NH2  | 6.90  | 123.75      | 120.30   |
| 2   | V     | 75  | PHE  | CB-CG-CD1  | -6.89 | 115.98      | 120.80   |
| 1   | A     | 332 | VAL  | N-CA-CB    | -6.88 | 96.36       | 111.50   |
| 1   | A     | 110 | GLU  | OE1-CD-OE2 | -6.87 | 115.06      | 123.30   |
| 2   | S     | 65  | ARG  | NE-CZ-NH1  | 6.86  | 123.73      | 120.30   |
| 1   | D     | 24  | TYR  | N-CA-CB    | -6.86 | 98.25       | 110.60   |
| 1   | C     | 99  | ALA  | CB-CA-C    | 6.86  | 120.39      | 110.10   |
| 1   | D     | 213 | ARG  | CB-CA-C    | 6.86  | 124.11      | 110.40   |
| 1   | A     | 84  | CYS  | CA-CB-SG   | -6.84 | 101.69      | 114.00   |
| 2   | T     | 100 | ARG  | N-CA-CB    | -6.83 | 98.31       | 110.60   |
| 2   | T     | 66  | TYR  | CB-CG-CD2  | 6.83  | 125.10      | 121.00   |
| 1   | D     | 213 | ARG  | NH1-CZ-NH2 | -6.82 | 111.90      | 119.40   |
| 1   | B     | 204 | GLU  | CG-CD-OE2  | -6.82 | 104.66      | 118.30   |
| 1   | A     | 341 | ILE  | O-C-N      | 6.81  | 133.60      | 122.70   |
| 1   | A     | 454 | GLU  | OE1-CD-OE2 | 6.81  | 131.47      | 123.30   |
| 1   | B     | 89  | ARG  | CA-CB-CG   | 6.81  | 128.38      | 113.40   |
| 1   | D     | 25  | TYR  | CB-CG-CD2  | 6.81  | 125.08      | 121.00   |
| 2   | U     | 109 | GLN  | CB-CG-CD   | 6.79  | 129.25      | 111.60   |
| 1   | A     | 292 | HIS  | CA-C-O     | -6.78 | 105.85      | 120.10   |
| 1   | A     | 95  | ASP  | CB-CG-OD2  | 6.78  | 124.40      | 118.30   |
| 1   | C     | 339 | ARG  | NH1-CZ-NH2 | 6.78  | 126.85      | 119.40   |
| 1   | D     | 165 | TYR  | CB-CG-CD2  | 6.77  | 125.06      | 121.00   |
| 1   | D     | 64  | GLY  | N-CA-C     | 6.77  | 130.02      | 113.10   |
| 1   | A     | 200 | THR  | CA-C-N     | 6.76  | 132.07      | 117.20   |
| 1   | C     | 121 | VAL  | N-CA-CB    | -6.76 | 96.63       | 111.50   |
| 2   | S     | 107 | VAL  | O-C-N      | 6.76  | 133.51      | 122.70   |
| 1   | A     | 125 | PHE  | CA-C-N     | 6.75  | 129.70      | 116.20   |
| 1   | A     | 101 | VAL  | CG1-CB-CG2 | 6.75  | 121.69      | 110.90   |
| 1   | C     | 74  | LEU  | CA-CB-CG   | 6.74  | 130.81      | 115.30   |
| 1   | A     | 207 | ASN  | OD1-CG-ND2 | 6.74  | 137.40      | 121.90   |
| 1   | C     | 153 | HIS  | CA-CB-CG   | -6.74 | 102.14      | 113.60   |
| 2   | S     | 48  | HIS  | CA-C-N     | -6.74 | 102.73      | 116.20   |
| 2   | U     | 98  | TRP  | N-CA-CB    | 6.73  | 122.72      | 110.60   |
| 2   | S     | 1   | MET  | CG-SD-CE   | 6.72  | 110.95      | 100.20   |
| 2   | V     | 21  | LEU  | CA-CB-CG   | 6.72  | 130.76      | 115.30   |
| 2   | V     | 7   | ILE  | N-CA-C     | 6.71  | 129.13      | 111.00   |
| 1   | D     | 110 | GLU  | CG-CD-OE2  | 6.71  | 131.72      | 118.30   |
| 2   | T     | 79  | ASP  | CB-CG-OD1  | -6.71 | 112.26      | 118.30   |
| 2   | U     | 7   | ILE  | CA-C-N     | 6.70  | 131.94      | 117.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 60  | GLU  | CG-CD-OE1  | -6.70 | 104.91      | 118.30   |
| 2   | V     | 61  | TYR  | O-C-N      | 6.69  | 133.41      | 122.70   |
| 1   | A     | 106 | ASP  | CB-CG-OD1  | 6.69  | 124.32      | 118.30   |
| 2   | V     | 42  | LEU  | CB-CG-CD1  | 6.69  | 122.37      | 111.00   |
| 1   | D     | 454 | GLU  | OE1-CD-OE2 | 6.68  | 131.32      | 123.30   |
| 2   | U     | 36  | ASN  | OD1-CG-ND2 | 6.67  | 137.25      | 121.90   |
| 1   | C     | 431 | ARG  | NE-CZ-NH2  | -6.67 | 116.97      | 120.30   |
| 1   | C     | 92  | GLY  | O-C-N      | 6.66  | 133.36      | 122.70   |
| 1   | A     | 173 | THR  | CA-CB-CG2  | 6.66  | 121.72      | 112.40   |
| 1   | B     | 377 | VAL  | CA-C-O     | 6.66  | 134.08      | 120.10   |
| 2   | V     | 13  | GLU  | CG-CD-OE2  | -6.66 | 104.99      | 118.30   |
| 1   | C     | 200 | THR  | CA-C-O     | -6.65 | 106.13      | 120.10   |
| 1   | C     | 89  | ARG  | CA-CB-CG   | 6.65  | 128.03      | 113.40   |
| 2   | S     | 89  | GLU  | CA-CB-CG   | 6.64  | 128.01      | 113.40   |
| 2   | V     | 34  | LEU  | CB-CA-C    | 6.64  | 122.82      | 110.20   |
| 2   | S     | 26  | LEU  | CB-CA-C    | 6.64  | 122.81      | 110.20   |
| 1   | B     | 204 | GLU  | CG-CD-OE1  | 6.64  | 131.57      | 118.30   |
| 1   | B     | 238 | HIS  | CA-C-N     | 6.63  | 131.78      | 117.20   |
| 1   | C     | 26  | THR  | CA-CB-CG2  | 6.63  | 121.68      | 112.40   |
| 1   | B     | 96  | GLN  | CA-CB-CG   | 6.63  | 127.98      | 113.40   |
| 1   | A     | 86  | ARG  | N-CA-CB    | 6.62  | 122.52      | 110.60   |
| 1   | B     | 360 | ARG  | NE-CZ-NH2  | 6.62  | 123.61      | 120.30   |
| 1   | D     | 387 | MET  | CA-CB-CG   | -6.62 | 102.06      | 113.30   |
| 2   | V     | 98  | TRP  | N-CA-C     | -6.61 | 93.15       | 111.00   |
| 1   | A     | 24  | TYR  | CB-CA-C    | 6.61  | 123.62      | 110.40   |
| 1   | B     | 153 | HIS  | CA-CB-CG   | -6.60 | 102.38      | 113.60   |
| 2   | V     | 44  | PHE  | CB-CG-CD2  | -6.60 | 116.18      | 120.80   |
| 1   | C     | 52  | GLU  | N-CA-CB    | 6.59  | 122.46      | 110.60   |
| 1   | A     | 97  | TYR  | CB-CA-C    | -6.59 | 97.23       | 110.40   |
| 1   | B     | 203 | ASP  | CB-CG-OD1  | 6.59  | 124.23      | 118.30   |
| 1   | A     | 278 | THR  | CA-CB-OG1  | -6.58 | 95.17       | 109.00   |
| 1   | B     | 91  | VAL  | O-C-N      | 6.58  | 134.39      | 123.20   |
| 1   | D     | 10  | SER  | N-CA-CB    | 6.58  | 120.37      | 110.50   |
| 2   | S     | 52  | TYR  | CA-CB-CG   | 6.58  | 125.89      | 113.40   |
| 1   | B     | 247 | CYS  | CA-CB-SG   | 6.58  | 125.84      | 114.00   |
| 1   | B     | 52  | GLU  | N-CA-CB    | 6.57  | 122.43      | 110.60   |
| 1   | C     | 218 | PHE  | CB-CG-CD1  | 6.57  | 125.40      | 120.80   |
| 2   | T     | 60  | GLY  | O-C-N      | -6.57 | 112.19      | 122.70   |
| 2   | T     | 108 | ARG  | NE-CZ-NH2  | 6.56  | 123.58      | 120.30   |
| 1   | B     | 24  | TYR  | CB-CA-C    | 6.55  | 123.51      | 110.40   |
| 1   | D     | 158 | GLU  | CG-CD-OE2  | 6.55  | 131.41      | 118.30   |
| 2   | V     | 86  | GLU  | OE1-CD-OE2 | 6.55  | 131.16      | 123.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | T     | 105 | ASP  | CB-CG-OD2  | -6.55 | 112.41      | 118.30   |
| 1   | C     | 324 | ASP  | CB-CG-OD1  | 6.54  | 124.19      | 118.30   |
| 1   | B     | 288 | GLY  | C-N-CA     | 6.53  | 138.01      | 121.70   |
| 1   | C     | 431 | ARG  | CG-CD-NE   | 6.53  | 125.51      | 111.80   |
| 1   | B     | 259 | GLU  | CB-CG-CD   | 6.52  | 131.81      | 114.20   |
| 1   | D     | 467 | PHE  | CB-CG-CD1  | -6.52 | 116.23      | 120.80   |
| 1   | D     | 280 | LEU  | CB-CA-C    | 6.51  | 122.58      | 110.20   |
| 2   | T     | 21  | LEU  | CA-CB-CG   | 6.51  | 130.27      | 115.30   |
| 1   | B     | 360 | ARG  | CD-NE-CZ   | -6.51 | 114.49      | 123.60   |
| 1   | D     | 431 | ARG  | CD-NE-CZ   | -6.50 | 114.49      | 123.60   |
| 1   | B     | 319 | ARG  | NH1-CZ-NH2 | -6.50 | 112.25      | 119.40   |
| 1   | B     | 13  | PHE  | O-C-N      | 6.50  | 133.10      | 122.70   |
| 1   | D     | 144 | TYR  | CG-CD1-CE1 | 6.50  | 126.50      | 121.30   |
| 2   | T     | 82  | GLN  | CB-CA-C    | 6.49  | 123.38      | 110.40   |
| 2   | T     | 50  | PHE  | O-C-N      | -6.48 | 112.33      | 122.70   |
| 1   | C     | 183 | LYS  | CA-CB-CG   | -6.47 | 99.17       | 113.40   |
| 2   | T     | 45  | GLU  | CA-CB-CG   | 6.47  | 127.63      | 113.40   |
| 1   | A     | 110 | GLU  | CG-CD-OE2  | 6.47  | 131.23      | 118.30   |
| 2   | U     | 75  | PHE  | O-C-N      | 6.47  | 134.19      | 123.20   |
| 2   | V     | 57  | LYS  | CA-C-O     | -6.47 | 106.52      | 120.10   |
| 1   | C     | 110 | GLU  | CA-CB-CG   | 6.46  | 127.62      | 113.40   |
| 1   | B     | 239 | TYR  | CB-CG-CD1  | 6.46  | 124.88      | 121.00   |
| 1   | A     | 212 | MET  | O-C-N      | 6.45  | 133.03      | 122.70   |
| 1   | C     | 135 | LEU  | CB-CA-C    | 6.45  | 122.45      | 110.20   |
| 1   | D     | 139 | ARG  | CD-NE-CZ   | -6.45 | 114.58      | 123.60   |
| 1   | A     | 203 | ASP  | N-CA-CB    | 6.44  | 122.19      | 110.60   |
| 1   | C     | 468 | ASN  | N-CA-CB    | 6.44  | 122.19      | 110.60   |
| 1   | D     | 436 | ASP  | CB-CG-OD1  | 6.43  | 124.09      | 118.30   |
| 1   | A     | 180 | LEU  | N-CA-CB    | -6.42 | 97.55       | 110.40   |
| 1   | D     | 189 | VAL  | CA-CB-CG1  | 6.42  | 120.53      | 110.90   |
| 2   | T     | 33  | LEU  | CA-CB-CG   | 6.42  | 130.06      | 115.30   |
| 1   | D     | 332 | VAL  | N-CA-CB    | -6.41 | 97.40       | 111.50   |
| 1   | B     | 347 | ASP  | CA-CB-CG   | 6.41  | 127.50      | 113.40   |
| 1   | C     | 156 | GLN  | CB-CG-CD   | 6.41  | 128.26      | 111.60   |
| 1   | A     | 215 | ARG  | CB-CG-CD   | 6.41  | 128.25      | 111.60   |
| 1   | B     | 159 | ARG  | NE-CZ-NH1  | -6.39 | 117.10      | 120.30   |
| 1   | B     | 225 | LEU  | CB-CG-CD2  | -6.39 | 100.13      | 111.00   |
| 1   | D     | 95  | ASP  | CB-CG-OD1  | -6.39 | 112.54      | 118.30   |
| 1   | C     | 89  | ARG  | O-C-N      | 6.39  | 132.92      | 122.70   |
| 1   | C     | 220 | PHE  | O-C-N      | 6.39  | 132.92      | 122.70   |
| 1   | C     | 357 | ASP  | CB-CG-OD1  | -6.38 | 112.56      | 118.30   |
| 1   | C     | 19  | GLU  | CA-CB-CG   | 6.38  | 127.43      | 113.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 281 | ALA  | N-CA-CB    | 6.38  | 119.03      | 110.10   |
| 1   | B     | 226 | TYR  | CA-C-O     | -6.38 | 106.71      | 120.10   |
| 2   | T     | 112 | CYS  | CA-CB-SG   | -6.37 | 102.54      | 114.00   |
| 2   | S     | 38  | TRP  | CB-CG-CD2  | -6.36 | 118.33      | 126.60   |
| 1   | D     | 326 | ILE  | N-CA-CB    | 6.36  | 125.44      | 110.80   |
| 1   | C     | 79  | ARG  | CG-CD-NE   | 6.36  | 125.16      | 111.80   |
| 2   | S     | 100 | ARG  | NE-CZ-NH2  | -6.36 | 117.12      | 120.30   |
| 1   | A     | 292 | HIS  | O-C-N      | 6.35  | 132.86      | 122.70   |
| 1   | B     | 159 | ARG  | NE-CZ-NH2  | 6.35  | 123.48      | 120.30   |
| 1   | B     | 194 | ARG  | NE-CZ-NH2  | 6.35  | 123.47      | 120.30   |
| 1   | D     | 60  | GLU  | CG-CD-OE2  | 6.35  | 131.00      | 118.30   |
| 2   | U     | 82  | GLN  | CB-CG-CD   | 6.34  | 128.08      | 111.60   |
| 1   | D     | 296 | ALA  | N-CA-CB    | -6.34 | 101.23      | 110.10   |
| 1   | B     | 201 | LYS  | N-CA-CB    | -6.33 | 99.21       | 110.60   |
| 1   | D     | 291 | LEU  | O-C-N      | 6.33  | 132.83      | 122.70   |
| 2   | U     | 111 | GLN  | N-CA-C     | -6.32 | 93.93       | 111.00   |
| 1   | D     | 350 | ARG  | CB-CG-CD   | -6.32 | 95.17       | 111.60   |
| 1   | D     | 92  | GLY  | O-C-N      | 6.32  | 132.81      | 122.70   |
| 1   | C     | 160 | ASP  | O-C-N      | 6.31  | 132.80      | 122.70   |
| 1   | D     | 41  | ARG  | CD-NE-CZ   | -6.31 | 114.77      | 123.60   |
| 2   | V     | 63  | ASP  | CA-CB-CG   | 6.31  | 127.28      | 113.40   |
| 1   | A     | 24  | TYR  | N-CA-CB    | -6.31 | 99.25       | 110.60   |
| 1   | D     | 159 | ARG  | CD-NE-CZ   | -6.30 | 114.78      | 123.60   |
| 2   | T     | 66  | TYR  | CB-CG-CD1  | -6.30 | 117.22      | 121.00   |
| 2   | V     | 100 | ARG  | CA-CB-CG   | 6.30  | 127.27      | 113.40   |
| 1   | D     | 328 | SER  | CA-C-O     | -6.29 | 106.88      | 120.10   |
| 1   | B     | 331 | VAL  | C-N-CA     | 6.29  | 137.41      | 121.70   |
| 2   | U     | 40  | PRO  | O-C-N      | 6.28  | 132.75      | 122.70   |
| 1   | A     | 194 | ARG  | N-CA-CB    | 6.28  | 121.90      | 110.60   |
| 2   | V     | 48  | HIS  | CA-CB-CG   | -6.28 | 102.92      | 113.60   |
| 2   | U     | 43  | GLU  | CA-CB-CG   | 6.28  | 127.21      | 113.40   |
| 1   | B     | 383 | HIS  | O-C-N      | 6.28  | 132.74      | 122.70   |
| 1   | B     | 88  | GLU  | O-C-N      | 6.27  | 132.73      | 122.70   |
| 1   | B     | 202 | ASP  | CB-CG-OD1  | 6.27  | 123.94      | 118.30   |
| 1   | B     | 194 | ARG  | NH1-CZ-NH2 | -6.27 | 112.51      | 119.40   |
| 2   | U     | 55  | ASN  | CA-CB-CG   | -6.26 | 99.62       | 113.40   |
| 2   | V     | 20  | ASP  | CB-CG-OD1  | -6.26 | 112.66      | 118.30   |
| 1   | D     | 193 | LEU  | CA-CB-CG   | 6.26  | 129.69      | 115.30   |
| 2   | U     | 7   | ILE  | CA-C-O     | -6.26 | 106.96      | 120.10   |
| 1   | D     | 269 | TYR  | CB-CG-CD1  | 6.26  | 124.75      | 121.00   |
| 2   | S     | 89  | GLU  | CG-CD-OE1  | -6.25 | 105.79      | 118.30   |
| 2   | U     | 94  | TYR  | CB-CG-CD1  | -6.25 | 117.25      | 121.00   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 83  | ARG  | CD-NE-CZ   | 6.25  | 132.35      | 123.60   |
| 1   | A     | 93  | GLU  | CA-C-N     | -6.25 | 103.45      | 117.20   |
| 1   | A     | 433 | GLU  | CB-CG-CD   | 6.25  | 131.06      | 114.20   |
| 1   | D     | 30  | GLN  | O-C-N      | 6.24  | 132.69      | 122.70   |
| 1   | D     | 394 | PHE  | CA-C-N     | 6.23  | 128.67      | 116.20   |
| 1   | C     | 447 | GLU  | CG-CD-OE1  | -6.22 | 105.86      | 118.30   |
| 1   | D     | 253 | ARG  | NH1-CZ-NH2 | 6.22  | 126.25      | 119.40   |
| 2   | V     | 94  | TYR  | CB-CG-CD1  | -6.22 | 117.27      | 121.00   |
| 2   | T     | 98  | TRP  | N-CA-CB    | 6.22  | 121.79      | 110.60   |
| 1   | C     | 445 | ILE  | CB-CA-C    | 6.21  | 124.03      | 111.60   |
| 1   | C     | 324 | ASP  | CB-CG-OD2  | -6.21 | 112.71      | 118.30   |
| 1   | A     | 88  | GLU  | CG-CD-OE1  | -6.21 | 105.88      | 118.30   |
| 2   | U     | 54  | GLU  | CG-CD-OE1  | -6.20 | 105.89      | 118.30   |
| 1   | A     | 213 | ARG  | CD-NE-CZ   | 6.20  | 132.28      | 123.60   |
| 2   | U     | 111 | GLN  | N-CA-CB    | 6.20  | 121.76      | 110.60   |
| 1   | D     | 319 | ARG  | NH1-CZ-NH2 | 6.20  | 126.21      | 119.40   |
| 1   | A     | 196 | GLY  | C-N-CA     | 6.19  | 137.18      | 121.70   |
| 1   | C     | 61  | SER  | CA-CB-OG   | -6.19 | 94.48       | 111.20   |
| 1   | A     | 469 | PHE  | N-CA-CB    | 6.19  | 121.75      | 110.60   |
| 1   | C     | 110 | GLU  | N-CA-CB    | -6.19 | 99.46       | 110.60   |
| 1   | D     | 334 | LYS  | CA-CB-CG   | 6.19  | 127.02      | 113.40   |
| 1   | A     | 409 | HIS  | CA-CB-CG   | 6.19  | 124.12      | 113.60   |
| 1   | D     | 294 | HIS  | O-C-N      | 6.18  | 132.60      | 122.70   |
| 1   | D     | 165 | TYR  | C-N-CA     | 6.18  | 135.28      | 122.30   |
| 1   | A     | 248 | GLU  | CA-CB-CG   | 6.18  | 126.99      | 113.40   |
| 1   | B     | 300 | VAL  | CG1-CB-CG2 | 6.17  | 120.78      | 110.90   |
| 1   | A     | 360 | ARG  | NH1-CZ-NH2 | 6.17  | 126.19      | 119.40   |
| 1   | A     | 135 | LEU  | CB-CA-C    | 6.17  | 121.92      | 110.20   |
| 2   | T     | 82  | GLN  | CA-CB-CG   | 6.17  | 126.96      | 113.40   |
| 2   | S     | 110 | VAL  | CA-CB-CG1  | 6.16  | 120.14      | 110.90   |
| 2   | V     | 43  | GLU  | CG-CD-OE1  | 6.16  | 130.63      | 118.30   |
| 1   | B     | 246 | THR  | O-C-N      | 6.16  | 132.56      | 122.70   |
| 1   | C     | 19  | GLU  | N-CA-CB    | 6.16  | 121.69      | 110.60   |
| 1   | D     | 296 | ALA  | CB-CA-C    | 6.16  | 119.34      | 110.10   |
| 1   | D     | 298 | HIS  | CA-CB-CG   | 6.16  | 124.07      | 113.60   |
| 1   | C     | 413 | ASN  | CA-CB-CG   | 6.16  | 126.94      | 113.40   |
| 1   | B     | 26  | THR  | CA-CB-CG2  | 6.15  | 121.01      | 112.40   |
| 1   | D     | 199 | PHE  | CB-CG-CD1  | -6.15 | 116.50      | 120.80   |
| 1   | C     | 187 | ARG  | CD-NE-CZ   | 6.14  | 132.20      | 123.60   |
| 1   | A     | 201 | LYS  | CB-CA-C    | -6.14 | 98.12       | 110.40   |
| 2   | V     | 20  | ASP  | CB-CG-OD2  | -6.14 | 112.77      | 118.30   |
| 2   | S     | 111 | GLN  | N-CA-C     | -6.14 | 94.43       | 111.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | U     | 44  | PHE  | CB-CG-CD2  | -6.14 | 116.50      | 120.80   |
| 2   | U     | 110 | VAL  | CG1-CB-CG2 | -6.13 | 101.08      | 110.90   |
| 2   | U     | 118 | TYR  | CB-CG-CD1  | 6.13  | 124.68      | 121.00   |
| 1   | C     | 281 | ALA  | CB-CA-C    | -6.13 | 100.90      | 110.10   |
| 1   | C     | 61  | SER  | CB-CA-C    | -6.12 | 98.46       | 110.10   |
| 1   | B     | 213 | ARG  | NE-CZ-NH2  | -6.12 | 117.24      | 120.30   |
| 2   | U     | 110 | VAL  | O-C-N      | 6.12  | 132.50      | 122.70   |
| 1   | B     | 396 | ASP  | CB-CG-OD1  | 6.12  | 123.81      | 118.30   |
| 1   | C     | 89  | ARG  | N-CA-CB    | 6.12  | 121.61      | 110.60   |
| 1   | D     | 136 | GLU  | CG-CD-OE2  | -6.12 | 106.06      | 118.30   |
| 1   | D     | 402 | PHE  | CA-C-O     | 6.12  | 132.95      | 120.10   |
| 1   | A     | 160 | ASP  | CB-CG-OD1  | -6.12 | 112.80      | 118.30   |
| 1   | C     | 159 | ARG  | NE-CZ-NH1  | -6.11 | 117.25      | 120.30   |
| 1   | C     | 435 | ARG  | CD-NE-CZ   | -6.10 | 115.05      | 123.60   |
| 1   | C     | 144 | TYR  | CB-CG-CD2  | 6.10  | 124.66      | 121.00   |
| 2   | T     | 100 | ARG  | NE-CZ-NH2  | -6.09 | 117.25      | 120.30   |
| 1   | C     | 207 | ASN  | CA-CB-CG   | 6.09  | 126.81      | 113.40   |
| 1   | A     | 217 | ARG  | NH1-CZ-NH2 | -6.09 | 112.70      | 119.40   |
| 1   | B     | 165 | TYR  | CB-CG-CD2  | 6.09  | 124.65      | 121.00   |
| 1   | D     | 103 | TYR  | CG-CD1-CE1 | 6.09  | 126.17      | 121.30   |
| 2   | T     | 75  | PHE  | CB-CG-CD1  | -6.08 | 116.54      | 120.80   |
| 2   | S     | 66  | TYR  | CG-CD2-CE2 | 6.08  | 126.16      | 121.30   |
| 1   | D     | 406 | THR  | CA-CB-CG2  | 6.08  | 120.91      | 112.40   |
| 1   | B     | 460 | GLU  | CG-CD-OE2  | 6.08  | 130.45      | 118.30   |
| 1   | C     | 326 | ILE  | N-CA-CB    | 6.08  | 124.77      | 110.80   |
| 2   | S     | 98  | TRP  | N-CA-CB    | 6.07  | 121.52      | 110.60   |
| 1   | D     | 201 | LYS  | N-CA-CB    | -6.06 | 99.70       | 110.60   |
| 2   | S     | 74  | MET  | CG-SD-CE   | 6.06  | 109.89      | 100.20   |
| 1   | B     | 303 | ARG  | CG-CD-NE   | -6.06 | 99.08       | 111.80   |
| 1   | C     | 201 | LYS  | CB-CA-C    | -6.06 | 98.29       | 110.40   |
| 1   | C     | 97  | TYR  | CB-CG-CD1  | 6.05  | 124.63      | 121.00   |
| 1   | C     | 321 | SER  | O-C-N      | -6.05 | 112.91      | 123.20   |
| 2   | U     | 82  | GLN  | CB-CA-C    | 6.05  | 122.51      | 110.40   |
| 2   | V     | 56  | ASN  | O-C-N      | 6.05  | 132.39      | 122.70   |
| 2   | V     | 47  | GLU  | CG-CD-OE2  | -6.05 | 106.19      | 118.30   |
| 1   | A     | 257 | ALA  | CB-CA-C    | 6.05  | 119.17      | 110.10   |
| 1   | D     | 469 | PHE  | N-CA-CB    | 6.05  | 121.49      | 110.60   |
| 1   | D     | 421 | ARG  | NH1-CZ-NH2 | 6.05  | 126.05      | 119.40   |
| 1   | B     | 19  | GLU  | CA-CB-CG   | 6.05  | 126.70      | 113.40   |
| 1   | A     | 201 | LYS  | N-CA-CB    | -6.04 | 99.72       | 110.60   |
| 1   | A     | 217 | ARG  | N-CA-CB    | 6.04  | 121.48      | 110.60   |
| 1   | C     | 355 | GLU  | N-CA-CB    | -6.03 | 99.74       | 110.60   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 139 | ARG  | CD-NE-CZ   | -6.03 | 115.16      | 123.60   |
| 1   | B     | 466 | VAL  | O-C-N      | 6.03  | 132.34      | 122.70   |
| 1   | B     | 133 | LEU  | O-C-N      | 6.02  | 132.33      | 122.70   |
| 1   | C     | 256 | PHE  | CB-CG-CD2  | -6.02 | 116.59      | 120.80   |
| 1   | C     | 265 | VAL  | O-C-N      | 6.02  | 132.33      | 122.70   |
| 1   | B     | 211 | PHE  | CB-CG-CD2  | 6.01  | 125.01      | 120.80   |
| 1   | C     | 190 | TYR  | CB-CG-CD2  | 6.01  | 124.61      | 121.00   |
| 1   | C     | 303 | ARG  | CG-CD-NE   | -6.01 | 99.18       | 111.80   |
| 1   | D     | 213 | ARG  | NE-CZ-NH1  | 6.00  | 123.30      | 120.30   |
| 2   | V     | 85  | ALA  | CA-C-N     | -6.00 | 103.99      | 117.20   |
| 1   | D     | 285 | ARG  | CD-NE-CZ   | -6.00 | 115.20      | 123.60   |
| 1   | A     | 167 | ARG  | NE-CZ-NH2  | 6.00  | 123.30      | 120.30   |
| 1   | A     | 138 | LEU  | CA-CB-CG   | 5.99  | 129.09      | 115.30   |
| 1   | A     | 431 | ARG  | NE-CZ-NH2  | -5.99 | 117.31      | 120.30   |
| 1   | B     | 350 | ARG  | CA-CB-CG   | 5.99  | 126.57      | 113.40   |
| 1   | A     | 357 | ASP  | CB-CG-OD2  | 5.98  | 123.69      | 118.30   |
| 2   | T     | 100 | ARG  | CA-CB-CG   | 5.98  | 126.56      | 113.40   |
| 1   | B     | 307 | HIS  | CB-CA-C    | -5.98 | 98.44       | 110.40   |
| 1   | D     | 32  | LYS  | N-CA-CB    | 5.98  | 121.36      | 110.60   |
| 1   | D     | 89  | ARG  | N-CA-CB    | 5.97  | 121.35      | 110.60   |
| 1   | D     | 244 | ALA  | O-C-N      | -5.97 | 113.06      | 123.20   |
| 1   | A     | 355 | GLU  | CG-CD-OE2  | -5.96 | 106.37      | 118.30   |
| 1   | B     | 97  | TYR  | CB-CA-C    | -5.96 | 98.47       | 110.40   |
| 1   | A     | 347 | ASP  | CB-CG-OD2  | -5.96 | 112.94      | 118.30   |
| 1   | C     | 203 | ASP  | N-CA-C     | -5.96 | 94.92       | 111.00   |
| 1   | A     | 194 | ARG  | CD-NE-CZ   | 5.95  | 131.93      | 123.60   |
| 1   | C     | 321 | SER  | CB-CA-C    | 5.95  | 121.40      | 110.10   |
| 1   | D     | 244 | ALA  | CA-C-O     | 5.95  | 132.59      | 120.10   |
| 2   | S     | 9   | LYS  | CA-CB-CG   | 5.94  | 126.47      | 113.40   |
| 1   | A     | 44  | PRO  | CA-C-N     | -5.94 | 104.14      | 117.20   |
| 2   | V     | 2   | GLN  | CA-CB-CG   | 5.93  | 126.45      | 113.40   |
| 1   | C     | 334 | LYS  | CA-CB-CG   | 5.93  | 126.44      | 113.40   |
| 1   | A     | 285 | ARG  | CG-CD-NE   | -5.93 | 99.36       | 111.80   |
| 1   | B     | 217 | ARG  | N-CA-CB    | 5.92  | 121.26      | 110.60   |
| 1   | B     | 409 | HIS  | CA-CB-CG   | 5.92  | 123.67      | 113.60   |
| 1   | C     | 52  | GLU  | N-CA-C     | -5.92 | 95.00       | 111.00   |
| 1   | C     | 311 | PHE  | CB-CG-CD1  | -5.92 | 116.65      | 120.80   |
| 1   | A     | 26  | THR  | CA-CB-CG2  | 5.92  | 120.69      | 112.40   |
| 1   | A     | 351 | ASP  | CB-CG-OD2  | -5.92 | 112.97      | 118.30   |
| 2   | V     | 20  | ASP  | OD1-CG-OD2 | 5.92  | 134.54      | 123.30   |
| 1   | B     | 347 | ASP  | OD1-CG-OD2 | -5.92 | 112.06      | 123.30   |
| 1   | B     | 340 | ASP  | O-C-N      | 5.92  | 132.16      | 122.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | V     | 2   | GLN  | CA-C-N     | -5.92 | 104.19      | 117.20   |
| 2   | S     | 49  | GLY  | CA-C-O     | -5.91 | 109.95      | 120.60   |
| 2   | S     | 109 | GLN  | CB-CG-CD   | 5.91  | 126.98      | 111.60   |
| 1   | D     | 217 | ARG  | NE-CZ-NH1  | 5.91  | 123.26      | 120.30   |
| 1   | C     | 350 | ARG  | CB-CG-CD   | -5.91 | 96.25       | 111.60   |
| 1   | C     | 293 | ILE  | C-N-CA     | 5.90  | 136.46      | 121.70   |
| 1   | B     | 29  | TYR  | CA-C-N     | -5.90 | 104.22      | 117.20   |
| 2   | V     | 105 | ASP  | CB-CG-OD2  | -5.90 | 112.99      | 118.30   |
| 1   | D     | 203 | ASP  | N-CA-C     | -5.90 | 95.07       | 111.00   |
| 1   | B     | 454 | GLU  | CG-CD-OE2  | -5.90 | 106.51      | 118.30   |
| 1   | A     | 93  | GLU  | CG-CD-OE2  | 5.90  | 130.09      | 118.30   |
| 1   | A     | 213 | ARG  | NH1-CZ-NH2 | -5.89 | 112.92      | 119.40   |
| 1   | A     | 202 | ASP  | CB-CG-OD2  | 5.89  | 123.60      | 118.30   |
| 1   | A     | 79  | ARG  | CB-CA-C    | -5.89 | 98.62       | 110.40   |
| 1   | D     | 391 | THR  | N-CA-CB    | 5.89  | 121.49      | 110.30   |
| 1   | B     | 253 | ARG  | NE-CZ-NH2  | -5.89 | 117.36      | 120.30   |
| 1   | D     | 406 | THR  | N-CA-CB    | 5.89  | 121.48      | 110.30   |
| 1   | A     | 194 | ARG  | NH1-CZ-NH2 | -5.88 | 112.93      | 119.40   |
| 1   | B     | 37  | LEU  | O-C-N      | 5.88  | 132.11      | 122.70   |
| 1   | C     | 469 | PHE  | N-CA-CB    | 5.88  | 121.19      | 110.60   |
| 1   | A     | 283 | TYR  | CB-CG-CD2  | -5.88 | 117.47      | 121.00   |
| 1   | B     | 121 | VAL  | N-CA-CB    | -5.88 | 98.56       | 111.50   |
| 1   | C     | 295 | ARG  | O-C-N      | 5.88  | 132.11      | 122.70   |
| 2   | V     | 77  | CYS  | CA-CB-SG   | -5.88 | 103.41      | 114.00   |
| 1   | C     | 165 | TYR  | C-N-CA     | 5.88  | 134.64      | 122.30   |
| 2   | U     | 65  | ARG  | CG-CD-NE   | 5.88  | 124.14      | 111.80   |
| 1   | D     | 204 | GLU  | CG-CD-OE1  | 5.88  | 130.06      | 118.30   |
| 1   | B     | 431 | ARG  | NE-CZ-NH1  | -5.88 | 117.36      | 120.30   |
| 1   | C     | 100 | TYR  | N-CA-CB    | 5.87  | 121.17      | 110.60   |
| 2   | U     | 98  | TRP  | N-CA-C     | -5.87 | 95.14       | 111.00   |
| 2   | V     | 32  | TYR  | CA-C-O     | 5.87  | 132.43      | 120.10   |
| 1   | C     | 234 | GLU  | OE1-CD-OE2 | 5.87  | 130.34      | 123.30   |
| 1   | B     | 357 | ASP  | CB-CG-OD1  | -5.87 | 113.02      | 118.30   |
| 2   | S     | 93  | ALA  | N-CA-CB    | 5.86  | 118.30      | 110.10   |
| 2   | V     | 93  | ALA  | N-CA-CB    | 5.86  | 118.30      | 110.10   |
| 1   | A     | 335 | LEU  | CA-CB-CG   | 5.86  | 128.77      | 115.30   |
| 1   | D     | 86  | ARG  | O-C-N      | 5.86  | 132.07      | 122.70   |
| 1   | D     | 203 | ASP  | CB-CG-OD2  | -5.85 | 113.03      | 118.30   |
| 1   | A     | 338 | GLU  | CA-C-O     | 5.85  | 132.39      | 120.10   |
| 1   | B     | 110 | GLU  | CG-CD-OE1  | -5.85 | 106.61      | 118.30   |
| 2   | T     | 2   | GLN  | N-CA-CB    | 5.85  | 121.12      | 110.60   |
| 2   | S     | 48  | HIS  | O-C-N      | 5.85  | 133.14      | 123.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | V     | 53  | ARG  | CD-NE-CZ    | -5.84 | 115.42      | 123.60   |
| 1   | A     | 187 | ARG  | CD-NE-CZ    | 5.84  | 131.78      | 123.60   |
| 1   | C     | 153 | HIS  | CB-CA-C     | -5.84 | 98.72       | 110.40   |
| 1   | D     | 258 | ARG  | NH1-CZ-NH2  | -5.84 | 112.98      | 119.40   |
| 1   | A     | 338 | GLU  | OE1-CD-OE2  | -5.84 | 116.29      | 123.30   |
| 1   | B     | 443 | GLU  | OE1-CD-OE2  | -5.84 | 116.30      | 123.30   |
| 2   | V     | 90  | ALA  | CB-CA-C     | 5.84  | 118.86      | 110.10   |
| 1   | A     | 82  | GLY  | N-CA-C      | -5.83 | 98.51       | 113.10   |
| 1   | C     | 93  | GLU  | CA-C-N      | -5.83 | 104.37      | 117.20   |
| 1   | D     | 433 | GLU  | OE1-CD-OE2  | 5.83  | 130.30      | 123.30   |
| 1   | B     | 193 | LEU  | CB-CG-CD1   | 5.83  | 120.91      | 111.00   |
| 2   | S     | 7   | ILE  | C-N-CA      | -5.83 | 107.13      | 121.70   |
| 1   | C     | 323 | GLY  | N-CA-C      | -5.83 | 98.53       | 113.10   |
| 1   | D     | 35  | ASP  | CB-CG-OD2   | 5.83  | 123.54      | 118.30   |
| 1   | C     | 108 | PHE  | CB-CG-CD2   | -5.82 | 116.72      | 120.80   |
| 1   | C     | 255 | VAL  | CG1-CB-CG2  | 5.82  | 120.22      | 110.90   |
| 1   | D     | 274 | PHE  | CB-CG-CD2   | -5.82 | 116.73      | 120.80   |
| 1   | C     | 220 | PHE  | CA-C-O      | -5.81 | 107.90      | 120.10   |
| 1   | A     | 253 | ARG  | NE-CZ-NH2   | 5.81  | 123.20      | 120.30   |
| 2   | S     | 82  | GLN  | CA-CB-CG    | 5.81  | 126.18      | 113.40   |
| 1   | A     | 355 | GLU  | OE1-CD-OE2  | 5.81  | 130.27      | 123.30   |
| 1   | A     | 63  | THR  | CA-C-O      | -5.80 | 107.91      | 120.10   |
| 2   | U     | 27  | LEU  | CA-CB-CG    | -5.80 | 101.96      | 115.30   |
| 1   | B     | 178 | LEU  | C-N-CA      | 5.80  | 134.48      | 122.30   |
| 1   | B     | 285 | ARG  | NE-CZ-NH1   | -5.80 | 117.40      | 120.30   |
| 1   | D     | 86  | ARG  | N-CA-CB     | 5.80  | 121.03      | 110.60   |
| 2   | U     | 114 | SER  | CB-CA-C     | 5.79  | 121.11      | 110.10   |
| 1   | C     | 332 | VAL  | N-CA-CB     | -5.79 | 98.75       | 111.50   |
| 1   | C     | 215 | ARG  | CD-NE-CZ    | -5.79 | 115.49      | 123.60   |
| 2   | S     | 2   | GLN  | N-CA-CB     | 5.79  | 121.02      | 110.60   |
| 2   | T     | 38  | TRP  | CD1-NE1-CE2 | -5.78 | 103.80      | 109.00   |
| 1   | C     | 289 | LEU  | CB-CG-CD1   | -5.78 | 101.17      | 111.00   |
| 1   | D     | 199 | PHE  | CG-CD1-CE1  | -5.78 | 114.44      | 120.80   |
| 1   | D     | 216 | ASP  | CB-CG-OD2   | 5.78  | 123.50      | 118.30   |
| 2   | U     | 65  | ARG  | NH1-CZ-NH2  | 5.78  | 125.75      | 119.40   |
| 1   | C     | 79  | ARG  | NE-CZ-NH2   | -5.78 | 117.41      | 120.30   |
| 2   | S     | 18  | LEU  | O-C-N       | 5.77  | 132.07      | 121.10   |
| 2   | T     | 7   | ILE  | N-CA-C      | 5.77  | 126.59      | 111.00   |
| 1   | C     | 460 | GLU  | CG-CD-OE2   | 5.77  | 129.84      | 118.30   |
| 2   | V     | 48  | HIS  | CA-C-N      | -5.77 | 104.66      | 116.20   |
| 2   | S     | 45  | GLU  | CG-CD-OE1   | 5.77  | 129.84      | 118.30   |
| 1   | A     | 89  | ARG  | NE-CZ-NH2   | 5.76  | 123.18      | 120.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | T     | 20  | ASP  | CB-CG-OD1  | 5.76  | 123.49      | 118.30   |
| 1   | A     | 215 | ARG  | NH1-CZ-NH2 | 5.75  | 125.73      | 119.40   |
| 2   | T     | 82  | GLN  | CB-CG-CD   | 5.75  | 126.55      | 111.60   |
| 1   | B     | 377 | VAL  | O-C-N      | -5.75 | 113.50      | 122.70   |
| 1   | A     | 199 | PHE  | CB-CG-CD1  | 5.75  | 124.82      | 120.80   |
| 1   | A     | 359 | SER  | CB-CA-C    | 5.75  | 121.02      | 110.10   |
| 1   | D     | 312 | ARG  | NH1-CZ-NH2 | 5.75  | 125.72      | 119.40   |
| 1   | B     | 180 | LEU  | CB-CG-CD2  | -5.74 | 101.24      | 111.00   |
| 1   | D     | 85  | TYR  | CB-CG-CD1  | 5.74  | 124.45      | 121.00   |
| 2   | S     | 105 | ASP  | CA-C-N     | 5.74  | 129.83      | 117.20   |
| 1   | C     | 168 | PRO  | N-CD-CG    | -5.74 | 94.60       | 103.20   |
| 1   | C     | 238 | HIS  | CG-ND1-CE1 | 5.73  | 116.23      | 108.20   |
| 1   | B     | 173 | THR  | CA-CB-CG2  | 5.73  | 120.42      | 112.40   |
| 1   | B     | 90  | VAL  | O-C-N      | 5.72  | 131.86      | 122.70   |
| 1   | B     | 155 | ILE  | CA-C-O     | -5.72 | 108.08      | 120.10   |
| 1   | C     | 259 | GLU  | CB-CG-CD   | 5.72  | 129.66      | 114.20   |
| 2   | T     | 33  | LEU  | CB-CA-C    | 5.72  | 121.07      | 110.20   |
| 2   | S     | 92  | LYS  | CA-C-O     | -5.71 | 108.10      | 120.10   |
| 1   | C     | 201 | LYS  | CG-CD-CE   | -5.71 | 94.76       | 111.90   |
| 1   | C     | 260 | LEU  | O-C-N      | -5.71 | 113.48      | 123.20   |
| 2   | U     | 12  | TYR  | CB-CG-CD2  | -5.71 | 117.57      | 121.00   |
| 1   | D     | 215 | ARG  | NH1-CZ-NH2 | -5.70 | 113.13      | 119.40   |
| 1   | A     | 350 | ARG  | CG-CD-NE   | 5.70  | 123.77      | 111.80   |
| 1   | C     | 29  | TYR  | C-N-CA     | 5.70  | 135.94      | 121.70   |
| 2   | V     | 120 | PRO  | N-CA-C     | -5.70 | 97.29       | 112.10   |
| 1   | A     | 286 | ASP  | CB-CG-OD1  | 5.70  | 123.43      | 118.30   |
| 1   | B     | 75  | THR  | O-C-N      | 5.69  | 131.81      | 122.70   |
| 1   | C     | 74  | LEU  | CB-CA-C    | 5.69  | 121.01      | 110.20   |
| 1   | C     | 91  | VAL  | CA-CB-CG1  | 5.69  | 119.43      | 110.90   |
| 1   | A     | 340 | ASP  | CB-CG-OD1  | 5.69  | 123.42      | 118.30   |
| 2   | T     | 34  | LEU  | CB-CA-C    | 5.68  | 121.00      | 110.20   |
| 2   | S     | 44  | PHE  | CB-CG-CD1  | -5.68 | 116.82      | 120.80   |
| 2   | U     | 26  | LEU  | CB-CA-C    | 5.68  | 120.99      | 110.20   |
| 1   | B     | 286 | ASP  | O-C-N      | 5.68  | 131.78      | 122.70   |
| 1   | C     | 239 | TYR  | CB-CG-CD2  | -5.67 | 117.60      | 121.00   |
| 1   | C     | 352 | ASP  | O-C-N      | 5.67  | 131.77      | 122.70   |
| 1   | A     | 283 | TYR  | CD1-CE1-CZ | -5.67 | 114.70      | 119.80   |
| 1   | A     | 35  | ASP  | CB-CA-C    | -5.66 | 99.08       | 110.40   |
| 1   | C     | 340 | ASP  | CB-CG-OD1  | 5.66  | 123.39      | 118.30   |
| 2   | S     | 82  | GLN  | CB-CA-C    | 5.66  | 121.71      | 110.40   |
| 1   | B     | 71  | THR  | O-C-N      | 5.66  | 131.75      | 122.70   |
| 1   | C     | 215 | ARG  | NH1-CZ-NH2 | 5.65  | 125.62      | 119.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 93  | GLU  | CA-C-N     | -5.65 | 104.77      | 117.20   |
| 1   | C     | 136 | GLU  | CG-CD-OE1  | 5.65  | 129.61      | 118.30   |
| 1   | D     | 280 | LEU  | CB-CG-CD1  | -5.65 | 101.39      | 111.00   |
| 1   | D     | 29  | TYR  | CA-C-N     | -5.65 | 104.77      | 117.20   |
| 1   | B     | 312 | ARG  | CD-NE-CZ   | -5.65 | 115.69      | 123.60   |
| 1   | C     | 84  | CYS  | CA-CB-SG   | -5.65 | 103.83      | 114.00   |
| 1   | C     | 44  | PRO  | N-CA-CB    | 5.64  | 110.07      | 103.30   |
| 1   | A     | 354 | VAL  | CA-C-N     | -5.64 | 104.79      | 117.20   |
| 2   | V     | 82  | GLN  | CB-CG-CD   | 5.64  | 126.26      | 111.60   |
| 1   | B     | 89  | ARG  | O-C-N      | 5.64  | 131.72      | 122.70   |
| 1   | B     | 231 | GLU  | OE1-CD-OE2 | 5.64  | 130.06      | 123.30   |
| 1   | D     | 89  | ARG  | NE-CZ-NH1  | 5.63  | 123.12      | 120.30   |
| 1   | B     | 89  | ARG  | NH1-CZ-NH2 | -5.63 | 113.21      | 119.40   |
| 1   | A     | 314 | LEU  | CB-CA-C    | 5.63  | 120.90      | 110.20   |
| 1   | C     | 286 | ASP  | O-C-N      | 5.63  | 131.71      | 122.70   |
| 1   | B     | 270 | LEU  | O-C-N      | 5.62  | 131.70      | 122.70   |
| 2   | T     | 110 | VAL  | CG1-CB-CG2 | -5.62 | 101.90      | 110.90   |
| 1   | C     | 454 | GLU  | OE1-CD-OE2 | 5.62  | 130.04      | 123.30   |
| 1   | C     | 180 | LEU  | N-CA-CB    | -5.62 | 99.17       | 110.40   |
| 1   | C     | 144 | TYR  | CB-CG-CD1  | -5.61 | 117.63      | 121.00   |
| 2   | T     | 98  | TRP  | N-CA-C     | -5.61 | 95.85       | 111.00   |
| 1   | B     | 445 | ILE  | CB-CA-C    | 5.61  | 122.82      | 111.60   |
| 1   | C     | 454 | GLU  | CG-CD-OE2  | -5.61 | 107.09      | 118.30   |
| 1   | A     | 193 | LEU  | N-CA-CB    | -5.60 | 99.19       | 110.40   |
| 1   | B     | 13  | PHE  | N-CA-CB    | 5.60  | 120.68      | 110.60   |
| 1   | A     | 116 | MET  | CG-SD-CE   | -5.60 | 91.24       | 100.20   |
| 1   | B     | 193 | LEU  | CA-C-O     | -5.60 | 108.34      | 120.10   |
| 1   | C     | 356 | GLN  | CA-C-N     | 5.60  | 129.52      | 117.20   |
| 1   | A     | 333 | GLY  | CA-C-O     | -5.60 | 110.52      | 120.60   |
| 2   | T     | 65  | ARG  | NE-CZ-NH2  | 5.60  | 123.10      | 120.30   |
| 1   | C     | 110 | GLU  | C-N-CA     | 5.60  | 134.05      | 122.30   |
| 2   | T     | 118 | TYR  | CB-CG-CD1  | 5.60  | 124.36      | 121.00   |
| 1   | D     | 401 | GLN  | CA-C-O     | 5.59  | 131.85      | 120.10   |
| 1   | A     | 88  | GLU  | CA-CB-CG   | 5.59  | 125.70      | 113.40   |
| 2   | V     | 55  | ASN  | CB-CG-OD1  | -5.59 | 110.41      | 121.60   |
| 1   | C     | 82  | GLY  | N-CA-C     | -5.59 | 99.12       | 113.10   |
| 1   | D     | 51  | GLU  | CA-CB-CG   | 5.59  | 125.70      | 113.40   |
| 2   | T     | 74  | MET  | CB-CA-C    | 5.59  | 121.58      | 110.40   |
| 1   | A     | 193 | LEU  | CA-C-N     | 5.59  | 129.49      | 117.20   |
| 1   | B     | 258 | ARG  | CB-CG-CD   | 5.59  | 126.12      | 111.60   |
| 2   | T     | 108 | ARG  | NE-CZ-NH1  | -5.59 | 117.51      | 120.30   |
| 2   | S     | 108 | ARG  | NE-CZ-NH1  | -5.58 | 117.51      | 120.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | S     | 32  | TYR  | CB-CG-CD1  | -5.57 | 117.66      | 121.00   |
| 1   | B     | 266 | MET  | N-CA-CB    | -5.57 | 100.57      | 110.60   |
| 1   | A     | 334 | LYS  | CA-CB-CG   | 5.57  | 125.66      | 113.40   |
| 1   | D     | 79  | ARG  | CA-CB-CG   | 5.57  | 125.65      | 113.40   |
| 1   | A     | 160 | ASP  | CB-CG-OD2  | 5.57  | 123.31      | 118.30   |
| 1   | A     | 319 | ARG  | CB-CG-CD   | 5.57  | 126.07      | 111.60   |
| 1   | B     | 52  | GLU  | CG-CD-OE1  | 5.57  | 129.43      | 118.30   |
| 1   | A     | 264 | ILE  | CA-CB-CG2  | 5.56  | 122.02      | 110.90   |
| 1   | B     | 44  | PRO  | CA-C-N     | -5.55 | 104.99      | 117.20   |
| 1   | C     | 28  | GLU  | OE1-CD-OE2 | 5.55  | 129.96      | 123.30   |
| 1   | C     | 211 | PHE  | CB-CG-CD2  | -5.55 | 116.92      | 120.80   |
| 1   | C     | 194 | ARG  | CD-NE-CZ   | 5.54  | 131.36      | 123.60   |
| 1   | D     | 396 | ASP  | CB-CG-OD2  | 5.54  | 123.28      | 118.30   |
| 1   | C     | 86  | ARG  | N-CA-CB    | 5.54  | 120.57      | 110.60   |
| 1   | C     | 406 | THR  | N-CA-CB    | 5.54  | 120.82      | 110.30   |
| 1   | D     | 120 | ILE  | CA-CB-CG1  | -5.53 | 100.49      | 111.00   |
| 1   | C     | 142 | PRO  | N-CD-CG    | -5.52 | 94.92       | 103.20   |
| 1   | D     | 328 | SER  | O-C-N      | 5.52  | 132.58      | 123.20   |
| 1   | D     | 218 | PHE  | CB-CG-CD1  | -5.52 | 116.94      | 120.80   |
| 1   | A     | 326 | ILE  | N-CA-CB    | 5.52  | 123.49      | 110.80   |
| 2   | S     | 45  | GLU  | O-C-N      | 5.51  | 131.52      | 122.70   |
| 1   | C     | 134 | ARG  | NH1-CZ-NH2 | 5.51  | 125.46      | 119.40   |
| 1   | D     | 77  | LEU  | CA-CB-CG   | 5.51  | 127.97      | 115.30   |
| 1   | A     | 169 | LEU  | CB-CA-C    | 5.51  | 120.66      | 110.20   |
| 1   | B     | 167 | ARG  | NH1-CZ-NH2 | -5.51 | 113.34      | 119.40   |
| 1   | C     | 64  | GLY  | N-CA-C     | 5.51  | 126.87      | 113.10   |
| 1   | B     | 91  | VAL  | N-CA-CB    | 5.50  | 123.61      | 111.50   |
| 1   | A     | 52  | GLU  | CG-CD-OE1  | 5.50  | 129.30      | 118.30   |
| 1   | B     | 314 | LEU  | CB-CA-C    | 5.50  | 120.65      | 110.20   |
| 1   | D     | 338 | GLU  | CA-C-O     | 5.49  | 131.63      | 120.10   |
| 2   | V     | 52  | TYR  | CG-CD1-CE1 | -5.49 | 116.91      | 121.30   |
| 2   | S     | 43  | GLU  | CA-CB-CG   | 5.49  | 125.48      | 113.40   |
| 2   | T     | 57  | LYS  | CA-C-O     | -5.49 | 108.57      | 120.10   |
| 1   | A     | 457 | ALA  | CB-CA-C    | 5.49  | 118.33      | 110.10   |
| 1   | D     | 319 | ARG  | CB-CA-C    | 5.48  | 121.36      | 110.40   |
| 2   | S     | 118 | TYR  | CB-CG-CD2  | -5.48 | 117.71      | 121.00   |
| 1   | C     | 394 | PHE  | CA-C-N     | 5.48  | 127.16      | 116.20   |
| 1   | A     | 319 | ARG  | NH1-CZ-NH2 | -5.48 | 113.38      | 119.40   |
| 1   | C     | 345 | PHE  | CB-CG-CD2  | -5.48 | 116.97      | 120.80   |
| 1   | D     | 137 | ASP  | N-CA-CB    | -5.47 | 100.75      | 110.60   |
| 1   | D     | 265 | VAL  | CA-CB-CG2  | -5.47 | 102.69      | 110.90   |
| 1   | D     | 137 | ASP  | CB-CG-OD1  | -5.47 | 113.38      | 118.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 32  | LYS  | N-CA-CB    | 5.47  | 120.45      | 110.60   |
| 1   | B     | 290 | LEU  | O-C-N      | 5.47  | 131.44      | 122.70   |
| 1   | D     | 268 | ASP  | CB-CG-OD2  | 5.47  | 123.22      | 118.30   |
| 1   | A     | 340 | ASP  | CB-CG-OD2  | -5.46 | 113.38      | 118.30   |
| 1   | B     | 371 | LEU  | CB-CG-CD1  | -5.46 | 101.72      | 111.00   |
| 2   | S     | 65  | ARG  | CD-NE-CZ   | -5.46 | 115.96      | 123.60   |
| 1   | B     | 78  | ASP  | CB-CG-OD1  | -5.46 | 113.39      | 118.30   |
| 1   | B     | 374 | VAL  | N-CA-CB    | -5.46 | 99.49       | 111.50   |
| 1   | D     | 52  | GLU  | N-CA-CB    | 5.46  | 120.43      | 110.60   |
| 2   | V     | 53  | ARG  | CA-C-O     | -5.46 | 108.64      | 120.10   |
| 1   | B     | 191 | GLU  | O-C-N      | -5.46 | 113.97      | 122.70   |
| 2   | T     | 93  | ALA  | N-CA-CB    | 5.45  | 117.73      | 110.10   |
| 1   | A     | 328 | SER  | CA-C-O     | -5.45 | 108.65      | 120.10   |
| 1   | B     | 296 | ALA  | CB-CA-C    | 5.45  | 118.28      | 110.10   |
| 1   | B     | 209 | GLN  | CA-CB-CG   | 5.45  | 125.39      | 113.40   |
| 2   | U     | 123 | TYR  | CB-CG-CD1  | -5.45 | 117.73      | 121.00   |
| 1   | B     | 238 | HIS  | CA-C-O     | -5.45 | 108.66      | 120.10   |
| 1   | A     | 216 | ASP  | CA-C-O     | -5.45 | 108.66      | 120.10   |
| 1   | A     | 268 | ASP  | CB-CG-OD2  | 5.45  | 123.20      | 118.30   |
| 1   | A     | 283 | TYR  | CZ-CE2-CD2 | -5.44 | 114.90      | 119.80   |
| 1   | B     | 326 | ILE  | N-CA-CB    | 5.44  | 123.31      | 110.80   |
| 1   | A     | 234 | GLU  | OE1-CD-OE2 | 5.44  | 129.83      | 123.30   |
| 1   | C     | 129 | ALA  | CA-C-N     | 5.44  | 129.17      | 117.20   |
| 1   | D     | 173 | THR  | CA-CB-CG2  | 5.44  | 120.02      | 112.40   |
| 1   | A     | 286 | ASP  | CA-C-O     | -5.44 | 108.68      | 120.10   |
| 2   | U     | 34  | LEU  | CB-CA-C    | 5.44  | 120.53      | 110.20   |
| 1   | B     | 277 | ASN  | CA-CB-CG   | -5.44 | 101.44      | 113.40   |
| 1   | D     | 160 | ASP  | CB-CG-OD1  | -5.43 | 113.41      | 118.30   |
| 2   | T     | 60  | GLY  | CA-C-O     | 5.43  | 130.38      | 120.60   |
| 1   | C     | 400 | LEU  | O-C-N      | 5.43  | 131.39      | 122.70   |
| 1   | C     | 268 | ASP  | CB-CG-OD2  | 5.43  | 123.18      | 118.30   |
| 1   | C     | 91  | VAL  | O-C-N      | 5.42  | 132.42      | 123.20   |
| 2   | U     | 106 | ASN  | CA-CB-CG   | -5.42 | 101.47      | 113.40   |
| 1   | D     | 82  | GLY  | N-CA-C     | -5.42 | 99.54       | 113.10   |
| 2   | S     | 7   | ILE  | N-CA-C     | 5.42  | 125.64      | 111.00   |
| 1   | B     | 271 | THR  | CA-CB-CG2  | -5.42 | 104.81      | 112.40   |
| 2   | V     | 98  | TRP  | O-C-N      | 5.42  | 131.37      | 122.70   |
| 1   | D     | 249 | GLU  | O-C-N      | 5.42  | 131.37      | 122.70   |
| 1   | A     | 307 | HIS  | CB-CA-C    | -5.42 | 99.57       | 110.40   |
| 1   | B     | 92  | GLY  | O-C-N      | 5.42  | 131.37      | 122.70   |
| 2   | V     | 121 | GLU  | CA-CB-CG   | 5.42  | 125.32      | 113.40   |
| 1   | A     | 442 | ASN  | CA-CB-CG   | -5.41 | 101.51      | 113.40   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | U     | 61  | TYR  | O-C-N     | 5.41  | 131.35      | 122.70   |
| 1   | A     | 39  | ALA  | CA-C-N    | 5.40  | 129.09      | 117.20   |
| 2   | T     | 49  | GLY  | CA-C-O    | -5.40 | 110.87      | 120.60   |
| 1   | C     | 283 | TYR  | CA-CB-CG  | -5.40 | 103.13      | 113.40   |
| 1   | A     | 113 | VAL  | O-C-N     | -5.40 | 114.06      | 122.70   |
| 1   | C     | 138 | LEU  | O-C-N     | 5.40  | 131.34      | 122.70   |
| 1   | D     | 28  | GLU  | CG-CD-OE1 | 5.40  | 129.10      | 118.30   |
| 1   | B     | 392 | GLU  | CA-CB-CG  | 5.40  | 125.27      | 113.40   |
| 1   | B     | 213 | ARG  | CD-NE-CZ  | -5.40 | 116.05      | 123.60   |
| 1   | C     | 401 | GLN  | N-CA-C    | 5.39  | 125.56      | 111.00   |
| 1   | A     | 26  | THR  | N-CA-CB   | -5.39 | 100.06      | 110.30   |
| 2   | T     | 7   | ILE  | CB-CA-C   | -5.39 | 100.81      | 111.60   |
| 1   | D     | 187 | ARG  | NE-CZ-NH2 | 5.39  | 123.00      | 120.30   |
| 2   | V     | 63  | ASP  | CB-CG-OD1 | 5.39  | 123.15      | 118.30   |
| 1   | C     | 352 | ASP  | N-CA-CB   | 5.39  | 120.30      | 110.60   |
| 1   | D     | 410 | PRO  | O-C-N     | 5.38  | 131.32      | 122.70   |
| 1   | A     | 239 | TYR  | CA-CB-CG  | 5.38  | 123.63      | 113.40   |
| 2   | U     | 48  | HIS  | CA-CB-CG  | -5.38 | 104.45      | 113.60   |
| 2   | U     | 65  | ARG  | CB-CG-CD  | -5.38 | 97.61       | 111.60   |
| 1   | D     | 197 | LEU  | CB-CG-CD2 | -5.38 | 101.86      | 111.00   |
| 1   | A     | 60  | GLU  | CG-CD-OE1 | -5.37 | 107.55      | 118.30   |
| 1   | D     | 183 | LYS  | CA-CB-CG  | -5.37 | 101.58      | 113.40   |
| 1   | A     | 85  | TYR  | CB-CG-CD2 | -5.37 | 117.78      | 121.00   |
| 1   | C     | 234 | GLU  | CA-CB-CG  | 5.37  | 125.22      | 113.40   |
| 1   | D     | 319 | ARG  | CA-CB-CG  | 5.37  | 125.22      | 113.40   |
| 1   | D     | 331 | VAL  | C-N-CA    | 5.37  | 135.13      | 121.70   |
| 1   | A     | 72  | ASP  | CB-CG-OD1 | 5.37  | 123.13      | 118.30   |
| 1   | A     | 201 | LYS  | CG-CD-CE  | -5.37 | 95.80       | 111.90   |
| 1   | C     | 165 | TYR  | CB-CG-CD1 | -5.36 | 117.78      | 121.00   |
| 2   | V     | 2   | GLN  | O-C-N     | 5.36  | 131.28      | 122.70   |
| 1   | D     | 399 | VAL  | CA-CB-CG1 | 5.36  | 118.94      | 110.90   |
| 2   | U     | 36  | ASN  | CB-CG-OD1 | -5.36 | 110.89      | 121.60   |
| 1   | D     | 163 | ASN  | O-C-N     | 5.36  | 131.27      | 122.70   |
| 2   | U     | 45  | GLU  | O-C-N     | 5.35  | 131.26      | 122.70   |
| 1   | B     | 50  | PRO  | O-C-N     | 5.35  | 131.26      | 122.70   |
| 1   | B     | 319 | ARG  | CA-CB-CG  | 5.35  | 125.17      | 113.40   |
| 1   | C     | 110 | GLU  | CB-CG-CD  | 5.35  | 128.65      | 114.20   |
| 2   | U     | 29  | GLU  | CG-CD-OE2 | 5.35  | 129.00      | 118.30   |
| 1   | A     | 363 | TYR  | CB-CG-CD2 | 5.35  | 124.21      | 121.00   |
| 1   | B     | 111 | GLY  | CA-C-O    | -5.35 | 110.97      | 120.60   |
| 2   | V     | 55  | ASN  | CA-CB-CG  | -5.35 | 101.64      | 113.40   |
| 1   | B     | 156 | GLN  | CG-CD-NE2 | -5.34 | 103.87      | 116.70   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 390 | LEU  | O-C-N      | 5.34  | 131.25      | 122.70   |
| 2   | U     | 32  | TYR  | CA-C-N     | -5.34 | 105.44      | 117.20   |
| 1   | C     | 20  | TYR  | CB-CG-CD1  | 5.34  | 124.20      | 121.00   |
| 1   | D     | 95  | ASP  | CA-CB-CG   | -5.34 | 101.65      | 113.40   |
| 1   | D     | 203 | ASP  | O-C-N      | 5.34  | 131.24      | 122.70   |
| 2   | U     | 48  | HIS  | O-C-N      | 5.34  | 132.27      | 123.20   |
| 1   | B     | 51  | GLU  | OE1-CD-OE2 | 5.33  | 129.70      | 123.30   |
| 1   | D     | 115 | ASN  | CB-CG-OD1  | 5.33  | 132.27      | 121.60   |
| 1   | B     | 79  | ARG  | NE-CZ-NH1  | 5.33  | 122.97      | 120.30   |
| 1   | A     | 89  | ARG  | N-CA-CB    | 5.33  | 120.19      | 110.60   |
| 1   | A     | 446 | ARG  | NE-CZ-NH1  | -5.33 | 117.64      | 120.30   |
| 1   | B     | 363 | TYR  | CB-CG-CD2  | 5.32  | 124.19      | 121.00   |
| 2   | T     | 8   | ASN  | O-C-N      | 5.32  | 131.22      | 122.70   |
| 2   | T     | 115 | PHE  | CG-CD1-CE1 | 5.32  | 126.65      | 120.80   |
| 2   | U     | 92  | LYS  | N-CA-C     | -5.32 | 96.63       | 111.00   |
| 1   | A     | 70  | TRP  | CD1-CG-CD2 | 5.32  | 110.56      | 106.30   |
| 1   | B     | 264 | ILE  | CA-CB-CG2  | 5.32  | 121.54      | 110.90   |
| 1   | D     | 183 | LYS  | O-C-N      | -5.32 | 114.19      | 122.70   |
| 1   | A     | 268 | ASP  | CB-CG-OD1  | -5.32 | 113.52      | 118.30   |
| 2   | U     | 8   | ASN  | O-C-N      | 5.31  | 131.20      | 122.70   |
| 1   | B     | 259 | GLU  | CA-CB-CG   | 5.31  | 125.09      | 113.40   |
| 2   | U     | 100 | ARG  | NE-CZ-NH1  | -5.31 | 117.64      | 120.30   |
| 2   | V     | 42  | LEU  | CA-CB-CG   | 5.31  | 127.52      | 115.30   |
| 1   | D     | 254 | ALA  | N-CA-CB    | 5.31  | 117.53      | 110.10   |
| 1   | B     | 170 | LEU  | N-CA-CB    | -5.31 | 99.78       | 110.40   |
| 1   | A     | 406 | THR  | N-CA-CB    | 5.30  | 120.38      | 110.30   |
| 2   | S     | 65  | ARG  | NH1-CZ-NH2 | 5.30  | 125.23      | 119.40   |
| 1   | C     | 270 | LEU  | CA-C-O     | -5.30 | 108.96      | 120.10   |
| 1   | B     | 89  | ARG  | N-CA-CB    | 5.30  | 120.14      | 110.60   |
| 1   | C     | 88  | GLU  | CA-CB-CG   | 5.30  | 125.07      | 113.40   |
| 2   | V     | 111 | GLN  | N-CA-C     | -5.30 | 96.69       | 111.00   |
| 1   | C     | 396 | ASP  | CB-CG-OD2  | -5.30 | 113.53      | 118.30   |
| 2   | T     | 34  | LEU  | CB-CG-CD2  | -5.30 | 101.99      | 111.00   |
| 1   | C     | 172 | CYS  | N-CA-CB    | -5.30 | 101.06      | 110.60   |
| 1   | D     | 345 | PHE  | O-C-N      | 5.30  | 131.17      | 122.70   |
| 1   | A     | 136 | GLU  | CA-CB-CG   | 5.29  | 125.04      | 113.40   |
| 2   | S     | 92  | LYS  | N-CA-C     | -5.29 | 96.71       | 111.00   |
| 1   | B     | 158 | GLU  | CG-CD-OE2  | 5.29  | 128.88      | 118.30   |
| 1   | D     | 127 | PHE  | CA-CB-CG   | -5.29 | 101.20      | 113.90   |
| 1   | A     | 211 | PHE  | CA-C-O     | -5.29 | 108.99      | 120.10   |
| 1   | B     | 334 | LYS  | CA-CB-CG   | 5.29  | 125.04      | 113.40   |
| 2   | S     | 94  | TYR  | CB-CA-C    | 5.29  | 120.98      | 110.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | S     | 100 | ARG  | CA-CB-CG   | 5.29  | 125.04      | 113.40   |
| 1   | A     | 281 | ALA  | N-CA-CB    | -5.29 | 102.70      | 110.10   |
| 1   | B     | 274 | PHE  | CB-CG-CD1  | -5.28 | 117.10      | 120.80   |
| 1   | C     | 401 | GLN  | N-CA-CB    | -5.28 | 101.09      | 110.60   |
| 2   | U     | 28  | SER  | N-CA-CB    | -5.28 | 102.57      | 110.50   |
| 1   | B     | 83  | ARG  | CG-CD-NE   | -5.28 | 100.71      | 111.80   |
| 1   | C     | 208 | SER  | CB-CA-C    | 5.28  | 120.13      | 110.10   |
| 1   | D     | 125 | PHE  | CA-C-N     | 5.28  | 126.75      | 116.20   |
| 2   | S     | 118 | TYR  | N-CA-CB    | -5.28 | 101.10      | 110.60   |
| 1   | A     | 127 | PHE  | CA-CB-CG   | -5.27 | 101.25      | 113.90   |
| 1   | A     | 91  | VAL  | CA-CB-CG1  | 5.27  | 118.81      | 110.90   |
| 2   | U     | 123 | TYR  | CA-C-O     | -5.27 | 109.03      | 120.10   |
| 1   | C     | 24  | TYR  | CB-CA-C    | 5.27  | 120.94      | 110.40   |
| 1   | C     | 254 | ALA  | N-CA-CB    | 5.27  | 117.47      | 110.10   |
| 1   | D     | 211 | PHE  | CB-CG-CD2  | -5.27 | 117.11      | 120.80   |
| 2   | V     | 66  | TYR  | O-C-N      | 5.26  | 131.12      | 122.70   |
| 1   | A     | 445 | ILE  | CB-CA-C    | 5.26  | 122.12      | 111.60   |
| 2   | T     | 105 | ASP  | CA-C-O     | -5.26 | 109.05      | 120.10   |
| 1   | A     | 238 | HIS  | CG-ND1-CE1 | 5.26  | 115.57      | 108.20   |
| 1   | B     | 324 | ASP  | CB-CG-OD2  | -5.26 | 113.56      | 118.30   |
| 1   | B     | 338 | GLU  | CA-C-O     | 5.26  | 131.15      | 120.10   |
| 1   | A     | 365 | THR  | O-C-N      | 5.26  | 131.12      | 122.70   |
| 1   | C     | 353 | PHE  | O-C-N      | 5.25  | 131.10      | 122.70   |
| 1   | B     | 178 | LEU  | CA-C-N     | 5.25  | 126.70      | 116.20   |
| 1   | A     | 93  | GLU  | OE1-CD-OE2 | -5.25 | 117.00      | 123.30   |
| 1   | B     | 217 | ARG  | CA-CB-CG   | 5.25  | 124.94      | 113.40   |
| 1   | D     | 119 | SER  | O-C-N      | 5.25  | 131.09      | 122.70   |
| 1   | B     | 211 | PHE  | CB-CG-CD1  | -5.24 | 117.13      | 120.80   |
| 1   | C     | 140 | ILE  | CA-CB-CG1  | 5.24  | 120.96      | 111.00   |
| 2   | T     | 115 | PHE  | CD1-CE1-CZ | -5.24 | 113.81      | 120.10   |
| 2   | T     | 38  | TRP  | CB-CA-C    | 5.24  | 120.88      | 110.40   |
| 1   | C     | 338 | GLU  | CA-C-O     | 5.24  | 131.11      | 120.10   |
| 2   | V     | 54  | GLU  | CG-CD-OE1  | -5.24 | 107.82      | 118.30   |
| 1   | B     | 167 | ARG  | O-C-N      | 5.24  | 131.06      | 121.10   |
| 1   | B     | 191 | GLU  | CB-CA-C    | 5.24  | 120.87      | 110.40   |
| 1   | D     | 324 | ASP  | CB-CG-OD2  | -5.24 | 113.59      | 118.30   |
| 1   | D     | 451 | TRP  | CB-CG-CD2  | -5.24 | 119.79      | 126.60   |
| 1   | A     | 79  | ARG  | CG-CD-NE   | 5.23  | 122.79      | 111.80   |
| 1   | A     | 174 | ILE  | CA-C-N     | 5.23  | 128.71      | 117.20   |
| 1   | B     | 259 | GLU  | N-CA-CB    | 5.23  | 120.01      | 110.60   |
| 1   | A     | 36  | ILE  | CA-C-O     | -5.23 | 109.12      | 120.10   |
| 2   | T     | 48  | HIS  | N-CA-CB    | 5.23  | 120.01      | 110.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 291 | LEU  | CA-C-O     | -5.23 | 109.13      | 120.10   |
| 1   | B     | 434 | GLY  | CA-C-O     | -5.22 | 111.19      | 120.60   |
| 1   | C     | 63  | THR  | CA-C-N     | 5.22  | 126.64      | 116.20   |
| 1   | D     | 291 | LEU  | N-CA-CB    | -5.22 | 99.96       | 110.40   |
| 2   | T     | 77  | CYS  | CA-CB-SG   | -5.22 | 104.61      | 114.00   |
| 2   | T     | 100 | ARG  | CB-CG-CD   | 5.21  | 125.16      | 111.60   |
| 2   | V     | 37  | GLY  | C-N-CA     | -5.21 | 108.66      | 121.70   |
| 1   | D     | 132 | ALA  | CB-CA-C    | 5.21  | 117.92      | 110.10   |
| 1   | D     | 371 | LEU  | N-CA-C     | -5.21 | 96.92       | 111.00   |
| 1   | D     | 199 | PHE  | CB-CA-C    | -5.21 | 99.98       | 110.40   |
| 1   | B     | 353 | PHE  | CB-CG-CD2  | -5.21 | 117.15      | 120.80   |
| 1   | C     | 290 | LEU  | N-CA-C     | -5.21 | 96.94       | 111.00   |
| 2   | V     | 79  | ASP  | CA-CB-CG   | -5.21 | 101.94      | 113.40   |
| 1   | A     | 289 | LEU  | CA-C-O     | -5.20 | 109.17      | 120.10   |
| 1   | A     | 203 | ASP  | N-CA-C     | -5.20 | 96.96       | 111.00   |
| 1   | D     | 367 | ASP  | CB-CG-OD2  | -5.20 | 113.62      | 118.30   |
| 1   | B     | 350 | ARG  | CA-C-N     | 5.20  | 128.64      | 117.20   |
| 1   | A     | 134 | ARG  | CD-NE-CZ   | -5.20 | 116.32      | 123.60   |
| 1   | D     | 149 | GLN  | O-C-N      | 5.20  | 132.03      | 123.20   |
| 1   | B     | 62  | SER  | O-C-N      | 5.19  | 131.01      | 122.70   |
| 1   | B     | 112 | SER  | N-CA-CB    | -5.19 | 102.71      | 110.50   |
| 1   | C     | 32  | LYS  | CA-C-N     | -5.19 | 105.78      | 117.20   |
| 2   | V     | 33  | LEU  | CB-CA-C    | 5.19  | 120.06      | 110.20   |
| 1   | A     | 269 | TYR  | CB-CG-CD2  | -5.19 | 117.89      | 121.00   |
| 1   | C     | 191 | GLU  | CA-C-O     | -5.18 | 109.21      | 120.10   |
| 2   | S     | 41  | CYS  | CA-CB-SG   | -5.18 | 104.67      | 114.00   |
| 1   | C     | 296 | ALA  | N-CA-CB    | -5.18 | 102.85      | 110.10   |
| 2   | V     | 59  | PRO  | CA-C-O     | -5.18 | 107.77      | 120.20   |
| 1   | C     | 95  | ASP  | CA-CB-CG   | -5.18 | 102.01      | 113.40   |
| 1   | D     | 79  | ARG  | NE-CZ-NH2  | -5.17 | 117.71      | 120.30   |
| 1   | C     | 131 | ARG  | NH1-CZ-NH2 | -5.17 | 113.71      | 119.40   |
| 1   | A     | 387 | MET  | CA-CB-CG   | -5.17 | 104.52      | 113.30   |
| 1   | C     | 79  | ARG  | CB-CA-C    | -5.17 | 100.06      | 110.40   |
| 1   | D     | 319 | ARG  | CG-CD-NE   | -5.17 | 100.95      | 111.80   |
| 2   | S     | 2   | GLN  | OE1-CD-NE2 | 5.16  | 133.77      | 121.90   |
| 2   | S     | 104 | PHE  | CB-CA-C    | -5.16 | 100.08      | 110.40   |
| 1   | B     | 354 | VAL  | CA-C-N     | -5.16 | 105.84      | 117.20   |
| 1   | A     | 263 | PRO  | CA-C-N     | 5.16  | 128.55      | 117.20   |
| 1   | A     | 351 | ASP  | CB-CG-OD1  | 5.16  | 122.94      | 118.30   |
| 1   | D     | 244 | ALA  | CB-CA-C    | 5.16  | 117.84      | 110.10   |
| 1   | A     | 88  | GLU  | O-C-N      | 5.16  | 130.95      | 122.70   |
| 1   | C     | 324 | ASP  | CB-CA-C    | 5.16  | 120.71      | 110.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 414 | ALA  | CB-CA-C    | 5.16  | 117.83      | 110.10   |
| 1   | B     | 268 | ASP  | CB-CG-OD1  | -5.15 | 113.66      | 118.30   |
| 1   | C     | 230 | ALA  | O-C-N      | 5.15  | 130.94      | 122.70   |
| 2   | V     | 111 | GLN  | N-CA-CB    | 5.15  | 119.88      | 110.60   |
| 1   | A     | 158 | GLU  | N-CA-CB    | 5.15  | 119.87      | 110.60   |
| 1   | C     | 434 | GLY  | CA-C-O     | -5.15 | 111.33      | 120.60   |
| 2   | V     | 92  | LYS  | N-CA-C     | -5.15 | 97.09       | 111.00   |
| 1   | D     | 354 | VAL  | O-C-N      | 5.15  | 130.94      | 122.70   |
| 1   | A     | 78  | ASP  | CB-CA-C    | 5.15  | 120.69      | 110.40   |
| 1   | A     | 245 | GLY  | CA-C-N     | 5.15  | 128.53      | 117.20   |
| 1   | A     | 319 | ARG  | CA-CB-CG   | 5.15  | 124.72      | 113.40   |
| 1   | A     | 325 | HIS  | CA-CB-CG   | 5.15  | 122.35      | 113.60   |
| 1   | D     | 234 | GLU  | N-CA-CB    | 5.14  | 119.86      | 110.60   |
| 1   | B     | 340 | ASP  | CB-CG-OD2  | -5.14 | 113.67      | 118.30   |
| 2   | S     | 40  | PRO  | O-C-N      | 5.13  | 130.91      | 122.70   |
| 1   | A     | 283 | TYR  | CA-CB-CG   | -5.13 | 103.65      | 113.40   |
| 1   | C     | 180 | LEU  | CA-C-N     | 5.13  | 128.49      | 117.20   |
| 1   | B     | 200 | THR  | N-CA-C     | -5.13 | 97.16       | 111.00   |
| 1   | B     | 442 | ASN  | CA-CB-CG   | -5.12 | 102.13      | 113.40   |
| 2   | U     | 101 | ILE  | CA-C-O     | -5.12 | 109.34      | 120.10   |
| 1   | D     | 61  | SER  | CA-CB-OG   | -5.12 | 97.37       | 111.20   |
| 1   | A     | 304 | GLN  | CB-CA-C    | 5.12  | 120.64      | 110.40   |
| 1   | A     | 468 | ASN  | N-CA-CB    | 5.12  | 119.81      | 110.60   |
| 1   | A     | 231 | GLU  | CG-CD-OE1  | -5.11 | 108.08      | 118.30   |
| 1   | A     | 436 | ASP  | CB-CG-OD1  | 5.11  | 122.90      | 118.30   |
| 2   | S     | 33  | LEU  | CB-CA-C    | 5.11  | 119.91      | 110.20   |
| 1   | B     | 295 | ARG  | NE-CZ-NH1  | 5.11  | 122.86      | 120.30   |
| 1   | D     | 260 | LEU  | O-C-N      | -5.11 | 114.51      | 123.20   |
| 2   | U     | 41  | CYS  | CA-CB-SG   | -5.11 | 104.80      | 114.00   |
| 1   | A     | 355 | GLU  | N-CA-CB    | -5.11 | 101.41      | 110.60   |
| 2   | T     | 52  | TYR  | CA-CB-CG   | 5.11  | 123.10      | 113.40   |
| 1   | D     | 10  | SER  | O-C-N      | 5.11  | 130.87      | 122.70   |
| 1   | D     | 26  | THR  | CA-CB-CG2  | 5.11  | 119.55      | 112.40   |
| 1   | D     | 239 | TYR  | CZ-CE2-CD2 | -5.11 | 115.20      | 119.80   |
| 1   | C     | 18  | LYS  | CD-CE-NZ   | 5.10  | 123.44      | 111.70   |
| 1   | B     | 385 | TRP  | CA-C-N     | 5.10  | 128.42      | 117.20   |
| 1   | C     | 134 | ARG  | CD-NE-CZ   | -5.10 | 116.46      | 123.60   |
| 1   | B     | 80  | TYR  | CB-CG-CD2  | 5.10  | 124.06      | 121.00   |
| 1   | A     | 52  | GLU  | N-CA-CB    | 5.09  | 119.76      | 110.60   |
| 1   | A     | 207 | ASN  | CB-CG-OD1  | -5.09 | 111.42      | 121.60   |
| 1   | C     | 132 | ALA  | O-C-N      | 5.09  | 130.84      | 122.70   |
| 2   | U     | 48  | HIS  | CA-C-N     | -5.09 | 106.02      | 116.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 360 | ARG  | NE-CZ-NH1  | -5.09 | 117.75      | 120.30   |
| 1   | B     | 301 | ILE  | CB-CG1-CD1 | -5.09 | 99.65       | 113.90   |
| 1   | C     | 446 | ARG  | NE-CZ-NH2  | 5.09  | 122.84      | 120.30   |
| 1   | B     | 178 | LEU  | CA-CB-CG   | 5.08  | 127.00      | 115.30   |
| 1   | B     | 264 | ILE  | CB-CG1-CD1 | -5.08 | 99.66       | 113.90   |
| 1   | C     | 207 | ASN  | CB-CA-C    | 5.08  | 120.57      | 110.40   |
| 1   | D     | 101 | VAL  | O-C-N      | 5.08  | 130.84      | 122.70   |
| 1   | A     | 309 | ILE  | O-C-N      | 5.08  | 130.83      | 122.70   |
| 2   | T     | 55  | ASN  | CA-CB-CG   | -5.08 | 102.22      | 113.40   |
| 1   | C     | 436 | ASP  | CB-CG-OD1  | 5.08  | 122.87      | 118.30   |
| 1   | A     | 45  | GLN  | CA-CB-CG   | 5.08  | 124.57      | 113.40   |
| 1   | D     | 119 | SER  | N-CA-CB    | 5.08  | 118.12      | 110.50   |
| 2   | U     | 2   | GLN  | CA-C-N     | -5.08 | 106.03      | 117.20   |
| 1   | A     | 223 | GLU  | CG-CD-OE2  | -5.08 | 108.15      | 118.30   |
| 1   | B     | 158 | GLU  | N-CA-CB    | 5.08  | 119.74      | 110.60   |
| 1   | D     | 97  | TYR  | CB-CG-CD2  | -5.07 | 117.96      | 121.00   |
| 1   | B     | 28  | GLU  | CG-CD-OE2  | -5.07 | 108.17      | 118.30   |
| 1   | D     | 44  | PRO  | CA-C-N     | -5.07 | 106.05      | 117.20   |
| 1   | C     | 258 | ARG  | CB-CG-CD   | 5.07  | 124.77      | 111.60   |
| 1   | D     | 327 | HIS  | CA-CB-CG   | 5.07  | 122.21      | 113.60   |
| 2   | S     | 103 | GLY  | CA-C-O     | -5.06 | 111.49      | 120.60   |
| 1   | C     | 468 | ASN  | O-C-N      | 5.06  | 130.80      | 122.70   |
| 1   | A     | 323 | GLY  | CA-C-O     | -5.06 | 111.49      | 120.60   |
| 1   | C     | 447 | GLU  | OE1-CD-OE2 | 5.06  | 129.37      | 123.30   |
| 2   | U     | 58  | SER  | N-CA-CB    | -5.06 | 102.92      | 110.50   |
| 1   | D     | 312 | ARG  | CD-NE-CZ   | -5.06 | 116.52      | 123.60   |
| 2   | T     | 58  | SER  | CB-CA-C    | 5.05  | 119.70      | 110.10   |
| 2   | U     | 83  | VAL  | CA-CB-CG2  | 5.05  | 118.48      | 110.90   |
| 2   | S     | 104 | PHE  | CB-CG-CD1  | -5.05 | 117.27      | 120.80   |
| 1   | A     | 32  | LYS  | N-CA-CB    | 5.05  | 119.68      | 110.60   |
| 1   | A     | 190 | TYR  | CA-C-O     | 5.05  | 130.70      | 120.10   |
| 1   | B     | 288 | GLY  | N-CA-C     | 5.05  | 125.71      | 113.10   |
| 1   | C     | 433 | GLU  | CB-CA-C    | -5.05 | 100.31      | 110.40   |
| 1   | B     | 387 | MET  | CA-CB-CG   | -5.04 | 104.73      | 113.30   |
| 1   | C     | 93  | GLU  | CG-CD-OE2  | 5.04  | 128.39      | 118.30   |
| 1   | B     | 83  | ARG  | CD-NE-CZ   | 5.04  | 130.66      | 123.60   |
| 2   | T     | 43  | GLU  | CG-CD-OE1  | -5.04 | 108.22      | 118.30   |
| 1   | C     | 224 | ALA  | CB-CA-C    | 5.04  | 117.66      | 110.10   |
| 1   | A     | 303 | ARG  | NE-CZ-NH1  | -5.04 | 117.78      | 120.30   |
| 1   | A     | 392 | GLU  | CA-CB-CG   | 5.04  | 124.48      | 113.40   |
| 1   | A     | 29  | TYR  | CA-C-N     | -5.03 | 106.12      | 117.20   |
| 1   | C     | 374 | VAL  | N-CA-CB    | -5.03 | 100.43      | 111.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 369 | VAL  | CA-C-O     | 5.03  | 130.67      | 120.10   |
| 2   | V     | 37  | GLY  | O-C-N      | 5.03  | 130.75      | 122.70   |
| 1   | D     | 386 | HIS  | CG-ND1-CE1 | 5.03  | 115.24      | 108.20   |
| 1   | C     | 117 | PHE  | N-CA-CB    | 5.03  | 119.65      | 110.60   |
| 1   | A     | 352 | ASP  | CB-CG-OD2  | 5.03  | 122.82      | 118.30   |
| 1   | B     | 465 | ILE  | CB-CA-C    | -5.02 | 101.55      | 111.60   |
| 1   | D     | 74  | LEU  | CB-CG-CD1  | 5.02  | 119.54      | 111.00   |
| 1   | C     | 376 | PRO  | N-CD-CG    | -5.02 | 95.67       | 103.20   |
| 1   | B     | 303 | ARG  | NE-CZ-NH1  | 5.02  | 122.81      | 120.30   |
| 1   | C     | 148 | PHE  | CD1-CE1-CZ | -5.02 | 114.08      | 120.10   |
| 2   | U     | 73  | PRO  | N-CA-C     | -5.02 | 99.06       | 112.10   |
| 1   | A     | 88  | GLU  | CA-C-O     | -5.02 | 109.57      | 120.10   |
| 1   | A     | 431 | ARG  | CD-NE-CZ   | -5.01 | 116.58      | 123.60   |
| 1   | A     | 105 | LEU  | CB-CG-CD2  | 5.01  | 119.52      | 111.00   |
| 1   | B     | 420 | ASN  | CB-CG-OD1  | -5.01 | 111.58      | 121.60   |
| 1   | C     | 407 | LEU  | N-CA-CB    | -5.01 | 100.38      | 110.40   |
| 2   | V     | 96  | GLN  | O-C-N      | 5.01  | 130.72      | 122.70   |
| 1   | D     | 297 | MET  | CA-CB-CG   | -5.01 | 104.79      | 113.30   |
| 1   | B     | 425 | GLU  | CG-CD-OE1  | 5.01  | 128.31      | 118.30   |
| 2   | V     | 55  | ASN  | OD1-CG-ND2 | 5.01  | 133.42      | 121.90   |
| 1   | B     | 200 | THR  | CA-C-O     | -5.00 | 109.59      | 120.10   |
| 2   | U     | 92  | LYS  | CA-C-O     | -5.00 | 109.60      | 120.10   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3628  | 0        | 3559     | 200     | 0            |
| 1   | B     | 3628  | 0        | 3558     | 225     | 1            |
| 1   | C     | 3628  | 0        | 3556     | 246     | 1            |
| 1   | D     | 3628  | 0        | 3557     | 242     | 0            |
| 2   | S     | 1024  | 0        | 991      | 67      | 0            |
| 2   | T     | 1024  | 0        | 991      | 85      | 0            |
| 2   | U     | 1024  | 0        | 991      | 95      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | V     | 1024  | 0        | 991      | 93      | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 21    | 0        | 6        | 2       | 0            |
| 4   | B     | 21    | 0        | 5        | 0       | 0            |
| 4   | C     | 21    | 0        | 6        | 1       | 0            |
| 4   | D     | 21    | 0        | 6        | 3       | 0            |
| 5   | A     | 3     | 0        | 0        | 1       | 0            |
| 5   | B     | 3     | 0        | 0        | 0       | 0            |
| 5   | C     | 3     | 0        | 0        | 1       | 0            |
| 5   | D     | 3     | 0        | 0        | 1       | 0            |
| All | All   | 18708 | 0        | 18217    | 1145    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1145) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:U:79:ASP:HB3   | 2:U:82:GLN:HE21  | 1.13                     | 1.10              |
| 1:A:79:ARG:HG2   | 1:A:79:ARG:HH11  | 1.18                     | 1.09              |
| 2:V:79:ASP:HB3   | 2:V:82:GLN:HE21  | 1.14                     | 1.09              |
| 1:D:79:ARG:HH11  | 1:D:79:ARG:HG2   | 1.15                     | 1.06              |
| 1:C:26:THR:HG22  | 1:C:29:TYR:HB2   | 1.37                     | 1.05              |
| 1:C:79:ARG:HH11  | 1:C:79:ARG:HG2   | 1.18                     | 1.04              |
| 1:C:90:VAL:HG21  | 1:C:96:GLN:HG2   | 1.37                     | 1.02              |
| 2:T:79:ASP:HB3   | 2:T:82:GLN:HE21  | 1.18                     | 1.02              |
| 1:D:176:PRO:HD2  | 1:D:180:LEU:HD22 | 1.43                     | 1.01              |
| 1:A:26:THR:HG22  | 1:A:29:TYR:HB2   | 1.43                     | 0.98              |
| 1:C:452:SER:HB3  | 1:C:455:LEU:HB3  | 1.48                     | 0.96              |
| 2:S:27:LEU:HD23  | 2:S:31:GLU:OE2   | 1.65                     | 0.96              |
| 2:S:79:ASP:HB3   | 2:S:82:GLN:HE21  | 1.32                     | 0.94              |
| 1:B:304:GLN:HE21 | 1:B:304:GLN:HA   | 1.34                     | 0.93              |
| 1:A:89:ARG:HB2   | 1:A:89:ARG:HH11  | 1.35                     | 0.92              |
| 2:V:79:ASP:CB    | 2:V:82:GLN:HE21  | 1.82                     | 0.92              |
| 1:B:29:TYR:OH    | 1:B:32:LYS:NZ    | 2.01                     | 0.92              |
| 2:S:56:ASN:ND2   | 2:S:58:SER:H     | 1.68                     | 0.92              |
| 1:B:155:ILE:HG12 | 1:B:375:LEU:HD13 | 1.51                     | 0.92              |
| 1:C:89:ARG:HH11  | 1:C:89:ARG:HB2   | 1.35                     | 0.91              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:293:ILE:HG21 | 1:D:318:LEU:CD1  | 2.00                     | 0.91              |
| 1:D:26:THR:HG22  | 1:D:29:TYR:HB2   | 1.53                     | 0.91              |
| 1:D:383:HIS:H    | 1:D:386:HIS:CD2  | 1.88                     | 0.91              |
| 1:D:452:SER:HB3  | 1:D:455:LEU:HB3  | 1.53                     | 0.91              |
| 1:C:414:ALA:HB3  | 1:C:415:PRO:HD3  | 1.53                     | 0.90              |
| 2:V:22:SER:H     | 2:V:25:GLN:HE21  | 1.18                     | 0.90              |
| 1:D:89:ARG:HH11  | 1:D:89:ARG:HB2   | 1.37                     | 0.90              |
| 1:D:383:HIS:H    | 1:D:386:HIS:HD2  | 1.13                     | 0.88              |
| 1:D:414:ALA:HB3  | 1:D:415:PRO:HD3  | 1.54                     | 0.88              |
| 2:U:11:LYS:HG3   | 2:U:17:TYR:CE1   | 2.09                     | 0.88              |
| 2:U:79:ASP:CB    | 2:U:82:GLN:HE21  | 1.87                     | 0.87              |
| 2:T:75:PHE:HD1   | 1:D:9:ALA:HB1    | 1.39                     | 0.87              |
| 1:C:431:ARG:HB2  | 1:C:437:LEU:HD21 | 1.57                     | 0.86              |
| 2:V:33:LEU:HD13  | 2:V:38:TRP:HB2   | 1.54                     | 0.86              |
| 1:D:457:ALA:O    | 1:D:461:VAL:HG23 | 1.74                     | 0.86              |
| 2:V:82:GLN:O     | 2:V:85:ALA:HB3   | 1.76                     | 0.86              |
| 1:C:26:THR:CG2   | 1:C:29:TYR:HB2   | 2.06                     | 0.86              |
| 2:T:60:GLY:O     | 2:T:65:ARG:NH2   | 2.09                     | 0.85              |
| 1:B:304:GLN:NE2  | 1:B:304:GLN:HA   | 1.89                     | 0.85              |
| 2:U:56:ASN:ND2   | 2:U:58:SER:H     | 1.73                     | 0.85              |
| 1:A:26:THR:O     | 1:A:26:THR:HG22  | 1.77                     | 0.85              |
| 1:C:455:LEU:HD12 | 1:C:455:LEU:O    | 1.77                     | 0.85              |
| 1:A:293:ILE:HG21 | 1:A:318:LEU:CD1  | 2.06                     | 0.84              |
| 2:S:22:SER:H     | 2:S:25:GLN:HE21  | 1.25                     | 0.84              |
| 1:B:383:HIS:H    | 1:B:386:HIS:HD2  | 1.20                     | 0.84              |
| 2:S:82:GLN:O     | 2:S:85:ALA:HB3   | 1.76                     | 0.84              |
| 2:U:33:LEU:HD13  | 2:U:38:TRP:HB2   | 1.58                     | 0.84              |
| 1:C:176:PRO:HD2  | 1:C:180:LEU:HD22 | 1.58                     | 0.84              |
| 1:C:293:ILE:HG21 | 1:C:318:LEU:CD1  | 2.08                     | 0.84              |
| 2:U:79:ASP:HB3   | 2:U:82:GLN:NE2   | 1.93                     | 0.83              |
| 1:C:448:ALA:HA   | 1:C:451:TRP:CD1  | 2.12                     | 0.83              |
| 1:D:26:THR:CG2   | 1:D:29:TYR:HB2   | 2.08                     | 0.83              |
| 2:T:92:LYS:O     | 2:T:93:ALA:HB3   | 1.78                     | 0.83              |
| 1:A:29:TYR:CD1   | 1:A:83:ARG:HD2   | 2.13                     | 0.83              |
| 1:D:448:ALA:HA   | 1:D:451:TRP:CD1  | 2.12                     | 0.83              |
| 1:A:26:THR:CG2   | 1:A:29:TYR:HB2   | 2.09                     | 0.83              |
| 1:C:155:ILE:HG12 | 1:C:375:LEU:HD13 | 1.58                     | 0.83              |
| 1:C:332:VAL:HG13 | 1:C:386:HIS:ND1  | 1.94                     | 0.82              |
| 2:V:56:ASN:HB3   | 2:V:61:TYR:CD2   | 2.13                     | 0.82              |
| 1:D:295:ARG:HG3  | 1:D:298:HIS:CD2  | 2.15                     | 0.82              |
| 1:D:79:ARG:HG2   | 1:D:79:ARG:NH1   | 1.92                     | 0.82              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:79:ASP:CB    | 2:T:82:GLN:HE21  | 1.93                     | 0.82              |
| 1:A:155:ILE:HG12 | 1:A:375:LEU:HD13 | 1.63                     | 0.81              |
| 1:D:414:ALA:O    | 1:D:418:VAL:HG23 | 1.81                     | 0.80              |
| 2:T:77:CYS:HB2   | 2:T:82:GLN:OE1   | 1.81                     | 0.80              |
| 1:B:293:ILE:HG21 | 1:B:318:LEU:CD1  | 2.11                     | 0.80              |
| 1:B:178:LEU:HD21 | 1:B:205:ASN:ND2  | 1.97                     | 0.80              |
| 1:D:201:LYS:HE2  | 1:D:202:ASP:O    | 1.81                     | 0.80              |
| 1:D:29:TYR:OH    | 1:D:32:LYS:NZ    | 2.13                     | 0.79              |
| 1:B:89:ARG:HB2   | 1:B:89:ARG:HH11  | 1.47                     | 0.79              |
| 1:C:79:ARG:HG2   | 1:C:79:ARG:NH1   | 1.96                     | 0.79              |
| 1:B:9:ALA:HB1    | 2:V:75:PHE:HD1   | 1.47                     | 0.79              |
| 1:C:195:GLY:HA3  | 1:C:417:ALA:HB3  | 1.65                     | 0.79              |
| 2:T:56:ASN:ND2   | 2:T:58:SER:H     | 1.81                     | 0.78              |
| 2:V:56:ASN:ND2   | 2:V:58:SER:H     | 1.81                     | 0.78              |
| 2:S:27:LEU:CD2   | 2:S:31:GLU:OE2   | 2.32                     | 0.78              |
| 2:T:39:VAL:HG21  | 1:D:9:ALA:CB     | 2.13                     | 0.78              |
| 1:A:79:ARG:NH1   | 1:A:79:ARG:HG2   | 1.95                     | 0.78              |
| 1:A:90:VAL:HG21  | 1:A:96:GLN:HG2   | 1.65                     | 0.78              |
| 1:B:383:HIS:H    | 1:B:386:HIS:CD2  | 2.02                     | 0.78              |
| 1:B:26:THR:HG21  | 1:B:83:ARG:HD3   | 1.63                     | 0.78              |
| 1:B:26:THR:HG22  | 1:B:29:TYR:HB2   | 1.64                     | 0.78              |
| 1:B:79:ARG:HG2   | 1:B:79:ARG:HH11  | 1.47                     | 0.77              |
| 1:A:293:ILE:HG21 | 1:A:318:LEU:HD13 | 1.65                     | 0.77              |
| 2:T:92:LYS:O     | 2:T:93:ALA:CB    | 2.32                     | 0.77              |
| 2:T:11:LYS:HG3   | 2:T:17:TYR:CE1   | 2.19                     | 0.77              |
| 1:B:452:SER:HB3  | 1:B:455:LEU:HB3  | 1.67                     | 0.77              |
| 1:D:293:ILE:HG13 | 1:D:318:LEU:HD11 | 1.67                     | 0.76              |
| 1:B:9:ALA:CB     | 2:V:39:VAL:HG21  | 2.15                     | 0.76              |
| 1:C:181:SER:HB2  | 1:D:156:GLN:HE22 | 1.49                     | 0.76              |
| 1:D:202:ASP:OD1  | 1:D:238:HIS:HE1  | 1.67                     | 0.76              |
| 2:S:77:CYS:HB2   | 2:S:82:GLN:OE1   | 1.84                     | 0.76              |
| 1:B:293:ILE:HG21 | 1:B:318:LEU:HD13 | 1.67                     | 0.76              |
| 1:B:202:ASP:OD1  | 1:B:238:HIS:HE1  | 1.69                     | 0.75              |
| 1:D:171:GLY:O    | 1:D:402:PHE:N    | 2.18                     | 0.75              |
| 1:C:387:MET:HB3  | 1:C:388:PRO:HD3  | 1.68                     | 0.75              |
| 2:U:33:LEU:C     | 2:U:33:LEU:HD12  | 2.07                     | 0.75              |
| 1:D:57:VAL:O     | 1:D:61:SER:HB2   | 1.85                     | 0.75              |
| 1:B:332:VAL:HG13 | 1:B:386:HIS:ND1  | 2.01                     | 0.75              |
| 1:B:71:THR:O     | 1:B:74:LEU:HB2   | 1.85                     | 0.75              |
| 1:C:435:ARG:HD2  | 1:C:440:GLU:OE1  | 1.87                     | 0.75              |
| 2:U:98:TRP:HD1   | 2:U:116:ILE:HD11 | 1.51                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:448:ALA:HA   | 1:A:451:TRP:CD1  | 2.22                     | 0.74              |
| 1:A:71:THR:O     | 1:A:74:LEU:HB2   | 1.87                     | 0.74              |
| 2:U:22:SER:H     | 2:U:25:GLN:HE21  | 1.33                     | 0.74              |
| 1:A:43:THR:HG22  | 1:A:131:ARG:HG3  | 1.68                     | 0.74              |
| 1:D:332:VAL:HG13 | 1:D:332:VAL:O    | 1.86                     | 0.74              |
| 1:A:251:ILE:O    | 1:A:255:VAL:HG23 | 1.87                     | 0.74              |
| 1:A:414:ALA:HB3  | 1:A:415:PRO:HD3  | 1.70                     | 0.73              |
| 1:D:26:THR:HG21  | 1:D:83:ARG:HD3   | 1.67                     | 0.73              |
| 2:S:92:LYS:O     | 2:S:93:ALA:HB3   | 1.88                     | 0.73              |
| 1:C:43:THR:HG22  | 1:C:131:ARG:HG3  | 1.70                     | 0.73              |
| 2:U:93:ALA:C     | 2:U:95:PRO:HD3   | 2.09                     | 0.73              |
| 1:B:77:LEU:O     | 1:B:81:LYS:HG2   | 1.89                     | 0.73              |
| 1:C:29:TYR:CD1   | 1:C:83:ARG:HD2   | 2.23                     | 0.73              |
| 1:B:193:LEU:HD13 | 1:B:200:THR:HG23 | 1.70                     | 0.73              |
| 1:B:155:ILE:HG12 | 1:B:375:LEU:CD1  | 2.18                     | 0.73              |
| 1:C:26:THR:O     | 1:C:26:THR:HG22  | 1.89                     | 0.73              |
| 2:S:33:LEU:HD13  | 2:S:38:TRP:HB2   | 1.70                     | 0.73              |
| 1:A:383:HIS:H    | 1:A:386:HIS:HD2  | 1.36                     | 0.73              |
| 2:U:82:GLN:O     | 2:U:85:ALA:HB3   | 1.89                     | 0.73              |
| 2:S:93:ALA:C     | 2:S:95:PRO:HD3   | 2.10                     | 0.72              |
| 1:A:455:LEU:O    | 1:A:455:LEU:HD12 | 1.89                     | 0.72              |
| 2:T:75:PHE:HD1   | 1:D:9:ALA:CB     | 2.01                     | 0.72              |
| 2:V:94:TYR:HB3   | 2:V:97:ALA:HB2   | 1.71                     | 0.72              |
| 1:A:26:THR:HG21  | 1:A:83:ARG:HD3   | 1.70                     | 0.72              |
| 2:T:93:ALA:C     | 2:T:95:PRO:HD3   | 2.09                     | 0.72              |
| 1:C:304:GLN:NE2  | 1:C:304:GLN:HA   | 2.05                     | 0.71              |
| 1:D:171:GLY:O    | 1:D:401:GLN:HA   | 1.90                     | 0.71              |
| 2:V:93:ALA:C     | 2:V:95:PRO:HD3   | 2.09                     | 0.71              |
| 1:B:414:ALA:HB3  | 1:B:415:PRO:HD3  | 1.72                     | 0.71              |
| 1:A:19:GLU:HB3   | 1:A:52:GLU:OE1   | 1.90                     | 0.71              |
| 1:B:332:VAL:HG13 | 1:B:332:VAL:O    | 1.91                     | 0.71              |
| 1:B:448:ALA:HA   | 1:B:451:TRP:CD1  | 2.25                     | 0.71              |
| 1:C:181:SER:CB   | 1:D:156:GLN:HE22 | 2.03                     | 0.71              |
| 2:U:86:GLU:OE1   | 2:U:86:GLU:HA    | 1.90                     | 0.71              |
| 2:S:79:ASP:CB    | 2:S:82:GLN:HE21  | 2.03                     | 0.70              |
| 1:A:29:TYR:CE2   | 1:A:31:THR:HA    | 2.25                     | 0.70              |
| 2:U:3:VAL:HG21   | 2:V:70:TRP:CE3   | 2.27                     | 0.70              |
| 1:C:120:ILE:HG22 | 1:C:121:VAL:HG23 | 1.73                     | 0.70              |
| 1:C:383:HIS:H    | 1:C:386:HIS:CD2  | 2.10                     | 0.70              |
| 1:A:293:ILE:HG13 | 1:A:318:LEU:HD11 | 1.73                     | 0.70              |
| 1:C:173:THR:HA   | 1:C:201:LYS:HG2  | 1.73                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:414:ALA:O    | 1:C:418:VAL:HG23 | 1.91                     | 0.70              |
| 2:T:75:PHE:CD1   | 1:D:9:ALA:CB     | 2.74                     | 0.70              |
| 1:D:29:TYR:CD1   | 1:D:83:ARG:HD2   | 2.27                     | 0.70              |
| 1:C:79:ARG:CG    | 1:C:79:ARG:HH11  | 1.91                     | 0.70              |
| 2:V:77:CYS:HB2   | 2:V:82:GLN:OE1   | 1.92                     | 0.70              |
| 1:C:171:GLY:O    | 1:C:401:GLN:HA   | 1.91                     | 0.69              |
| 1:C:26:THR:HG21  | 1:C:83:ARG:HD3   | 1.74                     | 0.69              |
| 2:V:79:ASP:HB3   | 2:V:82:GLN:NE2   | 1.98                     | 0.69              |
| 1:D:26:THR:HG22  | 1:D:26:THR:O     | 1.92                     | 0.69              |
| 1:B:200:THR:OG1  | 1:B:238:HIS:HD2  | 1.74                     | 0.69              |
| 2:U:77:CYS:HB2   | 2:U:82:GLN:OE1   | 1.93                     | 0.69              |
| 1:B:332:VAL:CG1  | 1:B:332:VAL:O    | 2.40                     | 0.69              |
| 1:D:431:ARG:HB2  | 1:D:437:LEU:HD21 | 1.75                     | 0.69              |
| 1:C:293:ILE:HG21 | 1:C:318:LEU:HD13 | 1.73                     | 0.69              |
| 1:D:305:LYS:HG2  | 1:D:305:LYS:O    | 1.91                     | 0.68              |
| 2:S:84:LEU:HD23  | 2:S:84:LEU:O     | 1.93                     | 0.68              |
| 1:C:412:GLY:HA3  | 2:V:72:LEU:HD11  | 1.75                     | 0.68              |
| 1:B:29:TYR:CD1   | 1:B:83:ARG:HD2   | 2.29                     | 0.68              |
| 1:B:387:MET:HB3  | 1:B:388:PRO:HD3  | 1.74                     | 0.68              |
| 1:B:431:ARG:HB2  | 1:B:437:LEU:HD21 | 1.75                     | 0.68              |
| 1:C:383:HIS:H    | 1:C:386:HIS:HD2  | 1.39                     | 0.68              |
| 1:B:19:GLU:HB3   | 1:B:52:GLU:OE1   | 1.94                     | 0.68              |
| 2:U:92:LYS:O     | 2:U:93:ALA:HB3   | 1.93                     | 0.68              |
| 2:V:79:ASP:H     | 2:V:82:GLN:NE2   | 1.91                     | 0.68              |
| 1:B:178:LEU:CD2  | 1:B:205:ASN:ND2  | 2.57                     | 0.68              |
| 1:D:293:ILE:HG21 | 1:D:318:LEU:HD13 | 1.72                     | 0.68              |
| 2:S:11:LYS:HG3   | 2:S:17:TYR:CE1   | 2.28                     | 0.68              |
| 1:A:332:VAL:HG13 | 1:A:386:HIS:ND1  | 2.08                     | 0.67              |
| 1:A:443:GLU:O    | 1:A:447:GLU:HG3  | 1.94                     | 0.67              |
| 1:B:194:ARG:NH2  | 2:T:4:TRP:O      | 2.26                     | 0.67              |
| 2:T:94:TYR:N     | 2:T:95:PRO:HD3   | 2.09                     | 0.67              |
| 1:A:26:THR:CG2   | 1:A:26:THR:O     | 2.40                     | 0.67              |
| 1:D:32:LYS:NZ    | 1:D:35:ASP:OD1   | 2.25                     | 0.67              |
| 2:S:43:GLU:OE1   | 2:S:100:ARG:NH1  | 2.27                     | 0.67              |
| 1:B:414:ALA:O    | 1:B:418:VAL:HG23 | 1.94                     | 0.67              |
| 1:A:431:ARG:HB2  | 1:A:437:LEU:HD21 | 1.75                     | 0.67              |
| 1:D:293:ILE:HG21 | 1:D:318:LEU:HD11 | 1.77                     | 0.67              |
| 1:D:90:VAL:HG21  | 1:D:96:GLN:HG2   | 1.75                     | 0.67              |
| 1:C:209:GLN:HB3  | 1:C:210:PRO:CD   | 2.24                     | 0.67              |
| 1:D:435:ARG:HD2  | 1:D:440:GLU:OE1  | 1.95                     | 0.67              |
| 1:C:339:ARG:O    | 1:C:343:LEU:HG   | 1.95                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:176:PRO:HD2  | 1:D:180:LEU:CD2  | 2.23                     | 0.66              |
| 1:D:466:VAL:HG23 | 1:D:468:ASN:H    | 1.59                     | 0.66              |
| 2:S:33:LEU:CD1   | 2:S:38:TRP:HB2   | 2.25                     | 0.66              |
| 1:A:194:ARG:NH2  | 2:S:4:TRP:O      | 2.27                     | 0.66              |
| 1:A:436:ASP:OD1  | 1:A:438:ALA:N    | 2.28                     | 0.66              |
| 2:S:92:LYS:O     | 2:S:93:ALA:CB    | 2.43                     | 0.66              |
| 1:B:195:GLY:HA3  | 1:B:417:ALA:HB3  | 1.76                     | 0.66              |
| 1:C:89:ARG:NH1   | 1:C:89:ARG:HB2   | 2.09                     | 0.66              |
| 2:U:43:GLU:OE1   | 2:U:100:ARG:NH1  | 2.26                     | 0.66              |
| 1:C:293:ILE:HG21 | 1:C:318:LEU:HD11 | 1.76                     | 0.66              |
| 1:B:202:ASP:OD2  | 1:B:217:ARG:NH2  | 2.29                     | 0.66              |
| 2:T:33:LEU:HD13  | 2:T:38:TRP:HB2   | 1.78                     | 0.66              |
| 1:D:151:PRO:HG2  | 1:D:372:PRO:HB2  | 1.78                     | 0.65              |
| 1:B:466:VAL:HG23 | 1:B:467:PHE:N    | 2.11                     | 0.65              |
| 1:A:293:ILE:HG21 | 1:A:318:LEU:HD11 | 1.78                     | 0.65              |
| 1:D:332:VAL:CG1  | 1:D:332:VAL:O    | 2.44                     | 0.65              |
| 1:A:440:GLU:O    | 1:A:444:ILE:HG13 | 1.96                     | 0.65              |
| 1:B:383:HIS:O    | 1:B:386:HIS:N    | 2.25                     | 0.65              |
| 1:A:89:ARG:HB2   | 1:A:89:ARG:NH1   | 2.10                     | 0.65              |
| 1:D:451:TRP:CH2  | 2:V:19:PRO:HD3   | 2.31                     | 0.65              |
| 1:D:383:HIS:N    | 1:D:386:HIS:HD2  | 1.92                     | 0.65              |
| 1:C:71:THR:O     | 1:C:74:LEU:HB2   | 1.96                     | 0.64              |
| 1:D:455:LEU:HD12 | 1:D:455:LEU:O    | 1.96                     | 0.64              |
| 1:A:383:HIS:H    | 1:A:386:HIS:CD2  | 2.13                     | 0.64              |
| 1:B:142:PRO:HB3  | 1:B:369:VAL:HG11 | 1.79                     | 0.64              |
| 2:V:43:GLU:HA    | 2:V:68:THR:O     | 1.96                     | 0.64              |
| 1:C:436:ASP:OD1  | 1:C:438:ALA:N    | 2.30                     | 0.64              |
| 1:D:193:LEU:HD13 | 1:D:200:THR:HG23 | 1.79                     | 0.64              |
| 2:T:22:SER:H     | 2:T:25:GLN:HE21  | 1.45                     | 0.64              |
| 1:C:457:ALA:O    | 1:C:461:VAL:HG23 | 1.98                     | 0.64              |
| 1:D:79:ARG:HH11  | 1:D:79:ARG:CG    | 1.85                     | 0.64              |
| 2:U:56:ASN:HB3   | 2:U:61:TYR:CD1   | 2.33                     | 0.64              |
| 1:B:176:PRO:HD2  | 1:B:180:LEU:HD22 | 1.78                     | 0.64              |
| 1:B:304:GLN:NE2  | 1:B:304:GLN:CA   | 2.60                     | 0.64              |
| 1:C:202:ASP:OD1  | 1:C:238:HIS:HE1  | 1.81                     | 0.64              |
| 1:C:292:HIS:HA   | 1:C:325:HIS:HB2  | 1.80                     | 0.64              |
| 1:C:440:GLU:O    | 1:C:444:ILE:HG13 | 1.96                     | 0.64              |
| 1:B:297:MET:O    | 1:B:297:MET:CG   | 2.46                     | 0.64              |
| 1:B:79:ARG:HG2   | 1:B:79:ARG:NH1   | 2.13                     | 0.64              |
| 1:D:29:TYR:OH    | 1:D:35:ASP:OD2   | 2.14                     | 0.64              |
| 1:D:443:GLU:O    | 1:D:446:ARG:HB3  | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:79:ASP:HB3   | 2:T:82:GLN:NE2   | 2.02                     | 0.64              |
| 2:U:27:LEU:O     | 2:U:31:GLU:HB2   | 1.97                     | 0.64              |
| 1:D:195:GLY:HA3  | 1:D:417:ALA:HB3  | 1.80                     | 0.64              |
| 2:T:56:ASN:HB3   | 2:T:61:TYR:CD1   | 2.33                     | 0.64              |
| 1:B:29:TYR:CE2   | 1:B:31:THR:HA    | 2.33                     | 0.63              |
| 1:C:52:GLU:O     | 1:C:53:ALA:C     | 2.36                     | 0.63              |
| 1:D:251:ILE:O    | 1:D:255:VAL:HG23 | 1.98                     | 0.63              |
| 2:T:75:PHE:CD1   | 1:D:9:ALA:HB1    | 2.27                     | 0.63              |
| 2:U:98:TRP:HD1   | 2:U:116:ILE:CD1  | 2.10                     | 0.63              |
| 1:C:19:GLU:HB3   | 1:C:52:GLU:OE1   | 1.98                     | 0.63              |
| 2:S:23:GLN:O     | 2:S:27:LEU:HB2   | 1.98                     | 0.63              |
| 2:T:43:GLU:OE1   | 2:T:100:ARG:NH1  | 2.31                     | 0.63              |
| 2:V:99:ILE:O     | 2:V:116:ILE:HG13 | 1.98                     | 0.63              |
| 1:B:305:LYS:HG2  | 1:B:305:LYS:O    | 1.99                     | 0.63              |
| 1:A:29:TYR:CG    | 1:A:83:ARG:HD2   | 2.32                     | 0.63              |
| 2:U:98:TRP:CD1   | 2:U:116:ILE:HD11 | 2.32                     | 0.63              |
| 1:B:9:ALA:CB     | 2:V:75:PHE:HD1   | 2.12                     | 0.63              |
| 2:V:71:LYS:O     | 2:V:72:LEU:HD12  | 1.98                     | 0.63              |
| 1:C:414:ALA:HB3  | 1:C:415:PRO:CD   | 2.28                     | 0.63              |
| 1:D:43:THR:HG22  | 1:D:131:ARG:HG3  | 1.81                     | 0.63              |
| 2:U:33:LEU:CD1   | 2:U:38:TRP:HB2   | 2.29                     | 0.63              |
| 1:A:435:ARG:HD2  | 1:A:440:GLU:OE1  | 1.99                     | 0.63              |
| 1:C:379:SER:OG   | 1:C:401:GLN:HB2  | 1.99                     | 0.63              |
| 1:C:425:GLU:OE1  | 2:U:17:TYR:HB2   | 1.99                     | 0.62              |
| 1:C:90:VAL:HG23  | 1:C:96:GLN:O     | 1.99                     | 0.62              |
| 1:A:176:PRO:HD2  | 1:A:180:LEU:HD22 | 1.79                     | 0.62              |
| 1:C:332:VAL:HG13 | 1:C:332:VAL:O    | 1.99                     | 0.62              |
| 1:C:382:ILE:HD12 | 1:C:390:LEU:CD1  | 2.29                     | 0.62              |
| 1:C:23:THR:HG22  | 1:C:81:LYS:NZ    | 2.14                     | 0.62              |
| 1:A:62:SER:O     | 1:D:178:LEU:HD22 | 2.00                     | 0.62              |
| 1:B:151:PRO:HB3  | 1:B:323:GLY:O    | 1.99                     | 0.62              |
| 1:B:435:ARG:HD2  | 1:B:440:GLU:OE1  | 2.00                     | 0.62              |
| 1:C:379:SER:HB3  | 4:C:490:CAP:O3   | 2.00                     | 0.62              |
| 1:C:51:GLU:HA    | 1:C:87:ILE:HD11  | 1.81                     | 0.62              |
| 2:S:96:GLN:OE1   | 2:S:96:GLN:N     | 2.28                     | 0.62              |
| 1:B:363:TYR:CD1  | 1:B:363:TYR:N    | 2.67                     | 0.62              |
| 1:C:192:CYS:HB3  | 1:C:197:LEU:HD23 | 1.82                     | 0.62              |
| 1:A:429:LYS:NZ   | 2:S:29:GLU:OE1   | 2.33                     | 0.62              |
| 1:A:207:ASN:O    | 1:A:217:ARG:NH2  | 2.26                     | 0.61              |
| 1:B:443:GLU:OE1  | 1:B:446:ARG:NH2  | 2.33                     | 0.61              |
| 1:C:305:LYS:O    | 1:C:305:LYS:HG2  | 1.98                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:207:ASN:O    | 1:B:217:ARG:NH1  | 2.27                     | 0.61              |
| 1:C:269:TYR:CD1  | 1:C:293:ILE:CG2  | 2.84                     | 0.61              |
| 1:A:195:GLY:HA3  | 1:A:417:ALA:HB3  | 1.81                     | 0.61              |
| 1:D:166:GLY:O    | 1:D:167:ARG:HB3  | 1.99                     | 0.61              |
| 2:U:117:ALA:O    | 2:U:118:TYR:HB2  | 2.00                     | 0.61              |
| 2:U:60:GLY:O     | 2:U:65:ARG:NH2   | 2.33                     | 0.61              |
| 1:A:134:ARG:HG3  | 1:A:135:LEU:N    | 2.15                     | 0.61              |
| 1:B:440:GLU:O    | 1:B:444:ILE:HG13 | 2.00                     | 0.61              |
| 1:B:90:VAL:HG21  | 1:B:96:GLN:HG2   | 1.82                     | 0.61              |
| 2:U:84:LEU:O     | 2:U:84:LEU:HD23  | 2.00                     | 0.61              |
| 1:B:297:MET:HG3  | 1:B:297:MET:O    | 1.99                     | 0.61              |
| 2:T:75:PHE:CE1   | 1:D:9:ALA:HB2    | 2.36                     | 0.61              |
| 1:D:387:MET:N    | 1:D:388:PRO:HD2  | 2.16                     | 0.61              |
| 1:C:158:GLU:OE2  | 1:C:325:HIS:NE2  | 2.28                     | 0.61              |
| 1:D:199:PHE:HA   | 1:D:237:GLY:O    | 2.00                     | 0.61              |
| 2:T:77:CYS:CB    | 2:T:82:GLN:OE1   | 2.48                     | 0.61              |
| 1:A:449:CYS:CB   | 1:A:459:CYS:SG   | 2.88                     | 0.61              |
| 1:D:430:ALA:HB1  | 1:D:444:ILE:HD13 | 1.81                     | 0.61              |
| 1:C:304:GLN:HE21 | 1:C:304:GLN:HA   | 1.65                     | 0.61              |
| 1:D:38:ALA:HB2   | 1:D:138:LEU:HD23 | 1.82                     | 0.61              |
| 1:A:45:GLN:OE1   | 1:A:131:ARG:HB3  | 2.01                     | 0.60              |
| 1:B:368:TRP:O    | 1:B:369:VAL:C    | 2.38                     | 0.60              |
| 1:C:382:ILE:HD12 | 1:C:390:LEU:HD13 | 1.83                     | 0.60              |
| 1:D:430:ALA:CB   | 1:D:444:ILE:HD13 | 2.30                     | 0.60              |
| 1:C:193:LEU:HD13 | 1:C:200:THR:HG23 | 1.82                     | 0.60              |
| 1:C:90:VAL:CG2   | 1:C:96:GLN:HG2   | 2.24                     | 0.60              |
| 2:V:11:LYS:HG3   | 2:V:17:TYR:CE1   | 2.37                     | 0.60              |
| 1:B:57:VAL:O     | 1:B:61:SER:HB2   | 2.02                     | 0.60              |
| 1:C:66:TRP:CE3   | 1:C:67:THR:HB    | 2.36                     | 0.60              |
| 2:T:79:ASP:H     | 2:T:82:GLN:NE2   | 2.00                     | 0.60              |
| 1:A:429:LYS:CE   | 2:S:29:GLU:OE1   | 2.50                     | 0.60              |
| 1:D:26:THR:CG2   | 1:D:26:THR:O     | 2.49                     | 0.60              |
| 1:A:181:SER:HB2  | 1:B:156:GLN:HE22 | 1.67                     | 0.60              |
| 1:A:425:GLU:OE1  | 2:S:17:TYR:HB2   | 2.02                     | 0.60              |
| 1:B:271:THR:HG1  | 1:C:118:THR:HG1  | 1.50                     | 0.60              |
| 1:B:363:TYR:HD1  | 1:B:363:TYR:N    | 2.00                     | 0.60              |
| 1:D:120:ILE:HG22 | 1:D:121:VAL:HG23 | 1.84                     | 0.60              |
| 2:S:83:VAL:O     | 2:S:86:GLU:HB2   | 2.02                     | 0.60              |
| 2:U:79:ASP:H     | 2:U:82:GLN:NE2   | 1.99                     | 0.60              |
| 2:V:113:ILE:O    | 2:V:114:SER:HB2  | 2.02                     | 0.60              |
| 1:C:383:HIS:NE2  | 1:C:465:ILE:HB   | 2.17                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:155:ILE:HG12 | 1:D:375:LEU:HD13 | 1.84                     | 0.59              |
| 2:S:60:GLY:O     | 2:S:65:ARG:NH2   | 2.35                     | 0.59              |
| 1:C:385:TRP:CZ2  | 1:C:459:CYS:HB3  | 2.37                     | 0.59              |
| 2:U:6:PRO:HG3    | 2:V:44:PHE:CE2   | 2.37                     | 0.59              |
| 2:U:79:ASP:H     | 2:U:82:GLN:HE22  | 1.50                     | 0.59              |
| 2:U:92:LYS:O     | 2:U:93:ALA:CB    | 2.49                     | 0.59              |
| 1:D:190:TYR:O    | 1:D:194:ARG:HG2  | 2.02                     | 0.59              |
| 1:D:295:ARG:O    | 1:D:298:HIS:HB3  | 2.01                     | 0.59              |
| 1:B:381:GLY:HA2  | 1:C:66:TRP:CD1   | 2.37                     | 0.59              |
| 1:B:9:ALA:CB     | 2:V:75:PHE:CD1   | 2.84                     | 0.59              |
| 1:D:190:TYR:CE1  | 1:D:227:LYS:HD3  | 2.38                     | 0.59              |
| 1:A:101:VAL:HG12 | 1:A:102:ALA:N    | 2.16                     | 0.59              |
| 1:C:462:TRP:O    | 1:C:465:ILE:HG12 | 2.02                     | 0.59              |
| 1:B:208:SER:O    | 1:C:109:GLU:HB2  | 2.02                     | 0.59              |
| 1:C:387:MET:HB3  | 1:C:388:PRO:CD   | 2.31                     | 0.59              |
| 2:V:60:GLY:O     | 2:V:65:ARG:NH2   | 2.36                     | 0.59              |
| 1:B:443:GLU:O    | 1:B:447:GLU:HG3  | 2.01                     | 0.59              |
| 2:V:27:LEU:O     | 2:V:31:GLU:HB2   | 2.03                     | 0.59              |
| 1:A:452:SER:HB3  | 1:A:455:LEU:HB3  | 1.84                     | 0.59              |
| 2:S:79:ASP:H     | 2:S:82:GLN:NE2   | 2.01                     | 0.59              |
| 2:T:77:CYS:SG    | 2:T:78:THR:N     | 2.75                     | 0.59              |
| 1:C:19:GLU:HB3   | 1:C:52:GLU:CD    | 2.23                     | 0.58              |
| 1:D:234:GLU:O    | 1:D:236:LYS:HG2  | 2.03                     | 0.58              |
| 1:D:440:GLU:O    | 1:D:444:ILE:HG13 | 2.02                     | 0.58              |
| 2:T:96:GLN:N     | 2:T:96:GLN:OE1   | 2.28                     | 0.58              |
| 2:V:56:ASN:ND2   | 2:V:58:SER:OG    | 2.36                     | 0.58              |
| 1:B:171:GLY:O    | 1:B:401:GLN:HA   | 2.03                     | 0.58              |
| 1:D:385:TRP:CZ2  | 1:D:459:CYS:HB3  | 2.38                     | 0.58              |
| 1:B:378:ALA:HB3  | 1:B:400:LEU:HD23 | 1.86                     | 0.58              |
| 1:D:436:ASP:OD1  | 1:D:438:ALA:N    | 2.36                     | 0.58              |
| 1:B:66:TRP:CE3   | 1:B:67:THR:HB    | 2.38                     | 0.58              |
| 1:B:79:ARG:HH11  | 1:B:79:ARG:CG    | 2.15                     | 0.58              |
| 1:C:448:ALA:HA   | 1:C:451:TRP:HD1  | 1.65                     | 0.58              |
| 2:V:27:LEU:HD12  | 2:V:84:LEU:CD1   | 2.33                     | 0.58              |
| 1:A:137:ASP:OD1  | 1:A:138:LEU:N    | 2.35                     | 0.58              |
| 1:D:97:TYR:O     | 1:D:98:ILE:HD13  | 2.03                     | 0.58              |
| 2:U:23:GLN:O     | 2:U:27:LEU:HB2   | 2.04                     | 0.58              |
| 2:V:33:LEU:CD1   | 2:V:38:TRP:HB2   | 2.31                     | 0.58              |
| 1:C:10:SER:O     | 1:C:11:VAL:HB    | 2.04                     | 0.58              |
| 1:C:459:CYS:O    | 1:C:463:LYS:HB2  | 2.04                     | 0.58              |
| 1:B:209:GLN:HB3  | 1:B:210:PRO:CD   | 2.34                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:56:ASN:HB3   | 2:V:61:TYR:CG    | 2.39                     | 0.58              |
| 1:C:443:GLU:O    | 1:C:447:GLU:N    | 2.32                     | 0.58              |
| 1:D:429:LYS:NZ   | 2:V:29:GLU:OE1   | 2.37                     | 0.58              |
| 1:A:414:ALA:O    | 1:A:418:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:19:GLU:HB3   | 1:A:52:GLU:CD    | 2.23                     | 0.57              |
| 1:C:209:GLN:HB3  | 1:C:210:PRO:HD2  | 1.86                     | 0.57              |
| 1:D:332:VAL:HG13 | 1:D:386:HIS:ND1  | 2.19                     | 0.57              |
| 2:S:77:CYS:SG    | 2:S:82:GLN:NE2   | 2.77                     | 0.57              |
| 1:A:466:VAL:HG23 | 1:A:468:ASN:H    | 1.69                     | 0.57              |
| 1:C:19:GLU:HB3   | 1:C:52:GLU:OE2   | 2.04                     | 0.57              |
| 2:T:39:VAL:HG21  | 1:D:9:ALA:HB2    | 1.85                     | 0.57              |
| 1:C:26:THR:HG22  | 1:C:29:TYR:CB    | 2.25                     | 0.57              |
| 1:C:32:LYS:NZ    | 1:C:35:ASP:OD1   | 2.35                     | 0.57              |
| 1:C:443:GLU:O    | 1:C:446:ARG:HB3  | 2.04                     | 0.57              |
| 1:D:23:THR:HB    | 1:D:24:TYR:CD1   | 2.39                     | 0.57              |
| 1:D:71:THR:O     | 1:D:74:LEU:HB2   | 2.05                     | 0.57              |
| 2:U:96:GLN:OE1   | 2:U:96:GLN:N     | 2.31                     | 0.57              |
| 1:D:133:LEU:O    | 1:D:307:HIS:HA   | 2.04                     | 0.57              |
| 1:A:443:GLU:O    | 1:A:447:GLU:N    | 2.37                     | 0.57              |
| 1:B:127:PHE:CE1  | 1:C:335:LEU:HD21 | 2.40                     | 0.57              |
| 1:D:378:ALA:HB3  | 1:D:400:LEU:HD23 | 1.85                     | 0.57              |
| 2:V:92:LYS:O     | 2:V:93:ALA:HB3   | 2.05                     | 0.57              |
| 1:C:57:VAL:O     | 1:C:61:SER:HB2   | 2.04                     | 0.57              |
| 1:C:94:LYS:O     | 1:C:96:GLN:N     | 2.38                     | 0.57              |
| 1:D:202:ASP:OD1  | 1:D:238:HIS:CE1  | 2.55                     | 0.57              |
| 2:T:27:LEU:HD12  | 2:T:84:LEU:CD1   | 2.35                     | 0.57              |
| 2:U:43:GLU:HA    | 2:U:68:THR:O     | 2.04                     | 0.57              |
| 1:B:429:LYS:HE3  | 2:T:21:LEU:HD22  | 1.87                     | 0.57              |
| 1:D:304:GLN:HA   | 1:D:304:GLN:NE2  | 2.19                     | 0.57              |
| 1:D:89:ARG:NH1   | 1:D:89:ARG:HB2   | 2.16                     | 0.57              |
| 1:C:155:ILE:HG12 | 1:C:375:LEU:CD1  | 2.31                     | 0.57              |
| 2:T:94:TYR:HB3   | 2:T:97:ALA:HB2   | 1.85                     | 0.57              |
| 1:C:293:ILE:HG13 | 1:C:318:LEU:HD11 | 1.85                     | 0.56              |
| 1:A:120:ILE:HD13 | 1:A:138:LEU:HD21 | 1.86                     | 0.56              |
| 1:A:193:LEU:HD13 | 1:A:200:THR:HG23 | 1.87                     | 0.56              |
| 1:B:387:MET:HB3  | 1:B:388:PRO:CD   | 2.35                     | 0.56              |
| 1:C:264:ILE:HG13 | 1:C:290:LEU:O    | 2.05                     | 0.56              |
| 2:U:94:TYR:N     | 2:U:95:PRO:HD3   | 2.20                     | 0.56              |
| 1:D:383:HIS:NE2  | 1:D:465:ILE:HB   | 2.20                     | 0.56              |
| 1:A:449:CYS:HB3  | 1:A:459:CYS:SG   | 2.45                     | 0.56              |
| 1:B:425:GLU:OE1  | 2:T:17:TYR:N     | 2.36                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:332:VAL:CG1  | 1:C:332:VAL:O    | 2.53                     | 0.56              |
| 2:T:86:GLU:HA    | 2:T:86:GLU:OE1   | 2.05                     | 0.56              |
| 2:V:94:TYR:N     | 2:V:95:PRO:HD3   | 2.20                     | 0.56              |
| 2:T:77:CYS:SG    | 2:T:82:GLN:NE2   | 2.79                     | 0.56              |
| 1:C:26:THR:CG2   | 1:C:26:THR:O     | 2.51                     | 0.56              |
| 2:V:33:LEU:HD12  | 2:V:33:LEU:C     | 2.25                     | 0.56              |
| 1:A:305:LYS:O    | 1:A:305:LYS:HG2  | 2.06                     | 0.56              |
| 1:C:447:GLU:O    | 1:C:450:LYS:HB2  | 2.06                     | 0.56              |
| 2:T:101:ILE:HG13 | 2:T:117:ALA:HB2  | 1.87                     | 0.56              |
| 1:A:181:SER:CB   | 1:B:156:GLN:HE22 | 2.18                     | 0.56              |
| 1:B:466:VAL:HG23 | 1:B:468:ASN:H    | 1.71                     | 0.56              |
| 1:C:431:ARG:CB   | 1:C:437:LEU:HD21 | 2.34                     | 0.56              |
| 2:S:94:TYR:N     | 2:S:95:PRO:HD3   | 2.21                     | 0.56              |
| 1:B:387:MET:N    | 1:B:388:PRO:HD2  | 2.21                     | 0.55              |
| 1:D:331:VAL:HG12 | 1:D:332:VAL:N    | 2.20                     | 0.55              |
| 1:D:90:VAL:HG23  | 1:D:97:TYR:HA    | 1.87                     | 0.55              |
| 1:C:306:ASN:OD1  | 1:C:306:ASN:N    | 2.33                     | 0.55              |
| 1:C:45:GLN:OE1   | 1:C:131:ARG:HB3  | 2.07                     | 0.55              |
| 1:C:383:HIS:O    | 1:C:386:HIS:N    | 2.36                     | 0.55              |
| 1:C:443:GLU:O    | 1:C:447:GLU:HG3  | 2.06                     | 0.55              |
| 1:A:209:GLN:HB3  | 1:A:210:PRO:HD2  | 1.88                     | 0.55              |
| 1:C:378:ALA:HB3  | 1:C:400:LEU:HD23 | 1.87                     | 0.55              |
| 1:D:94:LYS:O     | 1:D:95:ASP:C     | 2.45                     | 0.55              |
| 1:B:173:THR:HA   | 1:B:201:LYS:HG2  | 1.88                     | 0.55              |
| 1:C:466:VAL:HG23 | 1:C:468:ASN:H    | 1.72                     | 0.55              |
| 1:A:63:THR:HA    | 1:D:177:LYS:HB2  | 1.89                     | 0.55              |
| 2:S:103:GLY:HA3  | 2:S:113:ILE:HG22 | 1.88                     | 0.55              |
| 2:U:83:VAL:O     | 2:U:86:GLU:HB2   | 2.06                     | 0.55              |
| 1:B:60:GLU:OE2   | 1:B:65:THR:HA    | 2.07                     | 0.55              |
| 1:C:214:TRP:CD2  | 1:C:253:ARG:HG2  | 2.42                     | 0.55              |
| 1:D:304:GLN:HA   | 1:D:304:GLN:HE21 | 1.72                     | 0.55              |
| 2:T:42:LEU:HB3   | 2:T:70:TRP:HB3   | 1.88                     | 0.55              |
| 1:B:293:ILE:HG21 | 1:B:318:LEU:HD11 | 1.88                     | 0.55              |
| 1:C:234:GLU:OE2  | 1:C:421:ARG:NH2  | 2.38                     | 0.55              |
| 1:D:166:GLY:O    | 1:D:167:ARG:CB   | 2.54                     | 0.55              |
| 1:A:94:LYS:O     | 1:A:96:GLN:N     | 2.40                     | 0.55              |
| 1:C:298:HIS:CG   | 1:C:299:ALA:N    | 2.75                     | 0.55              |
| 1:D:173:THR:HA   | 1:D:201:LYS:HG2  | 1.88                     | 0.55              |
| 1:D:448:ALA:HA   | 1:D:451:TRP:HD1  | 1.70                     | 0.55              |
| 1:A:190:TYR:O    | 1:A:194:ARG:HG2  | 2.06                     | 0.54              |
| 1:B:445:ILE:HG13 | 1:B:446:ARG:N    | 2.22                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:U:56:ASN:HD21  | 2:U:58:SER:CB    | 2.19                     | 0.54              |
| 1:A:42:VAL:HG13  | 1:A:97:TYR:HB2   | 1.90                     | 0.54              |
| 1:B:201:LYS:HE2  | 1:B:202:ASP:O    | 2.07                     | 0.54              |
| 1:A:295:ARG:O    | 1:A:298:HIS:HB3  | 2.08                     | 0.54              |
| 2:T:39:VAL:CG2   | 1:D:9:ALA:CB     | 2.85                     | 0.54              |
| 2:V:77:CYS:SG    | 2:V:78:THR:N     | 2.80                     | 0.54              |
| 2:U:6:PRO:HG3    | 2:V:44:PHE:HE2   | 1.72                     | 0.54              |
| 1:A:138:LEU:O    | 1:A:316:LYS:NZ   | 2.40                     | 0.54              |
| 1:D:94:LYS:O     | 1:D:96:GLN:N     | 2.40                     | 0.54              |
| 1:B:425:GLU:OE1  | 2:T:17:TYR:HB2   | 2.07                     | 0.54              |
| 1:C:201:LYS:HE2  | 1:C:202:ASP:O    | 2.08                     | 0.54              |
| 1:D:190:TYR:CZ   | 1:D:194:ARG:HD2  | 2.43                     | 0.54              |
| 1:D:29:TYR:CG    | 1:D:83:ARG:HD2   | 2.43                     | 0.54              |
| 1:C:454:GLU:CD   | 1:C:454:GLU:H    | 2.10                     | 0.54              |
| 2:U:79:ASP:CB    | 2:U:82:GLN:NE2   | 2.61                     | 0.54              |
| 1:C:382:ILE:HG13 | 1:C:402:PHE:CE1  | 2.43                     | 0.54              |
| 1:D:449:CYS:HA   | 1:D:455:LEU:HG   | 1.89                     | 0.54              |
| 1:D:298:HIS:ND1  | 1:D:302:ASP:OD2  | 2.21                     | 0.54              |
| 1:D:368:TRP:O    | 1:D:369:VAL:C    | 2.46                     | 0.54              |
| 2:T:69:MET:CE    | 2:T:72:LEU:HD12  | 2.38                     | 0.54              |
| 1:D:45:GLN:OE1   | 1:D:131:ARG:HB3  | 2.09                     | 0.53              |
| 2:U:56:ASN:ND2   | 2:U:58:SER:OG    | 2.41                     | 0.53              |
| 2:S:77:CYS:CB    | 2:S:82:GLN:OE1   | 2.55                     | 0.53              |
| 2:U:3:VAL:HG22   | 2:V:71:LYS:H     | 1.74                     | 0.53              |
| 1:A:319:ARG:HD2  | 1:A:371:LEU:HD23 | 1.89                     | 0.53              |
| 1:A:79:ARG:CG    | 1:A:79:ARG:HH11  | 1.97                     | 0.53              |
| 1:B:43:THR:O     | 1:B:43:THR:HG22  | 2.06                     | 0.53              |
| 1:B:9:ALA:HB3    | 2:V:39:VAL:HG21  | 1.91                     | 0.53              |
| 1:C:251:ILE:O    | 1:C:255:VAL:HG23 | 2.09                     | 0.53              |
| 1:C:29:TYR:CE2   | 1:C:31:THR:HA    | 2.43                     | 0.53              |
| 1:D:101:VAL:HG12 | 1:D:102:ALA:N    | 2.24                     | 0.53              |
| 1:D:214:TRP:CD2  | 1:D:253:ARG:HG2  | 2.44                     | 0.53              |
| 1:D:383:HIS:O    | 1:D:386:HIS:N    | 2.41                     | 0.53              |
| 2:V:79:ASP:HB3   | 2:V:82:GLN:HB3   | 1.89                     | 0.53              |
| 1:B:190:TYR:CE1  | 1:B:227:LYS:HD3  | 2.44                     | 0.53              |
| 1:B:443:GLU:O    | 1:B:447:GLU:N    | 2.39                     | 0.53              |
| 2:U:79:ASP:O     | 2:U:82:GLN:N     | 2.42                     | 0.53              |
| 1:B:298:HIS:ND1  | 1:B:302:ASP:OD2  | 2.33                     | 0.53              |
| 2:V:113:ILE:HG13 | 2:V:114:SER:N    | 2.23                     | 0.53              |
| 2:V:84:LEU:O     | 2:V:84:LEU:HD23  | 2.09                     | 0.53              |
| 1:A:383:HIS:NE2  | 1:A:465:ILE:HB   | 2.23                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:23:THR:HG22  | 1:C:81:LYS:HZ3   | 1.74                     | 0.53              |
| 1:C:411:TRP:CH2  | 2:U:2:GLN:OE1    | 2.62                     | 0.53              |
| 1:A:209:GLN:HB3  | 1:A:210:PRO:CD   | 2.39                     | 0.53              |
| 1:A:202:ASP:OD1  | 1:A:238:HIS:HE1  | 1.92                     | 0.53              |
| 1:B:397:ASP:OD2  | 2:T:108:ARG:NH2  | 2.42                     | 0.53              |
| 1:A:9:ALA:N      | 1:A:73:GLY:O     | 2.42                     | 0.52              |
| 1:C:29:TYR:CG    | 1:C:83:ARG:HD2   | 2.44                     | 0.52              |
| 1:C:133:LEU:O    | 1:C:307:HIS:HA   | 2.10                     | 0.52              |
| 1:C:429:LYS:HE3  | 2:U:21:LEU:HD22  | 1.90                     | 0.52              |
| 2:U:107:VAL:O    | 2:U:107:VAL:HG12 | 2.08                     | 0.52              |
| 1:C:429:LYS:NZ   | 2:U:29:GLU:OE1   | 2.42                     | 0.52              |
| 1:D:178:LEU:HD21 | 1:D:205:ASN:ND2  | 2.25                     | 0.52              |
| 1:A:94:LYS:O     | 1:A:95:ASP:C     | 2.47                     | 0.52              |
| 1:B:69:VAL:HA    | 1:C:407:LEU:O    | 2.09                     | 0.52              |
| 1:C:332:VAL:CG1  | 1:C:386:HIS:ND1  | 2.71                     | 0.52              |
| 1:C:430:ALA:CB   | 1:C:444:ILE:HD13 | 2.39                     | 0.52              |
| 1:C:76:SER:OG    | 1:C:76:SER:O     | 2.23                     | 0.52              |
| 1:D:134:ARG:HA   | 1:D:308:GLY:O    | 2.10                     | 0.52              |
| 2:S:86:GLU:OE1   | 2:S:86:GLU:HA    | 2.08                     | 0.52              |
| 2:U:119:LYS:HD2  | 2:U:123:TYR:C    | 2.29                     | 0.52              |
| 2:V:113:ILE:HG13 | 2:V:114:SER:H    | 1.73                     | 0.52              |
| 2:V:89:GLU:O     | 2:V:92:LYS:NZ    | 2.35                     | 0.52              |
| 1:B:214:TRP:CD2  | 1:B:253:ARG:HG2  | 2.44                     | 0.52              |
| 1:B:410:PRO:HD3  | 1:B:461:VAL:HG21 | 1.90                     | 0.52              |
| 1:D:192:CYS:SG   | 1:D:413:ASN:ND2  | 2.83                     | 0.52              |
| 2:S:34:LEU:O     | 2:S:36:ASN:N     | 2.42                     | 0.52              |
| 2:T:75:PHE:CD1   | 1:D:9:ALA:HB2    | 2.43                     | 0.52              |
| 1:A:155:ILE:HG12 | 1:A:375:LEU:CD1  | 2.38                     | 0.52              |
| 1:B:466:VAL:HG23 | 1:B:468:ASN:N    | 2.25                     | 0.52              |
| 1:B:335:LEU:HD21 | 1:C:127:PHE:CE1  | 2.45                     | 0.52              |
| 1:D:190:TYR:HB2  | 1:D:224:ALA:HB1  | 1.92                     | 0.52              |
| 1:A:397:ASP:OD2  | 2:S:108:ARG:NH2  | 2.43                     | 0.52              |
| 1:B:32:LYS:O     | 1:B:35:ASP:HB2   | 2.10                     | 0.52              |
| 1:C:214:TRP:CE3  | 1:C:253:ARG:HG2  | 2.45                     | 0.52              |
| 2:S:27:LEU:O     | 2:S:31:GLU:HB2   | 2.10                     | 0.52              |
| 2:T:22:SER:OG    | 2:T:25:GLN:HB2   | 2.09                     | 0.52              |
| 1:C:227:LYS:HE2  | 2:V:66:TYR:O     | 2.10                     | 0.52              |
| 1:A:241:ASN:ND2  | 1:A:243:THR:H    | 2.08                     | 0.52              |
| 1:A:387:MET:HB3  | 1:A:388:PRO:HD3  | 1.92                     | 0.52              |
| 1:A:50:PRO:HG3   | 1:A:97:TYR:CZ    | 2.45                     | 0.52              |
| 1:C:153:HIS:N    | 1:C:324:ASP:OD1  | 2.41                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:10:SER:O     | 1:D:11:VAL:HB    | 2.09                     | 0.52              |
| 2:T:77:CYS:SG    | 2:T:82:GLN:CD    | 2.88                     | 0.52              |
| 1:C:449:CYS:HA   | 1:C:455:LEU:HG   | 1.92                     | 0.52              |
| 1:C:94:LYS:O     | 1:C:95:ASP:C     | 2.49                     | 0.52              |
| 1:D:19:GLU:HB3   | 1:D:52:GLU:CD    | 2.31                     | 0.52              |
| 2:S:56:ASN:ND2   | 2:S:58:SER:OG    | 2.42                     | 0.52              |
| 1:B:9:ALA:HB2    | 2:V:75:PHE:CE1   | 2.45                     | 0.51              |
| 1:C:166:GLY:O    | 1:C:167:ARG:HB3  | 2.09                     | 0.51              |
| 1:C:60:GLU:OE2   | 1:C:65:THR:HA    | 2.09                     | 0.51              |
| 1:D:214:TRP:CE3  | 1:D:253:ARG:HG2  | 2.45                     | 0.51              |
| 2:S:98:TRP:HD1   | 2:S:116:ILE:HD11 | 1.74                     | 0.51              |
| 2:V:27:LEU:HD12  | 2:V:84:LEU:HD12  | 1.92                     | 0.51              |
| 2:V:77:CYS:CB    | 2:V:82:GLN:OE1   | 2.58                     | 0.51              |
| 1:C:153:HIS:CD2  | 1:C:290:LEU:HD23 | 2.45                     | 0.51              |
| 1:C:178:LEU:HD21 | 1:C:205:ASN:ND2  | 2.26                     | 0.51              |
| 1:D:181:SER:O    | 1:D:182:ALA:C    | 2.49                     | 0.51              |
| 1:C:90:VAL:HG23  | 1:C:96:GLN:C     | 2.31                     | 0.51              |
| 2:U:89:GLU:O     | 2:U:92:LYS:HB3   | 2.09                     | 0.51              |
| 1:A:21:LYS:HB2   | 1:A:52:GLU:OE1   | 2.10                     | 0.51              |
| 1:A:24:TYR:HB2   | 1:A:55:ALA:HB1   | 1.93                     | 0.51              |
| 1:B:442:ASN:OD1  | 1:B:446:ARG:NH1  | 2.40                     | 0.51              |
| 1:B:443:GLU:OE2  | 1:B:446:ARG:NE   | 2.42                     | 0.51              |
| 1:C:269:TYR:CD1  | 1:C:293:ILE:HG21 | 2.46                     | 0.51              |
| 2:T:23:GLN:O     | 2:T:27:LEU:HB2   | 2.09                     | 0.51              |
| 1:B:93:GLU:HA    | 1:B:93:GLU:OE1   | 2.10                     | 0.51              |
| 1:C:331:VAL:HG12 | 1:C:332:VAL:N    | 2.24                     | 0.51              |
| 2:S:26:LEU:HD23  | 2:S:26:LEU:C     | 2.31                     | 0.51              |
| 1:A:440:GLU:O    | 1:A:441:GLY:C    | 2.49                     | 0.51              |
| 1:B:411:TRP:CH2  | 2:T:2:GLN:OE1    | 2.63                     | 0.51              |
| 1:A:43:THR:HG22  | 1:A:131:ARG:CG   | 2.38                     | 0.51              |
| 1:B:133:LEU:O    | 1:B:307:HIS:HA   | 2.11                     | 0.51              |
| 1:D:209:GLN:HB3  | 1:D:210:PRO:HD2  | 1.93                     | 0.51              |
| 1:D:459:CYS:O    | 1:D:463:LYS:HB2  | 2.11                     | 0.51              |
| 2:S:34:LEU:O     | 2:S:35:LYS:C     | 2.48                     | 0.51              |
| 1:D:446:ARG:O    | 1:D:446:ARG:HG3  | 2.11                     | 0.51              |
| 2:U:35:LYS:HD2   | 2:U:35:LYS:O     | 2.11                     | 0.51              |
| 2:V:25:GLN:O     | 2:V:28:SER:HB2   | 2.11                     | 0.51              |
| 1:D:189:VAL:HG13 | 1:D:200:THR:OG1  | 2.10                     | 0.51              |
| 1:D:269:TYR:CD1  | 1:D:293:ILE:CG2  | 2.94                     | 0.51              |
| 2:V:86:GLU:O     | 2:V:89:GLU:HB3   | 2.11                     | 0.51              |
| 1:A:412:GLY:HA3  | 2:T:72:LEU:HD11  | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:317:ALA:HA   | 1:D:320:MET:CE   | 2.41                     | 0.50              |
| 1:D:385:TRP:HZ2  | 1:D:459:CYS:HB3  | 1.75                     | 0.50              |
| 1:B:17:VAL:HG12  | 1:B:18:LYS:N     | 2.27                     | 0.50              |
| 1:B:190:TYR:HB2  | 1:B:224:ALA:HB1  | 1.94                     | 0.50              |
| 1:B:229:GLN:HE21 | 1:B:236:LYS:H    | 1.58                     | 0.50              |
| 1:B:26:THR:O     | 1:B:26:THR:HG22  | 2.11                     | 0.50              |
| 1:C:241:ASN:HD22 | 1:C:242:ALA:N    | 2.09                     | 0.50              |
| 1:C:330:THR:O    | 1:C:331:VAL:HB   | 2.11                     | 0.50              |
| 1:A:72:ASP:HB3   | 1:A:77:LEU:HD21  | 1.94                     | 0.50              |
| 1:B:19:GLU:HB3   | 1:B:52:GLU:CD    | 2.31                     | 0.50              |
| 1:B:363:TYR:HD1  | 1:B:363:TYR:H    | 1.57                     | 0.50              |
| 1:B:422:VAL:O    | 1:B:423:ALA:C    | 2.48                     | 0.50              |
| 1:D:299:ALA:HA   | 1:D:302:ASP:OD1  | 2.12                     | 0.50              |
| 2:U:11:LYS:HG3   | 2:U:17:TYR:HE1   | 1.73                     | 0.50              |
| 1:A:26:THR:HG22  | 1:A:29:TYR:CB    | 2.29                     | 0.50              |
| 1:B:455:LEU:HD12 | 1:B:455:LEU:O    | 2.12                     | 0.50              |
| 1:C:190:TYR:CE1  | 1:C:227:LYS:HD3  | 2.46                     | 0.50              |
| 2:U:26:LEU:HD23  | 2:U:26:LEU:C     | 2.32                     | 0.50              |
| 1:B:138:LEU:O    | 1:B:316:LYS:NZ   | 2.44                     | 0.50              |
| 1:C:43:THR:HG22  | 1:C:43:THR:O     | 2.10                     | 0.50              |
| 1:C:336:GLU:OE2  | 1:C:472:VAL:HB   | 2.12                     | 0.50              |
| 1:A:60:GLU:OE1   | 1:D:334:LYS:HE3  | 2.12                     | 0.50              |
| 1:D:9:ALA:N      | 1:D:73:GLY:O     | 2.45                     | 0.50              |
| 2:V:83:VAL:O     | 2:V:86:GLU:HB2   | 2.12                     | 0.50              |
| 1:B:436:ASP:C    | 1:B:436:ASP:OD1  | 2.50                     | 0.50              |
| 1:C:304:GLN:NE2  | 1:C:304:GLN:CA   | 2.73                     | 0.50              |
| 1:D:19:GLU:HB3   | 1:D:52:GLU:OE2   | 2.12                     | 0.50              |
| 2:T:12:TYR:HE2   | 2:T:98:TRP:NE1   | 2.10                     | 0.50              |
| 1:A:151:PRO:O    | 1:A:285:ARG:NH1  | 2.45                     | 0.50              |
| 1:A:60:GLU:O     | 1:D:177:LYS:HE3  | 2.11                     | 0.50              |
| 1:B:436:ASP:OD1  | 1:B:438:ALA:N    | 2.44                     | 0.50              |
| 1:B:127:PHE:CD1  | 1:C:335:LEU:HD23 | 2.47                     | 0.50              |
| 1:C:345:PHE:HA   | 1:C:348:LEU:HB2  | 1.92                     | 0.50              |
| 1:C:9:ALA:N      | 1:C:73:GLY:O     | 2.45                     | 0.50              |
| 2:S:44:PHE:HA    | 2:S:98:TRP:O     | 2.11                     | 0.50              |
| 1:B:120:ILE:HG22 | 1:B:121:VAL:HG23 | 1.94                     | 0.50              |
| 1:C:442:ASN:O    | 1:C:446:ARG:HB2  | 2.12                     | 0.50              |
| 2:S:33:LEU:HD12  | 2:S:33:LEU:C     | 2.32                     | 0.50              |
| 2:S:77:CYS:SG    | 2:S:78:THR:N     | 2.84                     | 0.50              |
| 2:U:33:LEU:C     | 2:U:33:LEU:CD1   | 2.79                     | 0.50              |
| 1:A:60:GLU:OE2   | 1:A:65:THR:HA    | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:31:GLU:OE2   | 2:T:80:ALA:HB2   | 2.12                     | 0.50              |
| 1:A:190:TYR:CZ   | 1:A:194:ARG:HD2  | 2.47                     | 0.49              |
| 1:A:151:PRO:HB3  | 1:A:323:GLY:O    | 2.11                     | 0.49              |
| 1:A:378:ALA:HB3  | 1:A:400:LEU:HD23 | 1.92                     | 0.49              |
| 1:C:41:ARG:HG2   | 1:C:41:ARG:O     | 2.12                     | 0.49              |
| 2:V:86:GLU:HA    | 2:V:86:GLU:OE1   | 2.12                     | 0.49              |
| 1:A:181:SER:O    | 1:A:182:ALA:C    | 2.51                     | 0.49              |
| 1:B:157:VAL:O    | 1:B:161:LYS:HG2  | 2.13                     | 0.49              |
| 1:A:336:GLU:OE2  | 1:A:472:VAL:HB   | 2.12                     | 0.49              |
| 1:C:194:ARG:NH2  | 2:U:4:TRP:O      | 2.39                     | 0.49              |
| 2:U:72:LEU:HG    | 2:U:73:PRO:HD2   | 1.94                     | 0.49              |
| 1:A:127:PHE:HA   | 1:D:335:LEU:HD23 | 1.94                     | 0.49              |
| 1:A:51:GLU:HA    | 1:A:87:ILE:HD11  | 1.95                     | 0.49              |
| 1:D:317:ALA:HA   | 1:D:320:MET:HE3  | 1.94                     | 0.49              |
| 1:D:98:ILE:HG22  | 1:D:100:TYR:CE1  | 2.47                     | 0.49              |
| 1:A:185:TYR:O    | 1:A:189:VAL:HG23 | 2.12                     | 0.49              |
| 1:C:423:ALA:O    | 1:C:426:ALA:HB3  | 2.11                     | 0.49              |
| 1:C:429:LYS:CE   | 2:U:29:GLU:OE1   | 2.61                     | 0.49              |
| 1:D:207:ASN:O    | 1:D:217:ARG:NH2  | 2.30                     | 0.49              |
| 2:V:26:LEU:O     | 2:V:29:GLU:HB2   | 2.12                     | 0.49              |
| 2:V:56:ASN:HD21  | 2:V:58:SER:CB    | 2.25                     | 0.49              |
| 2:V:79:ASP:CB    | 2:V:82:GLN:NE2   | 2.65                     | 0.49              |
| 1:A:60:GLU:HG3   | 1:A:127:PHE:CZ   | 2.47                     | 0.49              |
| 1:B:134:ARG:HA   | 1:B:308:GLY:O    | 2.12                     | 0.49              |
| 1:B:332:VAL:CG1  | 1:B:386:HIS:ND1  | 2.73                     | 0.49              |
| 1:C:43:THR:HG22  | 1:C:131:ARG:CG   | 2.40                     | 0.49              |
| 1:D:26:THR:HG22  | 1:D:29:TYR:CB    | 2.34                     | 0.49              |
| 1:D:29:TYR:CE2   | 1:D:31:THR:HA    | 2.48                     | 0.49              |
| 2:V:23:GLN:O     | 2:V:27:LEU:HB2   | 2.13                     | 0.49              |
| 1:A:298:HIS:CG   | 1:A:299:ALA:N    | 2.81                     | 0.49              |
| 1:A:466:VAL:HG23 | 1:A:467:PHE:N    | 2.28                     | 0.49              |
| 1:D:86:ARG:HG3   | 1:D:86:ARG:HH11  | 1.78                     | 0.49              |
| 2:T:56:ASN:HD21  | 2:T:58:SER:CB    | 2.25                     | 0.49              |
| 1:A:66:TRP:CE3   | 1:A:67:THR:HB    | 2.48                     | 0.49              |
| 1:B:317:ALA:HA   | 1:B:320:MET:CE   | 2.43                     | 0.49              |
| 1:C:142:PRO:HB3  | 1:C:369:VAL:HG11 | 1.94                     | 0.49              |
| 1:D:455:LEU:O    | 1:D:458:ALA:HB3  | 2.13                     | 0.49              |
| 2:S:91:LYS:HD2   | 2:S:118:TYR:CD2  | 2.48                     | 0.49              |
| 1:A:190:TYR:HB2  | 1:A:224:ALA:HB1  | 1.95                     | 0.49              |
| 1:A:142:PRO:HB3  | 1:A:369:VAL:HG11 | 1.94                     | 0.49              |
| 1:B:190:TYR:CZ   | 1:B:227:LYS:HD3  | 2.47                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:167:ARG:O    | 1:D:167:ARG:HG3  | 2.12                     | 0.49              |
| 1:D:193:LEU:CD1  | 1:D:200:THR:HG23 | 2.43                     | 0.49              |
| 1:D:339:ARG:O    | 1:D:343:LEU:HG   | 2.12                     | 0.49              |
| 1:A:118:THR:HG21 | 1:D:204:GLU:O    | 2.13                     | 0.49              |
| 1:A:202:ASP:OD2  | 1:A:217:ARG:NH1  | 2.46                     | 0.49              |
| 1:A:190:TYR:CE1  | 1:A:227:LYS:HD3  | 2.48                     | 0.49              |
| 1:B:24:TYR:CD2   | 1:B:59:ALA:HB2   | 2.48                     | 0.49              |
| 1:B:251:ILE:O    | 1:B:255:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:26:THR:CG2   | 1:B:29:TYR:HB2   | 2.38                     | 0.49              |
| 1:B:42:VAL:HG13  | 1:B:97:TYR:HB2   | 1.95                     | 0.49              |
| 1:D:331:VAL:HG21 | 1:D:339:ARG:HA   | 1.95                     | 0.49              |
| 1:D:60:GLU:OE2   | 1:D:65:THR:HA    | 2.13                     | 0.49              |
| 2:V:79:ASP:N     | 2:V:82:GLN:NE2   | 2.61                     | 0.49              |
| 1:A:336:GLU:OE2  | 1:A:473:ASP:N    | 2.46                     | 0.48              |
| 1:A:436:ASP:O    | 1:A:440:GLU:HB2  | 2.12                     | 0.48              |
| 1:A:97:TYR:O     | 1:A:98:ILE:HD13  | 2.12                     | 0.48              |
| 1:B:317:ALA:HA   | 1:B:320:MET:HE2  | 1.94                     | 0.48              |
| 1:B:454:GLU:CD   | 1:B:454:GLU:H    | 2.16                     | 0.48              |
| 2:V:33:LEU:HD22  | 2:V:113:ILE:HG21 | 1.94                     | 0.48              |
| 1:A:368:TRP:O    | 1:A:369:VAL:C    | 2.49                     | 0.48              |
| 1:A:223:GLU:OE1  | 2:T:65:ARG:HD3   | 2.12                     | 0.48              |
| 1:A:61:SER:HB3   | 1:A:103:TYR:HE1  | 1.78                     | 0.48              |
| 1:B:429:LYS:NZ   | 2:T:29:GLU:OE1   | 2.46                     | 0.48              |
| 1:C:229:GLN:HE21 | 1:C:236:LYS:H    | 1.60                     | 0.48              |
| 1:C:202:ASP:OD1  | 1:C:238:HIS:CE1  | 2.64                     | 0.48              |
| 1:D:203:ASP:HA   | 5:D:492:FMT:O1   | 2.13                     | 0.48              |
| 2:U:86:GLU:O     | 2:U:89:GLU:HB3   | 2.12                     | 0.48              |
| 1:C:454:GLU:CD   | 1:C:454:GLU:N    | 2.66                     | 0.48              |
| 1:D:42:VAL:HG23  | 1:D:130:LEU:HD22 | 1.95                     | 0.48              |
| 2:V:11:LYS:HE3   | 2:V:17:TYR:CZ    | 2.48                     | 0.48              |
| 1:A:153:HIS:CD2  | 1:A:290:LEU:HD23 | 2.48                     | 0.48              |
| 1:A:414:ALA:O    | 1:A:417:ALA:HB3  | 2.13                     | 0.48              |
| 1:A:462:TRP:O    | 1:A:465:ILE:HG12 | 2.13                     | 0.48              |
| 1:B:295:ARG:O    | 1:B:298:HIS:HB3  | 2.14                     | 0.48              |
| 1:A:97:TYR:C     | 1:A:98:ILE:HD13  | 2.33                     | 0.48              |
| 1:B:192:CYS:HB3  | 1:B:197:LEU:HD23 | 1.96                     | 0.48              |
| 1:B:177:LYS:HB2  | 1:C:63:THR:HA    | 1.95                     | 0.48              |
| 1:D:23:THR:HB    | 1:D:24:TYR:CE1   | 2.49                     | 0.48              |
| 1:A:162:LEU:O    | 1:A:164:LYS:HG3  | 2.13                     | 0.48              |
| 1:A:339:ARG:O    | 1:A:343:LEU:HG   | 2.14                     | 0.48              |
| 1:B:167:ARG:O    | 1:B:167:ARG:HG3  | 2.13                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:387:MET:HB3  | 1:D:388:PRO:HD3  | 1.95                     | 0.48              |
| 2:T:44:PHE:HA    | 2:T:98:TRP:O     | 2.14                     | 0.48              |
| 2:V:22:SER:H     | 2:V:25:GLN:NE2   | 1.98                     | 0.48              |
| 1:B:331:VAL:HG12 | 1:B:332:VAL:N    | 2.29                     | 0.48              |
| 1:B:86:ARG:HG3   | 1:B:86:ARG:NH1   | 2.29                     | 0.48              |
| 1:D:202:ASP:OD2  | 1:D:217:ARG:NH1  | 2.46                     | 0.48              |
| 1:B:120:ILE:HD13 | 1:B:138:LEU:CD2  | 2.44                     | 0.48              |
| 1:B:48:VAL:HA    | 1:B:49:PRO:HD2   | 1.78                     | 0.48              |
| 1:D:175:LYS:NZ   | 4:D:490:CAP:O1   | 2.41                     | 0.48              |
| 2:S:77:CYS:SG    | 2:S:82:GLN:CD    | 2.92                     | 0.48              |
| 2:T:98:TRP:HD1   | 2:T:116:ILE:HD11 | 1.78                     | 0.48              |
| 2:U:73:PRO:HG2   | 2:U:75:PHE:CE2   | 2.49                     | 0.48              |
| 2:U:77:CYS:SG    | 2:U:78:THR:N     | 2.86                     | 0.48              |
| 1:A:90:VAL:HG23  | 1:A:97:TYR:HA    | 1.96                     | 0.48              |
| 1:D:239:TYR:CE2  | 1:D:292:HIS:CD2  | 3.02                     | 0.48              |
| 2:U:84:LEU:C     | 2:U:84:LEU:HD23  | 2.34                     | 0.48              |
| 1:A:133:LEU:O    | 1:A:307:HIS:HA   | 2.14                     | 0.47              |
| 1:B:94:LYS:O     | 1:B:95:ASP:C     | 2.50                     | 0.47              |
| 1:C:445:ILE:HD12 | 1:C:449:CYS:SG   | 2.53                     | 0.47              |
| 2:T:39:VAL:CG2   | 1:D:9:ALA:HB3    | 2.44                     | 0.47              |
| 2:V:92:LYS:O     | 2:V:93:ALA:CB    | 2.62                     | 0.47              |
| 1:C:389:ALA:O    | 1:C:392:GLU:HB3  | 2.13                     | 0.47              |
| 1:B:43:THR:HG22  | 1:B:131:ARG:HG3  | 1.96                     | 0.47              |
| 1:B:327:HIS:HA   | 1:B:377:VAL:HB   | 1.97                     | 0.47              |
| 1:C:181:SER:HB2  | 1:D:156:GLN:NE2  | 2.23                     | 0.47              |
| 1:C:414:ALA:O    | 1:C:417:ALA:HB3  | 2.14                     | 0.47              |
| 1:D:19:GLU:HB3   | 1:D:52:GLU:OE1   | 2.13                     | 0.47              |
| 1:D:50:PRO:HB2   | 1:D:87:ILE:HG21  | 1.96                     | 0.47              |
| 2:T:82:GLN:O     | 2:T:85:ALA:HB3   | 2.15                     | 0.47              |
| 1:A:158:GLU:OE2  | 1:A:325:HIS:NE2  | 2.29                     | 0.47              |
| 1:A:332:VAL:HG13 | 1:A:332:VAL:O    | 2.14                     | 0.47              |
| 1:D:41:ARG:NH1   | 1:D:96:GLN:OE1   | 2.44                     | 0.47              |
| 1:B:440:GLU:O    | 1:B:441:GLY:C    | 2.52                     | 0.47              |
| 1:C:154:GLY:N    | 1:C:324:ASP:OD1  | 2.45                     | 0.47              |
| 1:C:52:GLU:O     | 1:C:55:ALA:N     | 2.48                     | 0.47              |
| 1:D:425:GLU:OE1  | 2:V:17:TYR:N     | 2.43                     | 0.47              |
| 1:D:429:LYS:CE   | 2:V:29:GLU:OE1   | 2.63                     | 0.47              |
| 1:A:443:GLU:OE1  | 1:A:446:ARG:NH2  | 2.48                     | 0.47              |
| 1:C:98:ILE:HG22  | 1:C:100:TYR:CE1  | 2.50                     | 0.47              |
| 1:C:190:TYR:HB2  | 1:C:224:ALA:HB1  | 1.95                     | 0.47              |
| 1:C:363:TYR:N    | 1:C:363:TYR:CD1  | 2.82                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:410:PRO:HD3  | 1:D:461:VAL:HG21 | 1.97                     | 0.47              |
| 1:D:43:THR:O     | 1:D:43:THR:HG22  | 2.13                     | 0.47              |
| 1:B:293:ILE:HG13 | 1:B:318:LEU:HD11 | 1.97                     | 0.47              |
| 1:C:411:TRP:O    | 1:C:415:PRO:HG2  | 2.15                     | 0.47              |
| 1:D:200:THR:OG1  | 1:D:238:HIS:HD2  | 1.98                     | 0.47              |
| 1:A:165:TYR:CD1  | 2:S:111:GLN:HB2  | 2.50                     | 0.47              |
| 2:U:106:ASN:C    | 2:U:106:ASN:OD1  | 2.52                     | 0.47              |
| 1:C:187:ARG:NH2  | 2:V:111:GLN:OE1  | 2.39                     | 0.47              |
| 1:A:295:ARG:HG3  | 1:A:298:HIS:CD2  | 2.49                     | 0.47              |
| 1:A:71:THR:HA    | 1:A:74:LEU:HD22  | 1.97                     | 0.47              |
| 1:A:93:GLU:HG2   | 1:A:96:GLN:OE1   | 2.15                     | 0.47              |
| 1:C:204:GLU:HB3  | 1:C:294:HIS:CD2  | 2.50                     | 0.47              |
| 1:C:151:PRO:HB3  | 1:C:323:GLY:O    | 2.14                     | 0.47              |
| 2:S:2:GLN:N      | 2:S:2:GLN:OE1    | 2.47                     | 0.47              |
| 1:B:382:ILE:HG13 | 1:B:402:PHE:CE1  | 2.49                     | 0.47              |
| 1:C:298:HIS:ND1  | 1:C:302:ASP:OD2  | 2.38                     | 0.47              |
| 1:C:436:ASP:C    | 1:C:436:ASP:OD1  | 2.53                     | 0.47              |
| 1:D:167:ARG:H    | 1:D:396:ASP:HB3  | 1.80                     | 0.47              |
| 1:D:97:TYR:C     | 1:D:98:ILE:HD13  | 2.34                     | 0.47              |
| 1:A:121:VAL:HG22 | 1:A:125:PHE:CE1  | 2.50                     | 0.47              |
| 1:A:101:VAL:CG1  | 1:A:102:ALA:N    | 2.78                     | 0.46              |
| 1:A:60:GLU:OE1   | 1:A:127:PHE:HZ   | 1.97                     | 0.46              |
| 1:D:229:GLN:HE21 | 1:D:236:LYS:H    | 1.62                     | 0.46              |
| 2:T:77:CYS:SG    | 2:T:82:GLN:OE1   | 2.74                     | 0.46              |
| 2:T:12:TYR:CE2   | 2:T:98:TRP:NE1   | 2.83                     | 0.46              |
| 1:D:397:ASP:OD2  | 2:V:108:ARG:NH2  | 2.48                     | 0.46              |
| 2:V:108:ARG:HB3  | 2:V:110:VAL:HG13 | 1.96                     | 0.46              |
| 1:A:19:GLU:HB3   | 1:A:52:GLU:OE2   | 2.15                     | 0.46              |
| 1:B:239:TYR:HE2  | 1:B:292:HIS:CE1  | 2.33                     | 0.46              |
| 1:B:239:TYR:CE2  | 1:B:292:HIS:CE1  | 3.03                     | 0.46              |
| 1:B:418:VAL:O    | 1:B:419:ALA:C    | 2.52                     | 0.46              |
| 1:C:385:TRP:HZ2  | 1:C:459:CYS:HB3  | 1.80                     | 0.46              |
| 2:S:22:SER:H     | 2:S:25:GLN:NE2   | 2.04                     | 0.46              |
| 1:B:214:TRP:CE3  | 1:B:253:ARG:HG2  | 2.50                     | 0.46              |
| 1:B:269:TYR:CD1  | 1:B:293:ILE:CG2  | 2.98                     | 0.46              |
| 1:D:407:LEU:HG   | 1:D:413:ASN:OD1  | 2.16                     | 0.46              |
| 2:U:77:CYS:CB    | 2:U:82:GLN:OE1   | 2.61                     | 0.46              |
| 1:C:105:LEU:O    | 1:C:107:LEU:N    | 2.48                     | 0.46              |
| 1:C:291:LEU:HG   | 1:C:293:ILE:HD11 | 1.97                     | 0.46              |
| 1:C:90:VAL:HG23  | 1:C:97:TYR:HA    | 1.98                     | 0.46              |
| 1:D:336:GLU:OE2  | 1:D:472:VAL:HB   | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:26:LEU:C     | 2:V:26:LEU:HD23  | 2.36                     | 0.46              |
| 1:A:41:ARG:HA    | 1:A:97:TYR:O     | 2.15                     | 0.46              |
| 1:B:333:GLY:O    | 1:C:128:LYS:NZ   | 2.26                     | 0.46              |
| 1:B:90:VAL:HG23  | 1:B:97:TYR:HA    | 1.96                     | 0.46              |
| 1:C:315:ALA:HB1  | 1:C:349:LEU:CD1  | 2.46                     | 0.46              |
| 1:D:414:ALA:HB3  | 1:D:415:PRO:CD   | 2.35                     | 0.46              |
| 1:B:204:GLU:HB3  | 1:B:294:HIS:CD2  | 2.50                     | 0.46              |
| 1:B:331:VAL:HG21 | 1:B:339:ARG:HA   | 1.96                     | 0.46              |
| 1:B:387:MET:CB   | 1:B:388:PRO:CD   | 2.91                     | 0.46              |
| 1:B:59:ALA:C     | 1:B:61:SER:H     | 2.19                     | 0.46              |
| 1:B:50:PRO:HB2   | 1:B:87:ILE:HG21  | 1.97                     | 0.46              |
| 1:D:296:ALA:O    | 1:D:297:MET:HB3  | 2.15                     | 0.46              |
| 1:D:376:PRO:HG2  | 1:D:376:PRO:O    | 2.14                     | 0.46              |
| 2:S:19:PRO:O     | 2:S:20:ASP:C     | 2.53                     | 0.46              |
| 2:S:42:LEU:HB3   | 2:S:70:TRP:HB3   | 1.98                     | 0.46              |
| 2:V:101:ILE:O    | 2:V:114:SER:HA   | 2.15                     | 0.46              |
| 1:B:178:LEU:HD22 | 1:B:205:ASN:HD21 | 1.79                     | 0.46              |
| 1:C:134:ARG:HG3  | 1:C:135:LEU:N    | 2.27                     | 0.46              |
| 1:C:425:GLU:OE1  | 2:U:17:TYR:N     | 2.47                     | 0.46              |
| 1:A:331:VAL:HG12 | 1:A:332:VAL:N    | 2.31                     | 0.46              |
| 1:A:429:LYS:HE2  | 2:S:29:GLU:OE1   | 2.15                     | 0.46              |
| 1:A:466:VAL:HG23 | 1:A:468:ASN:N    | 2.31                     | 0.46              |
| 1:C:388:PRO:HD3  | 1:C:445:ILE:HG21 | 1.97                     | 0.46              |
| 1:B:381:GLY:HA2  | 1:C:66:TRP:NE1   | 2.31                     | 0.46              |
| 1:D:436:ASP:C    | 1:D:436:ASP:OD1  | 2.53                     | 0.46              |
| 2:T:33:LEU:HD22  | 2:T:113:ILE:HG21 | 1.97                     | 0.46              |
| 2:V:105:ASP:HB2  | 2:V:112:CYS:SG   | 2.56                     | 0.46              |
| 1:A:312:ARG:HH11 | 1:A:312:ARG:HD3  | 1.55                     | 0.46              |
| 1:D:295:ARG:HD3  | 4:D:490:CAP:O6P  | 2.16                     | 0.46              |
| 1:D:466:VAL:HG23 | 1:D:468:ASN:N    | 2.28                     | 0.46              |
| 1:A:239:TYR:HB3  | 1:A:266:MET:HB2  | 1.98                     | 0.46              |
| 1:B:283:TYR:CD1  | 1:B:283:TYR:C    | 2.88                     | 0.46              |
| 1:B:463:LYS:HE2  | 1:B:463:LYS:HB3  | 1.44                     | 0.46              |
| 1:D:41:ARG:HD3   | 1:D:96:GLN:OE1   | 2.15                     | 0.46              |
| 2:S:84:LEU:HD23  | 2:S:84:LEU:C     | 2.36                     | 0.46              |
| 1:A:57:VAL:O     | 1:A:61:SER:HB2   | 2.15                     | 0.45              |
| 1:B:383:HIS:N    | 1:B:386:HIS:HD2  | 2.01                     | 0.45              |
| 1:C:195:GLY:HA3  | 1:C:417:ALA:CB   | 2.41                     | 0.45              |
| 1:D:192:CYS:HB3  | 1:D:197:LEU:HD23 | 1.97                     | 0.45              |
| 1:A:244:ALA:HB1  | 1:A:249:GLU:HB3  | 1.98                     | 0.45              |
| 1:A:269:TYR:CD1  | 1:A:293:ILE:CG2  | 2.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:318:LEU:C    | 1:B:320:MET:N    | 2.66                     | 0.45              |
| 1:C:463:LYS:HE2  | 1:C:463:LYS:HB3  | 1.39                     | 0.45              |
| 1:C:455:LEU:O    | 1:C:458:ALA:HB3  | 2.16                     | 0.45              |
| 1:C:203:ASP:HA   | 5:C:492:FMT:O1   | 2.16                     | 0.45              |
| 1:D:153:HIS:CD2  | 1:D:290:LEU:HD23 | 2.50                     | 0.45              |
| 2:T:79:ASP:HB3   | 2:T:82:GLN:HB3   | 1.98                     | 0.45              |
| 2:U:79:ASP:O     | 2:U:80:ALA:C     | 2.54                     | 0.45              |
| 1:A:120:ILE:HG22 | 1:A:121:VAL:HG23 | 1.99                     | 0.45              |
| 1:B:200:THR:OG1  | 1:B:238:HIS:CD2  | 2.63                     | 0.45              |
| 1:C:97:TYR:O     | 1:C:98:ILE:HD13  | 2.16                     | 0.45              |
| 1:D:291:LEU:HG   | 1:D:293:ILE:HD11 | 1.98                     | 0.45              |
| 2:U:91:LYS:HD2   | 2:U:118:TYR:CD2  | 2.52                     | 0.45              |
| 1:C:363:TYR:N    | 1:C:363:TYR:HD1  | 2.14                     | 0.45              |
| 1:D:151:PRO:HB3  | 1:D:323:GLY:O    | 2.16                     | 0.45              |
| 1:B:20:TYR:CD2   | 1:B:56:ALA:HA    | 2.51                     | 0.45              |
| 1:C:158:GLU:CD   | 1:C:325:HIS:HE2  | 2.18                     | 0.45              |
| 1:C:383:HIS:N    | 1:C:386:HIS:HD2  | 2.12                     | 0.45              |
| 2:T:12:TYR:OH    | 2:T:123:TYR:HB3  | 2.16                     | 0.45              |
| 2:T:69:MET:HE2   | 2:T:72:LEU:HD12  | 1.98                     | 0.45              |
| 1:A:20:TYR:CD2   | 1:A:56:ALA:HA    | 2.51                     | 0.45              |
| 1:B:429:LYS:CE   | 2:T:29:GLU:OE1   | 2.65                     | 0.45              |
| 2:T:91:LYS:H     | 2:T:91:LYS:HG2   | 1.63                     | 0.45              |
| 1:A:120:ILE:HD13 | 1:A:138:LEU:CD2  | 2.47                     | 0.45              |
| 1:D:301:ILE:CG2  | 1:D:309:ILE:HB   | 2.46                     | 0.45              |
| 1:D:313:VAL:O    | 1:D:314:LEU:C    | 2.55                     | 0.45              |
| 2:T:75:PHE:HE1   | 1:D:9:ALA:HB2    | 1.82                     | 0.45              |
| 1:B:451:TRP:CH2  | 2:T:19:PRO:HD3   | 2.52                     | 0.45              |
| 1:C:183:LYS:O    | 2:V:66:TYR:OH    | 2.30                     | 0.45              |
| 1:D:421:ARG:NH1  | 1:D:425:GLU:OE2  | 2.50                     | 0.45              |
| 1:B:215:ARG:HD2  | 1:B:215:ARG:HH11 | 1.34                     | 0.45              |
| 1:B:455:LEU:O    | 1:B:458:ALA:HB3  | 2.17                     | 0.45              |
| 1:B:66:TRP:CZ3   | 1:B:67:THR:HB    | 2.51                     | 0.45              |
| 1:C:190:TYR:CZ   | 1:C:194:ARG:HD2  | 2.52                     | 0.45              |
| 1:A:335:LEU:HD23 | 1:D:127:PHE:CD1  | 2.51                     | 0.45              |
| 1:D:169:LEU:HB2  | 1:D:399:VAL:HG22 | 1.99                     | 0.45              |
| 2:U:2:GLN:N      | 2:U:2:GLN:OE1    | 2.50                     | 0.45              |
| 2:U:68:THR:HG22  | 2:U:69:MET:O     | 2.17                     | 0.45              |
| 1:D:334:LYS:HB3  | 1:D:381:GLY:HA3  | 1.98                     | 0.44              |
| 2:U:44:PHE:HA    | 2:U:98:TRP:O     | 2.17                     | 0.44              |
| 1:A:105:LEU:HA   | 1:A:105:LEU:HD12 | 1.79                     | 0.44              |
| 1:A:407:LEU:HG   | 1:A:413:ASN:OD1  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:436:ASP:C    | 1:A:436:ASP:OD1  | 2.55                     | 0.44              |
| 4:A:490:CAP:O4   | 5:A:492:FMT:O2   | 2.35                     | 0.44              |
| 1:B:66:TRP:CD1   | 1:C:381:GLY:HA2  | 2.53                     | 0.44              |
| 1:B:76:SER:O     | 1:B:76:SER:OG    | 2.36                     | 0.44              |
| 1:D:141:PRO:HA   | 1:D:142:PRO:HD3  | 1.87                     | 0.44              |
| 2:T:27:LEU:HD12  | 2:T:84:LEU:HD12  | 1.99                     | 0.44              |
| 2:T:45:GLU:OE2   | 2:T:48:HIS:N     | 2.44                     | 0.44              |
| 1:C:451:TRP:CH2  | 2:U:19:PRO:HD3   | 2.52                     | 0.44              |
| 1:A:239:TYR:CE2  | 1:A:292:HIS:CE1  | 3.05                     | 0.44              |
| 1:A:318:LEU:C    | 1:A:320:MET:N    | 2.70                     | 0.44              |
| 1:B:10:SER:OG    | 1:B:11:VAL:HG23  | 2.17                     | 0.44              |
| 1:B:239:TYR:CE2  | 1:B:292:HIS:CD2  | 3.06                     | 0.44              |
| 1:B:264:ILE:HG21 | 1:B:264:ILE:HD13 | 1.52                     | 0.44              |
| 1:B:61:SER:HB3   | 1:B:103:TYR:HE1  | 1.82                     | 0.44              |
| 1:D:165:TYR:CD1  | 2:V:111:GLN:HB2  | 2.52                     | 0.44              |
| 1:D:387:MET:HE2  | 1:D:424:LEU:N    | 2.32                     | 0.44              |
| 1:D:414:ALA:CB   | 1:D:415:PRO:HD3  | 2.34                     | 0.44              |
| 4:D:490:CAP:O4   | 4:D:490:CAP:O2   | 2.33                     | 0.44              |
| 1:D:90:VAL:HG23  | 1:D:97:TYR:CA    | 2.48                     | 0.44              |
| 2:U:12:TYR:OH    | 2:U:123:TYR:HB3  | 2.18                     | 0.44              |
| 1:D:194:ARG:NH2  | 2:V:4:TRP:O      | 2.45                     | 0.44              |
| 1:A:157:VAL:O    | 1:A:161:LYS:HG2  | 2.18                     | 0.44              |
| 1:A:387:MET:HG2  | 1:A:424:LEU:HA   | 1.99                     | 0.44              |
| 1:B:421:ARG:HD2  | 1:B:421:ARG:HH11 | 1.58                     | 0.44              |
| 1:C:204:GLU:HG3  | 1:C:294:HIS:CE1  | 2.53                     | 0.44              |
| 1:D:452:SER:CB   | 1:D:455:LEU:HB3  | 2.35                     | 0.44              |
| 1:B:45:GLN:OE1   | 1:B:131:ARG:HB3  | 2.18                     | 0.44              |
| 1:C:387:MET:CB   | 1:C:388:PRO:CD   | 2.93                     | 0.44              |
| 1:B:150:GLY:HA3  | 1:B:371:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:191:GLU:O    | 1:C:194:ARG:HG2  | 2.18                     | 0.44              |
| 1:A:127:PHE:CE1  | 1:D:335:LEU:HD21 | 2.52                     | 0.44              |
| 1:D:90:VAL:HG23  | 1:D:96:GLN:O     | 2.18                     | 0.44              |
| 2:U:41:CYS:HB3   | 2:U:102:ILE:HD11 | 2.00                     | 0.44              |
| 1:A:173:THR:HA   | 1:A:201:LYS:HG2  | 1.99                     | 0.44              |
| 1:A:214:TRP:CD2  | 1:A:253:ARG:HG2  | 2.52                     | 0.44              |
| 1:B:118:THR:HG21 | 1:C:204:GLU:O    | 2.17                     | 0.44              |
| 1:C:239:TYR:HB3  | 1:C:266:MET:HB2  | 2.00                     | 0.44              |
| 2:S:41:CYS:SG    | 2:S:42:LEU:N     | 2.90                     | 0.44              |
| 1:A:214:TRP:CD2  | 1:A:215:ARG:N    | 2.86                     | 0.44              |
| 1:B:291:LEU:HG   | 1:B:293:ILE:HD11 | 2.00                     | 0.44              |
| 1:C:23:THR:CG2   | 1:C:81:LYS:HZ3   | 2.31                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:241:ASN:ND2  | 1:D:243:THR:H    | 2.16                     | 0.44              |
| 1:D:318:LEU:HD22 | 1:D:326:ILE:HD12 | 2.00                     | 0.44              |
| 1:B:239:TYR:CE2  | 1:B:292:HIS:CG   | 3.06                     | 0.44              |
| 1:C:414:ALA:CB   | 1:C:415:PRO:HD3  | 2.37                     | 0.44              |
| 1:D:142:PRO:HB3  | 1:D:369:VAL:HG11 | 2.00                     | 0.44              |
| 1:A:177:LYS:HB2  | 1:D:63:THR:HA    | 2.00                     | 0.44              |
| 2:U:84:LEU:O     | 2:U:87:VAL:HB    | 2.17                     | 0.44              |
| 1:A:227:LYS:HE2  | 2:T:66:TYR:O     | 2.18                     | 0.43              |
| 1:A:331:VAL:HG21 | 1:A:339:ARG:HA   | 2.00                     | 0.43              |
| 1:B:101:VAL:HG12 | 1:B:102:ALA:N    | 2.32                     | 0.43              |
| 1:B:127:PHE:CD1  | 1:C:335:LEU:CD2  | 3.01                     | 0.43              |
| 1:B:138:LEU:HD12 | 1:B:313:VAL:HG13 | 1.99                     | 0.43              |
| 1:B:382:ILE:HD12 | 1:B:390:LEU:HD13 | 1.99                     | 0.43              |
| 1:B:52:GLU:O     | 1:B:53:ALA:C     | 2.56                     | 0.43              |
| 1:C:101:VAL:HG12 | 1:C:102:ALA:N    | 2.33                     | 0.43              |
| 1:C:10:SER:OG    | 1:C:11:VAL:HG23  | 2.17                     | 0.43              |
| 1:C:310:HIS:CE1  | 1:C:312:ARG:CZ   | 3.00                     | 0.43              |
| 1:D:443:GLU:O    | 1:D:447:GLU:N    | 2.48                     | 0.43              |
| 1:D:63:THR:OG1   | 1:D:77:LEU:HD13  | 2.17                     | 0.43              |
| 2:U:102:ILE:HG22 | 2:U:114:SER:HB2  | 2.00                     | 0.43              |
| 2:U:56:ASN:ND2   | 2:U:58:SER:N     | 2.55                     | 0.43              |
| 1:D:411:TRP:CH2  | 2:V:2:GLN:OE1    | 2.70                     | 0.43              |
| 1:B:264:ILE:HG13 | 1:B:290:LEU:O    | 2.17                     | 0.43              |
| 1:B:336:GLU:OE2  | 1:B:472:VAL:HB   | 2.18                     | 0.43              |
| 1:B:86:ARG:HG3   | 1:B:86:ARG:HH11  | 1.83                     | 0.43              |
| 1:D:151:PRO:O    | 1:D:285:ARG:NH1  | 2.51                     | 0.43              |
| 1:D:311:PHE:O    | 1:D:312:ARG:C    | 2.55                     | 0.43              |
| 1:D:443:GLU:OE2  | 1:D:446:ARG:NE   | 2.50                     | 0.43              |
| 2:S:43:GLU:HA    | 2:S:68:THR:O     | 2.18                     | 0.43              |
| 2:T:101:ILE:O    | 2:T:114:SER:HA   | 2.17                     | 0.43              |
| 2:U:79:ASP:N     | 2:U:82:GLN:NE2   | 2.64                     | 0.43              |
| 1:A:183:LYS:O    | 2:T:66:TYR:OH    | 2.33                     | 0.43              |
| 1:A:41:ARG:O     | 1:A:41:ARG:HG2   | 2.18                     | 0.43              |
| 1:B:331:VAL:HA   | 1:B:337:GLY:O    | 2.18                     | 0.43              |
| 1:B:343:LEU:HD21 | 1:B:393:ILE:HG23 | 2.00                     | 0.43              |
| 1:D:440:GLU:O    | 1:D:441:GLY:C    | 2.56                     | 0.43              |
| 2:S:58:SER:O     | 2:S:59:PRO:C     | 2.55                     | 0.43              |
| 2:V:113:ILE:CG1  | 2:V:114:SER:N    | 2.81                     | 0.43              |
| 2:V:44:PHE:HA    | 2:V:98:TRP:O     | 2.18                     | 0.43              |
| 1:B:97:TYR:C     | 1:B:98:ILE:HD13  | 2.38                     | 0.43              |
| 1:C:23:THR:CG2   | 1:C:81:LYS:NZ    | 2.80                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:264:ILE:HG13 | 1:D:290:LEU:O    | 2.19                     | 0.43              |
| 2:T:39:VAL:HG21  | 1:D:9:ALA:HB3    | 1.96                     | 0.43              |
| 2:T:79:ASP:H     | 2:T:82:GLN:HE22  | 1.64                     | 0.43              |
| 1:B:454:GLU:CD   | 1:B:454:GLU:N    | 2.72                     | 0.43              |
| 2:T:29:GLU:HB3   | 2:T:115:PHE:CZ   | 2.53                     | 0.43              |
| 2:U:11:LYS:HG3   | 2:U:17:TYR:CZ    | 2.53                     | 0.43              |
| 2:U:10:LYS:HB3   | 2:U:50:PHE:CZ    | 2.53                     | 0.43              |
| 1:B:24:TYR:CG    | 1:B:59:ALA:HB2   | 2.54                     | 0.43              |
| 1:B:153:HIS:N    | 1:B:324:ASP:OD1  | 2.38                     | 0.43              |
| 1:B:389:ALA:O    | 1:B:393:ILE:HG13 | 2.19                     | 0.43              |
| 1:C:215:ARG:HH11 | 1:C:215:ARG:HD2  | 1.30                     | 0.43              |
| 1:D:190:TYR:CZ   | 1:D:227:LYS:HD3  | 2.52                     | 0.43              |
| 1:D:269:TYR:CD1  | 1:D:293:ILE:HG21 | 2.53                     | 0.43              |
| 1:A:421:ARG:HD2  | 1:A:421:ARG:HH11 | 1.58                     | 0.43              |
| 1:C:295:ARG:O    | 1:C:296:ALA:C    | 2.56                     | 0.43              |
| 1:C:375:LEU:HD12 | 1:C:375:LEU:HA   | 1.80                     | 0.43              |
| 1:D:383:HIS:N    | 1:D:386:HIS:CD2  | 2.71                     | 0.43              |
| 1:D:463:LYS:HB3  | 1:D:463:LYS:HE2  | 1.40                     | 0.43              |
| 2:U:41:CYS:HB2   | 2:U:104:PHE:HE2  | 1.82                     | 0.43              |
| 2:V:30:VAL:O     | 2:V:34:LEU:HB2   | 2.19                     | 0.43              |
| 1:A:298:HIS:ND1  | 1:A:302:ASP:OD2  | 2.35                     | 0.43              |
| 1:A:343:LEU:HD23 | 1:A:343:LEU:HA   | 1.72                     | 0.43              |
| 1:D:387:MET:HB3  | 1:D:388:PRO:CD   | 2.48                     | 0.43              |
| 1:D:86:ARG:HG3   | 1:D:86:ARG:NH1   | 2.34                     | 0.43              |
| 2:S:86:GLU:O     | 2:S:89:GLU:HB3   | 2.18                     | 0.43              |
| 2:V:103:GLY:HA3  | 2:V:113:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:410:PRO:HD3  | 1:A:461:VAL:HG21 | 2.01                     | 0.43              |
| 1:B:185:TYR:O    | 1:B:189:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:293:ILE:HA   | 1:B:293:ILE:HD13 | 1.79                     | 0.43              |
| 1:B:29:TYR:CG    | 1:B:83:ARG:HD2   | 2.54                     | 0.43              |
| 1:B:94:LYS:NZ    | 1:B:94:LYS:HB2   | 2.34                     | 0.43              |
| 1:C:178:LEU:CD2  | 1:C:205:ASN:ND2  | 2.81                     | 0.43              |
| 1:C:42:VAL:HG23  | 1:C:130:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:410:PRO:HD3  | 1:C:461:VAL:HG21 | 2.00                     | 0.43              |
| 1:D:193:LEU:HD13 | 1:D:200:THR:CG2  | 2.47                     | 0.43              |
| 2:U:117:ALA:O    | 2:U:118:TYR:CB   | 2.60                     | 0.43              |
| 1:C:167:ARG:HG2  | 2:U:14:THR:OG1   | 2.18                     | 0.43              |
| 2:V:11:LYS:HE3   | 2:V:17:TYR:CE1   | 2.54                     | 0.43              |
| 2:V:82:GLN:O     | 2:V:85:ALA:CB    | 2.59                     | 0.43              |
| 2:V:98:TRP:HD1   | 2:V:116:ILE:CD1  | 2.32                     | 0.43              |
| 1:A:158:GLU:CD   | 1:A:325:HIS:HE2  | 2.16                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:463:LYS:HE2  | 1:A:463:LYS:HB3  | 1.36                     | 0.43              |
| 1:B:190:TYR:O    | 1:B:194:ARG:HG2  | 2.19                     | 0.43              |
| 1:C:36:ILE:N     | 1:C:36:ILE:HD12  | 2.34                     | 0.43              |
| 1:C:44:PRO:O     | 1:C:131:ARG:HG2  | 2.19                     | 0.43              |
| 1:D:163:ASN:HA   | 1:D:163:ASN:HD22 | 1.61                     | 0.43              |
| 1:D:293:ILE:CG1  | 1:D:318:LEU:HD11 | 2.42                     | 0.43              |
| 2:U:15:LEU:C     | 2:U:17:TYR:H     | 2.22                     | 0.43              |
| 1:A:457:ALA:O    | 1:A:461:VAL:HG23 | 2.18                     | 0.42              |
| 1:D:280:LEU:HD12 | 1:D:280:LEU:HA   | 1.81                     | 0.42              |
| 1:D:336:GLU:OE2  | 1:D:473:ASP:N    | 2.52                     | 0.42              |
| 2:T:14:THR:HG22  | 2:T:15:LEU:HG    | 2.01                     | 0.42              |
| 2:U:89:GLU:O     | 2:U:92:LYS:O     | 2.37                     | 0.42              |
| 2:V:42:LEU:HB3   | 2:V:70:TRP:HB3   | 2.01                     | 0.42              |
| 1:A:268:ASP:HA   | 1:A:294:HIS:O    | 2.19                     | 0.42              |
| 1:A:332:VAL:O    | 1:A:332:VAL:CG1  | 2.66                     | 0.42              |
| 1:B:141:PRO:O    | 1:B:142:PRO:C    | 2.56                     | 0.42              |
| 1:B:239:TYR:CD2  | 1:B:292:HIS:CD2  | 3.07                     | 0.42              |
| 1:C:315:ALA:HB1  | 1:C:349:LEU:HD11 | 2.01                     | 0.42              |
| 1:C:86:ARG:NH1   | 1:C:86:ARG:HG3   | 2.33                     | 0.42              |
| 2:U:101:ILE:O    | 2:U:114:SER:HA   | 2.19                     | 0.42              |
| 1:A:45:GLN:HA    | 1:A:46:PRO:HD2   | 1.78                     | 0.42              |
| 1:B:112:SER:O    | 1:B:113:VAL:C    | 2.57                     | 0.42              |
| 1:B:435:ARG:HH11 | 1:B:435:ARG:HD2  | 1.61                     | 0.42              |
| 2:S:98:TRP:CD1   | 2:S:116:ILE:HD11 | 2.54                     | 0.42              |
| 2:U:41:CYS:SG    | 2:U:42:LEU:N     | 2.92                     | 0.42              |
| 2:U:79:ASP:HB3   | 2:U:82:GLN:HB3   | 2.01                     | 0.42              |
| 2:V:29:GLU:HB3   | 2:V:115:PHE:CZ   | 2.53                     | 0.42              |
| 2:V:43:GLU:OE2   | 2:V:100:ARG:NH1  | 2.45                     | 0.42              |
| 1:A:215:ARG:HD2  | 1:A:215:ARG:HH11 | 1.34                     | 0.42              |
| 1:B:190:TYR:CZ   | 1:B:194:ARG:HD2  | 2.55                     | 0.42              |
| 1:B:106:ASP:O    | 1:C:210:PRO:HD2  | 2.19                     | 0.42              |
| 1:D:264:ILE:HA   | 1:D:290:LEU:O    | 2.19                     | 0.42              |
| 1:D:454:GLU:CD   | 1:D:454:GLU:H    | 2.23                     | 0.42              |
| 2:T:33:LEU:HD22  | 2:T:113:ILE:CG2  | 2.49                     | 0.42              |
| 1:A:425:GLU:OE1  | 2:S:17:TYR:N     | 2.47                     | 0.42              |
| 1:B:94:LYS:O     | 1:B:96:GLN:N     | 2.52                     | 0.42              |
| 1:C:234:GLU:O    | 1:C:235:ILE:C    | 2.58                     | 0.42              |
| 1:C:295:ARG:CZ   | 1:C:298:HIS:CE1  | 3.03                     | 0.42              |
| 1:D:293:ILE:CG2  | 1:D:318:LEU:HD11 | 2.45                     | 0.42              |
| 2:V:113:ILE:O    | 2:V:114:SER:CB   | 2.66                     | 0.42              |
| 2:U:1:MET:SD     | 2:V:71:LYS:HB3   | 2.59                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:73:GLY:HA3   | 2:V:75:PHE:CE1   | 2.55                     | 0.42              |
| 1:A:318:LEU:HD22 | 1:A:326:ILE:HB   | 2.01                     | 0.42              |
| 1:A:345:PHE:O    | 1:A:348:LEU:HB2  | 2.18                     | 0.42              |
| 1:C:192:CYS:SG   | 1:C:413:ASN:ND2  | 2.93                     | 0.42              |
| 1:C:41:ARG:NH1   | 1:C:96:GLN:OE1   | 2.52                     | 0.42              |
| 1:D:443:GLU:O    | 1:D:447:GLU:HG3  | 2.19                     | 0.42              |
| 2:T:2:GLN:N      | 2:T:2:GLN:OE1    | 2.52                     | 0.42              |
| 2:T:56:ASN:ND2   | 2:T:58:SER:OG    | 2.49                     | 0.42              |
| 1:A:292:HIS:NE2  | 1:A:327:HIS:NE2  | 2.68                     | 0.42              |
| 1:A:318:LEU:HD22 | 1:A:326:ILE:HD12 | 2.00                     | 0.42              |
| 1:B:85:TYR:O     | 1:B:86:ARG:HB3   | 2.19                     | 0.42              |
| 1:C:442:ASN:O    | 1:C:446:ARG:CB   | 2.68                     | 0.42              |
| 1:D:134:ARG:HG3  | 1:D:135:LEU:N    | 2.33                     | 0.42              |
| 1:D:154:GLY:HA2  | 1:D:373:GLY:O    | 2.20                     | 0.42              |
| 1:D:66:TRP:CE3   | 1:D:67:THR:HB    | 2.54                     | 0.42              |
| 2:S:3:VAL:HG22   | 2:T:71:LYS:H     | 1.84                     | 0.42              |
| 1:B:89:ARG:HB2   | 1:B:89:ARG:NH1   | 2.25                     | 0.42              |
| 1:C:150:GLY:HA3  | 1:C:371:LEU:HD11 | 2.01                     | 0.42              |
| 1:D:167:ARG:HA   | 1:D:168:PRO:HD3  | 1.79                     | 0.42              |
| 1:D:421:ARG:O    | 1:D:425:GLU:HG3  | 2.19                     | 0.42              |
| 2:S:113:ILE:O    | 2:S:114:SER:HB2  | 2.20                     | 0.42              |
| 2:T:84:LEU:O     | 2:T:84:LEU:HD23  | 2.20                     | 0.42              |
| 1:B:9:ALA:N      | 1:B:73:GLY:O     | 2.53                     | 0.42              |
| 1:C:151:PRO:O    | 1:C:285:ARG:NH1  | 2.53                     | 0.42              |
| 1:C:190:TYR:CZ   | 1:C:227:LYS:HD3  | 2.55                     | 0.42              |
| 1:C:357:ASP:C    | 1:C:359:SER:N    | 2.73                     | 0.42              |
| 1:C:436:ASP:O    | 1:C:437:LEU:C    | 2.57                     | 0.42              |
| 1:C:441:GLY:O    | 1:C:444:ILE:HB   | 2.19                     | 0.42              |
| 1:D:239:TYR:HB3  | 1:D:266:MET:HB2  | 2.02                     | 0.42              |
| 1:A:167:ARG:HG2  | 2:S:14:THR:OG1   | 2.20                     | 0.42              |
| 2:S:26:LEU:O     | 2:S:29:GLU:HB2   | 2.20                     | 0.42              |
| 1:A:465:ILE:H    | 1:A:465:ILE:HG12 | 1.37                     | 0.42              |
| 1:C:330:THR:HG21 | 1:C:382:ILE:HG23 | 2.01                     | 0.42              |
| 1:A:17:VAL:C     | 1:A:18:LYS:HG3   | 2.39                     | 0.41              |
| 1:A:429:LYS:NZ   | 1:A:433:GLU:OE1  | 2.53                     | 0.41              |
| 1:C:41:ARG:HH11  | 1:C:41:ARG:HD3   | 1.43                     | 0.41              |
| 1:A:68:THR:O     | 1:D:408:GLY:HA2  | 2.19                     | 0.41              |
| 1:D:423:ALA:O    | 1:D:426:ALA:HB3  | 2.20                     | 0.41              |
| 2:S:3:VAL:HG21   | 2:T:70:TRP:CE3   | 2.55                     | 0.41              |
| 2:U:30:VAL:O     | 2:U:34:LEU:HD12  | 2.20                     | 0.41              |
| 1:A:280:LEU:HA   | 1:A:280:LEU:HD12 | 1.82                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:77:LEU:HD23  | 1:A:77:LEU:N     | 2.35                     | 0.41              |
| 1:B:225:LEU:HD12 | 1:B:225:LEU:C    | 2.40                     | 0.41              |
| 1:B:229:GLN:HG3  | 1:B:234:GLU:O    | 2.20                     | 0.41              |
| 1:B:411:TRP:CZ3  | 2:T:2:GLN:OE1    | 2.74                     | 0.41              |
| 1:C:269:TYR:CD1  | 1:C:293:ILE:HG22 | 2.55                     | 0.41              |
| 1:D:409:HIS:HA   | 1:D:410:PRO:HD2  | 1.74                     | 0.41              |
| 2:S:22:SER:OG    | 2:S:25:GLN:HB2   | 2.20                     | 0.41              |
| 2:S:33:LEU:HD13  | 2:S:38:TRP:CB    | 2.45                     | 0.41              |
| 2:U:105:ASP:HB2  | 2:U:112:CYS:SG   | 2.59                     | 0.41              |
| 1:B:251:ILE:HA   | 1:B:251:ILE:HD13 | 1.73                     | 0.41              |
| 1:C:440:GLU:O    | 1:C:441:GLY:C    | 2.59                     | 0.41              |
| 1:A:304:GLN:HA   | 1:A:304:GLN:NE2  | 2.35                     | 0.41              |
| 1:B:295:ARG:HG3  | 1:B:298:HIS:CD2  | 2.55                     | 0.41              |
| 1:C:27:PRO:HD2   | 1:C:28:GLU:OE2   | 2.20                     | 0.41              |
| 1:C:452:SER:HA   | 1:C:453:PRO:HD3  | 1.91                     | 0.41              |
| 1:D:465:ILE:H    | 1:D:465:ILE:HG12 | 1.67                     | 0.41              |
| 2:U:3:VAL:HG21   | 2:V:70:TRP:CZ3   | 2.55                     | 0.41              |
| 2:V:96:GLN:OE1   | 2:V:96:GLN:N     | 2.41                     | 0.41              |
| 1:B:407:LEU:HG   | 1:B:413:ASN:OD1  | 2.20                     | 0.41              |
| 1:C:436:ASP:CG   | 1:C:439:GLN:H    | 2.23                     | 0.41              |
| 1:C:45:GLN:HA    | 1:C:46:PRO:HD2   | 1.80                     | 0.41              |
| 1:D:360:ARG:HE   | 1:D:360:ARG:HB2  | 1.59                     | 0.41              |
| 1:D:363:TYR:N    | 1:D:363:TYR:CD1  | 2.89                     | 0.41              |
| 2:S:101:ILE:HG13 | 2:S:117:ALA:HB2  | 2.01                     | 0.41              |
| 2:V:55:ASN:N     | 2:V:63:ASP:OD2   | 2.45                     | 0.41              |
| 1:A:304:GLN:HA   | 1:A:304:GLN:HE21 | 1.84                     | 0.41              |
| 1:A:363:TYR:N    | 1:A:363:TYR:CD1  | 2.88                     | 0.41              |
| 1:A:435:ARG:HH22 | 1:A:447:GLU:CD   | 2.24                     | 0.41              |
| 1:A:24:TYR:CD2   | 1:A:59:ALA:HB2   | 2.55                     | 0.41              |
| 1:D:382:ILE:HG13 | 1:D:402:PHE:CE1  | 2.56                     | 0.41              |
| 1:A:451:TRP:CH2  | 2:S:19:PRO:HD3   | 2.56                     | 0.41              |
| 2:U:113:ILE:CG1  | 2:U:114:SER:N    | 2.83                     | 0.41              |
| 2:U:30:VAL:HG11  | 2:U:83:VAL:HG22  | 2.01                     | 0.41              |
| 2:V:19:PRO:O     | 2:V:20:ASP:C     | 2.58                     | 0.41              |
| 1:C:312:ARG:HD3  | 1:C:312:ARG:HH11 | 1.55                     | 0.41              |
| 1:C:397:ASP:OD2  | 2:U:108:ARG:NH2  | 2.53                     | 0.41              |
| 1:C:449:CYS:HB3  | 1:C:456:ALA:HA   | 2.01                     | 0.41              |
| 1:D:442:ASN:O    | 1:D:446:ARG:HB2  | 2.20                     | 0.41              |
| 2:S:29:GLU:HB3   | 2:S:115:PHE:CZ   | 2.56                     | 0.41              |
| 2:U:35:LYS:NZ    | 2:U:36:ASN:ND2   | 2.69                     | 0.41              |
| 1:A:264:ILE:HG21 | 1:A:264:ILE:HD13 | 1.88                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:335:LEU:HD21 | 1:D:127:PHE:CE1  | 2.55                     | 0.41              |
| 1:A:387:MET:N    | 1:A:388:PRO:HD2  | 2.36                     | 0.41              |
| 1:C:181:SER:O    | 1:C:182:ALA:C    | 2.59                     | 0.41              |
| 1:C:71:THR:HA    | 1:C:74:LEU:HD22  | 2.02                     | 0.41              |
| 1:A:128:LYS:HD2  | 1:D:333:GLY:O    | 2.20                     | 0.41              |
| 1:D:388:PRO:HD3  | 1:D:445:ILE:HG21 | 2.03                     | 0.41              |
| 1:B:17:VAL:O     | 1:B:18:LYS:HG3   | 2.21                     | 0.41              |
| 1:C:192:CYS:HB2  | 1:C:200:THR:HG21 | 2.03                     | 0.41              |
| 1:C:310:HIS:ND1  | 1:C:312:ARG:CZ   | 2.84                     | 0.41              |
| 1:C:388:PRO:O    | 1:C:392:GLU:HB2  | 2.21                     | 0.41              |
| 2:T:98:TRP:HD1   | 2:T:116:ILE:CD1  | 2.34                     | 0.41              |
| 2:U:11:LYS:HE3   | 2:U:17:TYR:CZ    | 2.56                     | 0.41              |
| 1:A:171:GLY:O    | 1:A:401:GLN:HA   | 2.21                     | 0.41              |
| 1:B:105:LEU:O    | 1:B:107:LEU:N    | 2.54                     | 0.41              |
| 1:B:213:ARG:HH11 | 1:B:213:ARG:HD2  | 1.60                     | 0.41              |
| 1:B:447:GLU:O    | 1:B:450:LYS:HB2  | 2.21                     | 0.41              |
| 1:C:201:LYS:HG3  | 1:C:202:ASP:O    | 2.21                     | 0.41              |
| 1:D:431:ARG:HG3  | 1:D:437:LEU:CD2  | 2.51                     | 0.41              |
| 2:U:119:LYS:HD2  | 2:U:123:TYR:OXT  | 2.20                     | 0.41              |
| 2:U:13:GLU:HB3   | 2:U:14:THR:H     | 1.67                     | 0.41              |
| 1:A:239:TYR:HE2  | 1:A:292:HIS:CE1  | 2.39                     | 0.41              |
| 1:B:171:GLY:HA2  | 1:B:199:PHE:O    | 2.20                     | 0.41              |
| 1:C:200:THR:OG1  | 1:C:238:HIS:HD2  | 2.04                     | 0.41              |
| 1:D:215:ARG:HH11 | 1:D:215:ARG:HD2  | 1.66                     | 0.41              |
| 1:D:304:GLN:NE2  | 1:D:304:GLN:CA   | 2.84                     | 0.41              |
| 2:T:11:LYS:HG3   | 2:T:17:TYR:CZ    | 2.56                     | 0.41              |
| 2:U:15:LEU:O     | 2:U:17:TYR:N     | 2.54                     | 0.41              |
| 1:D:451:TRP:CZ2  | 2:V:19:PRO:HD3   | 2.56                     | 0.41              |
| 1:B:121:VAL:HG13 | 1:C:300:VAL:HG21 | 2.01                     | 0.40              |
| 1:C:283:TYR:C    | 1:C:283:TYR:CD2  | 2.94                     | 0.40              |
| 1:C:371:LEU:HA   | 1:C:371:LEU:HD12 | 1.94                     | 0.40              |
| 1:D:343:LEU:HA   | 1:D:343:LEU:HD23 | 1.70                     | 0.40              |
| 2:T:33:LEU:C     | 2:T:33:LEU:HD12  | 2.41                     | 0.40              |
| 1:A:440:GLU:O    | 1:A:441:GLY:O    | 2.39                     | 0.40              |
| 1:B:26:THR:C     | 1:B:28:GLU:H     | 2.24                     | 0.40              |
| 1:C:51:GLU:HA    | 1:C:87:ILE:CD1   | 2.48                     | 0.40              |
| 1:D:152:PRO:O    | 1:D:285:ARG:NH1  | 2.51                     | 0.40              |
| 1:A:173:THR:HG21 | 4:A:490:CAP:O2   | 2.21                     | 0.40              |
| 1:B:9:ALA:HB2    | 2:V:75:PHE:CD1   | 2.56                     | 0.40              |
| 1:A:152:PRO:HA   | 1:A:285:ARG:HD3  | 2.03                     | 0.40              |
| 1:A:448:ALA:HA   | 1:A:451:TRP:HD1  | 1.82                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:48:VAL:HA    | 1:A:49:PRO:HD2   | 1.71                     | 0.40              |
| 1:B:105:LEU:HA   | 1:B:105:LEU:HD12 | 1.75                     | 0.40              |
| 1:B:163:ASN:HA   | 1:B:163:ASN:HD22 | 1.53                     | 0.40              |
| 1:B:165:TYR:CD1  | 2:T:111:GLN:HB2  | 2.56                     | 0.40              |
| 1:B:51:GLU:HA    | 1:B:87:ILE:CD1   | 2.51                     | 0.40              |
| 1:C:146:LYS:HA   | 1:C:146:LYS:HD2  | 1.83                     | 0.40              |
| 2:S:105:ASP:OD2  | 2:S:108:ARG:HD3  | 2.21                     | 0.40              |
| 1:B:429:LYS:HE2  | 2:T:29:GLU:OE1   | 2.22                     | 0.40              |
| 2:U:53:ARG:HD3   | 2:U:57:LYS:HG2   | 2.03                     | 0.40              |
| 2:V:107:VAL:O    | 2:V:107:VAL:HG12 | 2.21                     | 0.40              |
| 1:A:157:VAL:HA   | 1:A:160:ASP:HB2  | 2.04                     | 0.40              |
| 1:A:17:VAL:HG21  | 1:D:465:ILE:HD12 | 2.03                     | 0.40              |
| 1:C:357:ASP:OD2  | 1:C:360:ARG:HB2  | 2.21                     | 0.40              |
| 1:C:368:TRP:O    | 1:C:369:VAL:C    | 2.59                     | 0.40              |
| 1:C:466:VAL:HG23 | 1:C:468:ASN:N    | 2.37                     | 0.40              |
| 1:D:305:LYS:O    | 1:D:305:LYS:CG   | 2.66                     | 0.40              |
| 1:D:86:ARG:CG    | 1:D:86:ARG:HH11  | 2.33                     | 0.40              |
| 2:S:14:THR:HG22  | 2:S:15:LEU:HG    | 2.04                     | 0.40              |

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

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:B:446:ARG:NH2 | 1:C:30:GLN:NE2[3_654] | 2.00                     | 0.20              |

## 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     | 463/477 (97%) | 402 (87%) | 48 (10%) | 13 (3%)  | 6           | 14 |
| 1   | B     | 463/477 (97%) | 399 (86%) | 52 (11%) | 12 (3%)  | 6           | 15 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | C     | 463/477 (97%)   | 388 (84%)  | 63 (14%)  | 12 (3%)  | 6           | 15 |
| 1   | D     | 463/477 (97%)   | 400 (86%)  | 52 (11%)  | 11 (2%)  | 7           | 17 |
| 2   | S     | 121/123 (98%)   | 104 (86%)  | 14 (12%)  | 3 (2%)   | 6           | 17 |
| 2   | T     | 121/123 (98%)   | 102 (84%)  | 17 (14%)  | 2 (2%)   | 11          | 27 |
| 2   | U     | 121/123 (98%)   | 99 (82%)   | 19 (16%)  | 3 (2%)   | 6           | 17 |
| 2   | V     | 121/123 (98%)   | 100 (83%)  | 19 (16%)  | 2 (2%)   | 11          | 27 |
| All | All   | 2336/2400 (97%) | 1994 (85%) | 284 (12%) | 58 (2%)  | 6           | 17 |

All (58) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | PRO  |
| 1   | A     | 95  | ASP  |
| 1   | A     | 167 | ARG  |
| 2   | S     | 93  | ALA  |
| 1   | B     | 46  | PRO  |
| 1   | B     | 95  | ASP  |
| 1   | B     | 167 | ARG  |
| 2   | T     | 93  | ALA  |
| 1   | C     | 46  | PRO  |
| 1   | C     | 95  | ASP  |
| 1   | C     | 167 | ARG  |
| 2   | U     | 93  | ALA  |
| 1   | D     | 46  | PRO  |
| 1   | D     | 95  | ASP  |
| 1   | D     | 167 | ARG  |
| 2   | V     | 93  | ALA  |
| 1   | A     | 106 | ASP  |
| 1   | A     | 441 | GLY  |
| 1   | A     | 442 | ASN  |
| 1   | B     | 10  | SER  |
| 1   | B     | 106 | ASP  |
| 1   | B     | 441 | GLY  |
| 1   | B     | 442 | ASN  |
| 1   | C     | 86  | ARG  |
| 1   | C     | 106 | ASP  |
| 1   | C     | 441 | GLY  |
| 1   | C     | 442 | ASN  |
| 2   | U     | 16  | SER  |
| 1   | D     | 369 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 441 | GLY  |
| 1   | D     | 442 | ASN  |
| 1   | A     | 86  | ARG  |
| 1   | B     | 86  | ARG  |
| 2   | T     | 76  | GLY  |
| 2   | U     | 76  | GLY  |
| 1   | D     | 10  | SER  |
| 1   | D     | 86  | ARG  |
| 1   | A     | 10  | SER  |
| 2   | S     | 35  | LYS  |
| 2   | S     | 76  | GLY  |
| 1   | B     | 21  | LYS  |
| 1   | C     | 10  | SER  |
| 1   | A     | 11  | VAL  |
| 1   | B     | 11  | VAL  |
| 1   | B     | 369 | VAL  |
| 1   | C     | 11  | VAL  |
| 1   | C     | 384 | VAL  |
| 1   | C     | 385 | TRP  |
| 1   | D     | 11  | VAL  |
| 1   | D     | 166 | GLY  |
| 2   | V     | 16  | SER  |
| 1   | A     | 155 | ILE  |
| 1   | D     | 384 | VAL  |
| 1   | A     | 384 | VAL  |
| 1   | B     | 384 | VAL  |
| 1   | A     | 403 | GLY  |
| 1   | C     | 369 | VAL  |
| 1   | A     | 369 | VAL  |

### 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     | 373/386 (97%) | 326 (87%) | 47 (13%) | 5           | 12 |
| 1   | B     | 373/386 (97%) | 321 (86%) | 52 (14%) | 4           | 10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | C     | 373/386 (97%)   | 322 (86%)  | 51 (14%)  | 4           | 10 |
| 1   | D     | 373/386 (97%)   | 325 (87%)  | 48 (13%)  | 5           | 12 |
| 2   | S     | 109/109 (100%)  | 94 (86%)   | 15 (14%)  | 4           | 10 |
| 2   | T     | 109/109 (100%)  | 93 (85%)   | 16 (15%)  | 3           | 9  |
| 2   | U     | 109/109 (100%)  | 91 (84%)   | 18 (16%)  | 2           | 7  |
| 2   | V     | 109/109 (100%)  | 90 (83%)   | 19 (17%)  | 2           | 5  |
| All | All   | 1928/1980 (97%) | 1662 (86%) | 266 (14%) | 4           | 10 |

All (266) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | SER  |
| 1   | A     | 23  | THR  |
| 1   | A     | 46  | PRO  |
| 1   | A     | 51  | GLU  |
| 1   | A     | 61  | SER  |
| 1   | A     | 74  | LEU  |
| 1   | A     | 77  | LEU  |
| 1   | A     | 79  | ARG  |
| 1   | A     | 89  | ARG  |
| 1   | A     | 94  | LYS  |
| 1   | A     | 131 | ARG  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 139 | ARG  |
| 1   | A     | 142 | PRO  |
| 1   | A     | 152 | PRO  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 169 | LEU  |
| 1   | A     | 172 | CYS  |
| 1   | A     | 178 | LEU  |
| 1   | A     | 193 | LEU  |
| 1   | A     | 194 | ARG  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 201 | LYS  |
| 1   | A     | 203 | ASP  |
| 1   | A     | 213 | ARG  |
| 1   | A     | 215 | ARG  |
| 1   | A     | 241 | ASN  |
| 1   | A     | 258 | ARG  |
| 1   | A     | 285 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 295 | ARG  |
| 1   | A     | 312 | ARG  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 318 | LEU  |
| 1   | A     | 319 | ARG  |
| 1   | A     | 338 | GLU  |
| 1   | A     | 349 | LEU  |
| 1   | A     | 356 | GLN  |
| 1   | A     | 363 | TYR  |
| 1   | A     | 379 | SER  |
| 1   | A     | 384 | VAL  |
| 1   | A     | 421 | ARG  |
| 1   | A     | 429 | LYS  |
| 1   | A     | 433 | GLU  |
| 1   | A     | 437 | LEU  |
| 1   | A     | 442 | ASN  |
| 1   | A     | 445 | ILE  |
| 1   | A     | 466 | VAL  |
| 2   | S     | 2   | GLN  |
| 2   | S     | 6   | PRO  |
| 2   | S     | 27  | LEU  |
| 2   | S     | 29  | GLU  |
| 2   | S     | 33  | LEU  |
| 2   | S     | 35  | LYS  |
| 2   | S     | 54  | GLU  |
| 2   | S     | 77  | CYS  |
| 2   | S     | 78  | THR  |
| 2   | S     | 81  | THR  |
| 2   | S     | 82  | GLN  |
| 2   | S     | 91  | LYS  |
| 2   | S     | 92  | LYS  |
| 2   | S     | 96  | GLN  |
| 2   | S     | 110 | VAL  |
| 1   | B     | 10  | SER  |
| 1   | B     | 13  | PHE  |
| 1   | B     | 45  | GLN  |
| 1   | B     | 46  | PRO  |
| 1   | B     | 61  | SER  |
| 1   | B     | 74  | LEU  |
| 1   | B     | 77  | LEU  |
| 1   | B     | 79  | ARG  |
| 1   | B     | 89  | ARG  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 93  | GLU  |
| 1   | B     | 94  | LYS  |
| 1   | B     | 131 | ARG  |
| 1   | B     | 134 | ARG  |
| 1   | B     | 139 | ARG  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 169 | LEU  |
| 1   | B     | 172 | CYS  |
| 1   | B     | 178 | LEU  |
| 1   | B     | 185 | TYR  |
| 1   | B     | 193 | LEU  |
| 1   | B     | 194 | ARG  |
| 1   | B     | 197 | LEU  |
| 1   | B     | 201 | LYS  |
| 1   | B     | 203 | ASP  |
| 1   | B     | 213 | ARG  |
| 1   | B     | 215 | ARG  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 239 | TYR  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 285 | ARG  |
| 1   | B     | 295 | ARG  |
| 1   | B     | 304 | GLN  |
| 1   | B     | 312 | ARG  |
| 1   | B     | 314 | LEU  |
| 1   | B     | 318 | LEU  |
| 1   | B     | 319 | ARG  |
| 1   | B     | 335 | LEU  |
| 1   | B     | 338 | GLU  |
| 1   | B     | 349 | LEU  |
| 1   | B     | 356 | GLN  |
| 1   | B     | 359 | SER  |
| 1   | B     | 363 | TYR  |
| 1   | B     | 384 | VAL  |
| 1   | B     | 421 | ARG  |
| 1   | B     | 429 | LYS  |
| 1   | B     | 433 | GLU  |
| 1   | B     | 437 | LEU  |
| 1   | B     | 442 | ASN  |
| 1   | B     | 445 | ILE  |
| 1   | B     | 464 | GLU  |
| 1   | B     | 465 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 466 | VAL  |
| 2   | T     | 2   | GLN  |
| 2   | T     | 27  | LEU  |
| 2   | T     | 28  | SER  |
| 2   | T     | 29  | GLU  |
| 2   | T     | 33  | LEU  |
| 2   | T     | 35  | LYS  |
| 2   | T     | 42  | LEU  |
| 2   | T     | 65  | ARG  |
| 2   | T     | 72  | LEU  |
| 2   | T     | 77  | CYS  |
| 2   | T     | 78  | THR  |
| 2   | T     | 81  | THR  |
| 2   | T     | 82  | GLN  |
| 2   | T     | 91  | LYS  |
| 2   | T     | 92  | LYS  |
| 2   | T     | 96  | GLN  |
| 1   | C     | 10  | SER  |
| 1   | C     | 23  | THR  |
| 1   | C     | 32  | LYS  |
| 1   | C     | 45  | GLN  |
| 1   | C     | 46  | PRO  |
| 1   | C     | 61  | SER  |
| 1   | C     | 74  | LEU  |
| 1   | C     | 76  | SER  |
| 1   | C     | 77  | LEU  |
| 1   | C     | 79  | ARG  |
| 1   | C     | 89  | ARG  |
| 1   | C     | 93  | GLU  |
| 1   | C     | 94  | LYS  |
| 1   | C     | 131 | ARG  |
| 1   | C     | 134 | ARG  |
| 1   | C     | 139 | ARG  |
| 1   | C     | 142 | PRO  |
| 1   | C     | 163 | ASN  |
| 1   | C     | 169 | LEU  |
| 1   | C     | 172 | CYS  |
| 1   | C     | 178 | LEU  |
| 1   | C     | 193 | LEU  |
| 1   | C     | 197 | LEU  |
| 1   | C     | 200 | THR  |
| 1   | C     | 201 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 203 | ASP  |
| 1   | C     | 213 | ARG  |
| 1   | C     | 215 | ARG  |
| 1   | C     | 241 | ASN  |
| 1   | C     | 285 | ARG  |
| 1   | C     | 295 | ARG  |
| 1   | C     | 312 | ARG  |
| 1   | C     | 314 | LEU  |
| 1   | C     | 318 | LEU  |
| 1   | C     | 319 | ARG  |
| 1   | C     | 331 | VAL  |
| 1   | C     | 338 | GLU  |
| 1   | C     | 349 | LEU  |
| 1   | C     | 356 | GLN  |
| 1   | C     | 357 | ASP  |
| 1   | C     | 363 | TYR  |
| 1   | C     | 379 | SER  |
| 1   | C     | 384 | VAL  |
| 1   | C     | 421 | ARG  |
| 1   | C     | 429 | LYS  |
| 1   | C     | 437 | LEU  |
| 1   | C     | 442 | ASN  |
| 1   | C     | 445 | ILE  |
| 1   | C     | 464 | GLU  |
| 1   | C     | 465 | ILE  |
| 1   | C     | 466 | VAL  |
| 2   | U     | 2   | GLN  |
| 2   | U     | 6   | PRO  |
| 2   | U     | 23  | GLN  |
| 2   | U     | 27  | LEU  |
| 2   | U     | 28  | SER  |
| 2   | U     | 29  | GLU  |
| 2   | U     | 33  | LEU  |
| 2   | U     | 35  | LYS  |
| 2   | U     | 42  | LEU  |
| 2   | U     | 74  | MET  |
| 2   | U     | 77  | CYS  |
| 2   | U     | 78  | THR  |
| 2   | U     | 81  | THR  |
| 2   | U     | 82  | GLN  |
| 2   | U     | 91  | LYS  |
| 2   | U     | 92  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | U     | 96  | GLN  |
| 2   | U     | 110 | VAL  |
| 1   | D     | 10  | SER  |
| 1   | D     | 13  | PHE  |
| 1   | D     | 23  | THR  |
| 1   | D     | 37  | LEU  |
| 1   | D     | 45  | GLN  |
| 1   | D     | 46  | PRO  |
| 1   | D     | 61  | SER  |
| 1   | D     | 74  | LEU  |
| 1   | D     | 77  | LEU  |
| 1   | D     | 79  | ARG  |
| 1   | D     | 89  | ARG  |
| 1   | D     | 94  | LYS  |
| 1   | D     | 121 | VAL  |
| 1   | D     | 127 | PHE  |
| 1   | D     | 131 | ARG  |
| 1   | D     | 134 | ARG  |
| 1   | D     | 139 | ARG  |
| 1   | D     | 163 | ASN  |
| 1   | D     | 169 | LEU  |
| 1   | D     | 172 | CYS  |
| 1   | D     | 178 | LEU  |
| 1   | D     | 180 | LEU  |
| 1   | D     | 193 | LEU  |
| 1   | D     | 197 | LEU  |
| 1   | D     | 201 | LYS  |
| 1   | D     | 213 | ARG  |
| 1   | D     | 215 | ARG  |
| 1   | D     | 225 | LEU  |
| 1   | D     | 241 | ASN  |
| 1   | D     | 285 | ARG  |
| 1   | D     | 295 | ARG  |
| 1   | D     | 298 | HIS  |
| 1   | D     | 312 | ARG  |
| 1   | D     | 314 | LEU  |
| 1   | D     | 319 | ARG  |
| 1   | D     | 338 | GLU  |
| 1   | D     | 349 | LEU  |
| 1   | D     | 356 | GLN  |
| 1   | D     | 379 | SER  |
| 1   | D     | 384 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 421 | ARG  |
| 1   | D     | 429 | LYS  |
| 1   | D     | 433 | GLU  |
| 1   | D     | 437 | LEU  |
| 1   | D     | 442 | ASN  |
| 1   | D     | 445 | ILE  |
| 1   | D     | 465 | ILE  |
| 1   | D     | 466 | VAL  |
| 2   | V     | 2   | GLN  |
| 2   | V     | 6   | PRO  |
| 2   | V     | 23  | GLN  |
| 2   | V     | 27  | LEU  |
| 2   | V     | 29  | GLU  |
| 2   | V     | 33  | LEU  |
| 2   | V     | 35  | LYS  |
| 2   | V     | 52  | TYR  |
| 2   | V     | 65  | ARG  |
| 2   | V     | 77  | CYS  |
| 2   | V     | 78  | THR  |
| 2   | V     | 81  | THR  |
| 2   | V     | 82  | GLN  |
| 2   | V     | 91  | LYS  |
| 2   | V     | 92  | LYS  |
| 2   | V     | 96  | GLN  |
| 2   | V     | 100 | ARG  |
| 2   | V     | 110 | VAL  |
| 2   | V     | 121 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 153 | HIS  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 238 | HIS  |
| 1   | A     | 241 | ASN  |
| 1   | A     | 304 | GLN  |
| 1   | A     | 356 | GLN  |
| 2   | S     | 25  | GLN  |
| 2   | S     | 36  | ASN  |
| 2   | S     | 55  | ASN  |
| 2   | S     | 56  | ASN  |
| 2   | S     | 82  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S     | 111 | GLN  |
| 1   | B     | 153 | HIS  |
| 1   | B     | 156 | GLN  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 229 | GLN  |
| 1   | B     | 238 | HIS  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 304 | GLN  |
| 1   | B     | 356 | GLN  |
| 1   | B     | 420 | ASN  |
| 1   | B     | 439 | GLN  |
| 2   | T     | 23  | GLN  |
| 2   | T     | 25  | GLN  |
| 2   | T     | 36  | ASN  |
| 2   | T     | 56  | ASN  |
| 2   | T     | 82  | GLN  |
| 1   | C     | 163 | ASN  |
| 1   | C     | 229 | GLN  |
| 1   | C     | 238 | HIS  |
| 1   | C     | 241 | ASN  |
| 1   | C     | 304 | GLN  |
| 1   | C     | 356 | GLN  |
| 1   | C     | 420 | ASN  |
| 2   | U     | 25  | GLN  |
| 2   | U     | 36  | ASN  |
| 2   | U     | 55  | ASN  |
| 2   | U     | 56  | ASN  |
| 2   | U     | 82  | GLN  |
| 2   | U     | 111 | GLN  |
| 1   | D     | 156 | GLN  |
| 1   | D     | 163 | ASN  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 238 | HIS  |
| 1   | D     | 241 | ASN  |
| 1   | D     | 304 | GLN  |
| 1   | D     | 386 | HIS  |
| 1   | D     | 420 | ASN  |
| 2   | V     | 23  | GLN  |
| 2   | V     | 25  | GLN  |
| 2   | V     | 36  | ASN  |
| 2   | V     | 56  | ASN  |
| 2   | V     | 82  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 4   | CAP  | A     | 490 | 3    | 14,20,20     | 2.75 | 8 (57%)     | 17,31,31    | 4.28 | 9 (52%)     |
| 5   | FMT  | A     | 492 | 1,3  | 0,2,2        | 0.00 | -           | 0,1,1       | 0.00 | -           |
| 4   | CAP  | B     | 490 | 3    | 14,20,20     | 3.20 | 6 (42%)     | 17,31,31    | 4.65 | 9 (52%)     |
| 5   | FMT  | B     | 492 | 1,3  | 0,2,2        | 0.00 | -           | 0,1,1       | 0.00 | -           |
| 4   | CAP  | C     | 490 | 3    | 14,20,20     | 2.09 | 7 (50%)     | 17,31,31    | 5.12 | 10 (58%)    |
| 5   | FMT  | C     | 492 | 1,3  | 0,2,2        | 0.00 | -           | 0,1,1       | 0.00 | -           |
| 4   | CAP  | D     | 490 | 3    | 14,20,20     | 2.00 | 4 (28%)     | 17,31,31    | 4.89 | 8 (47%)     |
| 5   | FMT  | D     | 492 | 1,3  | 0,2,2        | 0.00 | -           | 0,1,1       | 0.00 | -           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | CAP  | A     | 490 | 3    | -       | 0/23/29/29 | 0/0/0/0 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | FMT  | A     | 492 | 1,3  | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | CAP  | B     | 490 | 3    | -       | 0/23/29/29 | 0/0/0/0 |
| 5   | FMT  | B     | 492 | 1,3  | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | CAP  | C     | 490 | 3    | -       | 0/23/29/29 | 0/0/0/0 |
| 5   | FMT  | C     | 492 | 1,3  | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | CAP  | D     | 490 | 3    | -       | 0/23/29/29 | 0/0/0/0 |
| 5   | FMT  | D     | 492 | 1,3  | -       | 0/0/0/0    | 0/0/0/0 |

All (25) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | B     | 490 | CAP  | C5-C4  | -6.84 | 1.41        | 1.51     |
| 4   | B     | 490 | CAP  | O2-C2  | -6.18 | 1.32        | 1.43     |
| 4   | A     | 490 | CAP  | O2-C2  | -5.59 | 1.33        | 1.43     |
| 4   | D     | 490 | CAP  | O2-C2  | -4.27 | 1.36        | 1.43     |
| 4   | C     | 490 | CAP  | O2-C2  | -3.71 | 1.37        | 1.43     |
| 4   | B     | 490 | CAP  | O5-C5  | -3.56 | 1.30        | 1.44     |
| 4   | A     | 490 | CAP  | C5-C4  | -3.55 | 1.46        | 1.51     |
| 4   | B     | 490 | CAP  | O3-C3  | -3.24 | 1.36        | 1.42     |
| 4   | D     | 490 | CAP  | O5-C5  | -2.65 | 1.34        | 1.44     |
| 4   | A     | 490 | CAP  | O1-C1  | -2.63 | 1.35        | 1.43     |
| 4   | A     | 490 | CAP  | O5-C5  | -2.62 | 1.34        | 1.44     |
| 4   | C     | 490 | CAP  | O5-C5  | -2.62 | 1.34        | 1.44     |
| 4   | C     | 490 | CAP  | C5-C4  | -2.61 | 1.47        | 1.51     |
| 4   | A     | 490 | CAP  | P1-O3P | -2.43 | 1.44        | 1.54     |
| 4   | C     | 490 | CAP  | P2-O4P | -2.41 | 1.42        | 1.50     |
| 4   | C     | 490 | CAP  | P1-O2P | -2.37 | 1.45        | 1.54     |
| 4   | A     | 490 | CAP  | P1-O2P | -2.37 | 1.45        | 1.54     |
| 4   | B     | 490 | CAP  | P2-O5P | 2.12  | 1.63        | 1.54     |
| 4   | C     | 490 | CAP  | P2-O5P | 2.23  | 1.64        | 1.54     |
| 4   | D     | 490 | CAP  | P2-O5P | 2.79  | 1.66        | 1.54     |
| 4   | C     | 490 | CAP  | P1-O1P | 2.81  | 1.60        | 1.50     |
| 4   | A     | 490 | CAP  | P2-O5P | 2.91  | 1.66        | 1.54     |
| 4   | A     | 490 | CAP  | P1-O1P | 3.84  | 1.63        | 1.50     |
| 4   | D     | 490 | CAP  | P1-O1P | 3.86  | 1.63        | 1.50     |
| 4   | B     | 490 | CAP  | P1-O1P | 4.18  | 1.65        | 1.50     |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4   | C     | 490 | CAP  | C5-C4-C3 | -14.64 | 81.95       | 112.05   |
| 4   | D     | 490 | CAP  | C5-C4-C3 | -13.06 | 85.20       | 112.05   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 4   | B     | 490 | CAP  | C5-C4-C3   | -11.72 | 87.95       | 112.05   |
| 4   | A     | 490 | CAP  | C5-C4-C3   | -11.46 | 88.49       | 112.05   |
| 4   | B     | 490 | CAP  | P1-O1-C1   | -4.83  | 104.98      | 118.30   |
| 4   | C     | 490 | CAP  | O3P-P1-O1  | -4.48  | 94.82       | 106.73   |
| 4   | D     | 490 | CAP  | P1-O1-C1   | -3.85  | 107.70      | 118.30   |
| 4   | C     | 490 | CAP  | O6P-P2-O5P | -3.68  | 92.75       | 107.61   |
| 4   | C     | 490 | CAP  | P1-O1-C1   | -3.36  | 109.03      | 118.30   |
| 4   | D     | 490 | CAP  | O6P-P2-O5P | -3.01  | 95.49       | 107.61   |
| 4   | A     | 490 | CAP  | P1-O1-C1   | -2.88  | 110.35      | 118.30   |
| 4   | D     | 490 | CAP  | O2P-P1-O1  | -2.82  | 99.23       | 106.73   |
| 4   | A     | 490 | CAP  | O6P-P2-O5  | -2.50  | 100.07      | 106.73   |
| 4   | A     | 490 | CAP  | O5P-P2-O4P | -2.50  | 100.73      | 110.50   |
| 4   | B     | 490 | CAP  | O3P-P1-O1  | -2.19  | 100.91      | 106.73   |
| 4   | B     | 490 | CAP  | O6P-P2-O5P | -2.07  | 99.26       | 107.61   |
| 4   | C     | 490 | CAP  | O5-P2-O4P  | 2.03   | 112.17      | 106.47   |
| 4   | C     | 490 | CAP  | O2P-P1-O1P | 2.29   | 119.46      | 110.50   |
| 4   | A     | 490 | CAP  | O5-P2-O4P  | 2.50   | 113.48      | 106.47   |
| 4   | C     | 490 | CAP  | O5P-P2-O4P | 2.65   | 120.87      | 110.50   |
| 4   | D     | 490 | CAP  | O6P-P2-O4P | 2.66   | 120.91      | 110.50   |
| 4   | C     | 490 | CAP  | O3P-P1-O2P | 2.72   | 118.59      | 107.61   |
| 4   | B     | 490 | CAP  | O5-C5-C4   | 2.80   | 116.84      | 109.36   |
| 4   | A     | 490 | CAP  | O6P-P2-O4P | 3.34   | 123.59      | 110.50   |
| 4   | B     | 490 | CAP  | O6P-P2-O4P | 3.41   | 123.85      | 110.50   |
| 4   | D     | 490 | CAP  | O3P-P1-O2P | 3.53   | 121.83      | 107.61   |
| 4   | B     | 490 | CAP  | O3P-P1-O2P | 4.26   | 124.79      | 107.61   |
| 4   | A     | 490 | CAP  | O3P-P1-O2P | 5.31   | 129.05      | 107.61   |
| 4   | A     | 490 | CAP  | O4-C4-C5   | 6.07   | 123.53      | 110.00   |
| 4   | C     | 490 | CAP  | O4-C4-C5   | 6.91   | 125.39      | 110.00   |
| 4   | D     | 490 | CAP  | O4-C4-C5   | 7.37   | 126.42      | 110.00   |
| 4   | B     | 490 | CAP  | O4-C4-C5   | 7.98   | 127.78      | 110.00   |
| 4   | A     | 490 | CAP  | P2-O5-C5   | 8.14   | 140.73      | 118.30   |
| 4   | B     | 490 | CAP  | P2-O5-C5   | 9.05   | 143.22      | 118.30   |
| 4   | C     | 490 | CAP  | P2-O5-C5   | 10.56  | 147.39      | 118.30   |
| 4   | D     | 490 | CAP  | P2-O5-C5   | 10.80  | 148.05      | 118.30   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 490 | CAP  | 2       | 0            |
| 5   | A     | 492 | FMT  | 1       | 0            |
| 4   | C     | 490 | CAP  | 1       | 0            |
| 5   | C     | 492 | FMT  | 1       | 0            |
| 4   | D     | 490 | CAP  | 3       | 0            |
| 5   | D     | 492 | FMT  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.