



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:25 AM UTC

PDB ID : 1BWF / pdb\_00001bwf  
Title : ESCHERICHIA COLI GLYCEROL KINASE MUTANT WITH BOUND ATP ANALOG SHOWING SUBSTANTIAL DOMAIN MOTION  
Authors : Bystrom, C.E.; Pettigrew, D.W.; Branchaud, B.P.; Remington, S.J.  
Deposited on : 1998-09-23  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

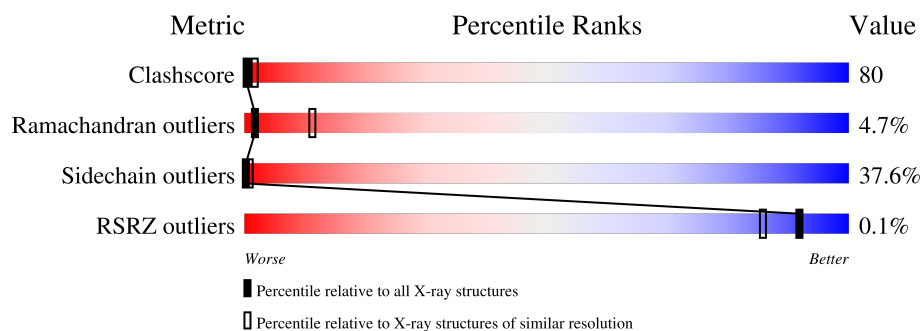
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

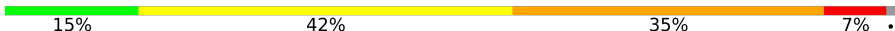
The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | O     | 501    |  |
| 1   | Y     | 501    |  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7900 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 GLYCEROL KINASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | Y     | 494      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3910  | 2470 | 683 | 738 | 19 |         |         |       |
| 1   | O     | 494      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3910  | 2470 | 683 | 738 | 19 |         |         |       |

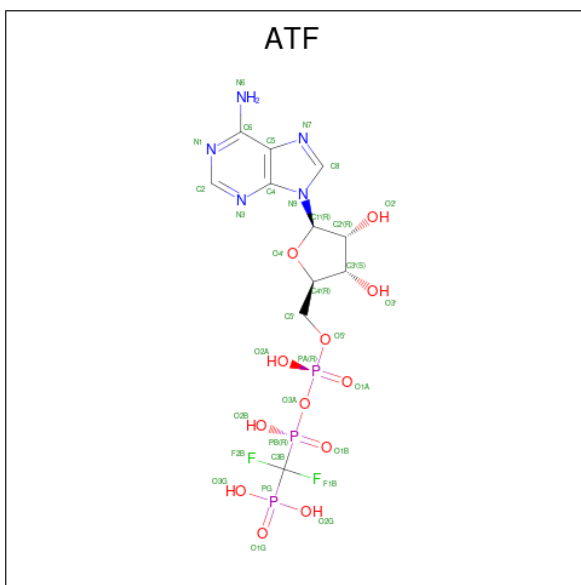
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| Y     | 58      | TRP      | SER    | engineered mutation | UNP P0A6F3 |
| O     | 58      | TRP      | SER    | engineered mutation | UNP P0A6F3 |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | Y     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | O     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is PHOSPHODIFLUOROMETHYLPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ATF) (formula: C<sub>11</sub>H<sub>16</sub>F<sub>2</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|--------|---------|---------|
| 3   | Y     | 1        | Total<br>33 | C<br>11 | F<br>2 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |
| 3   | O     | 1        | Total<br>33 | C<br>11 | F<br>2 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).

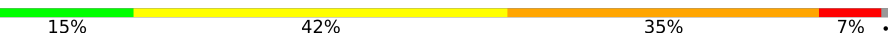


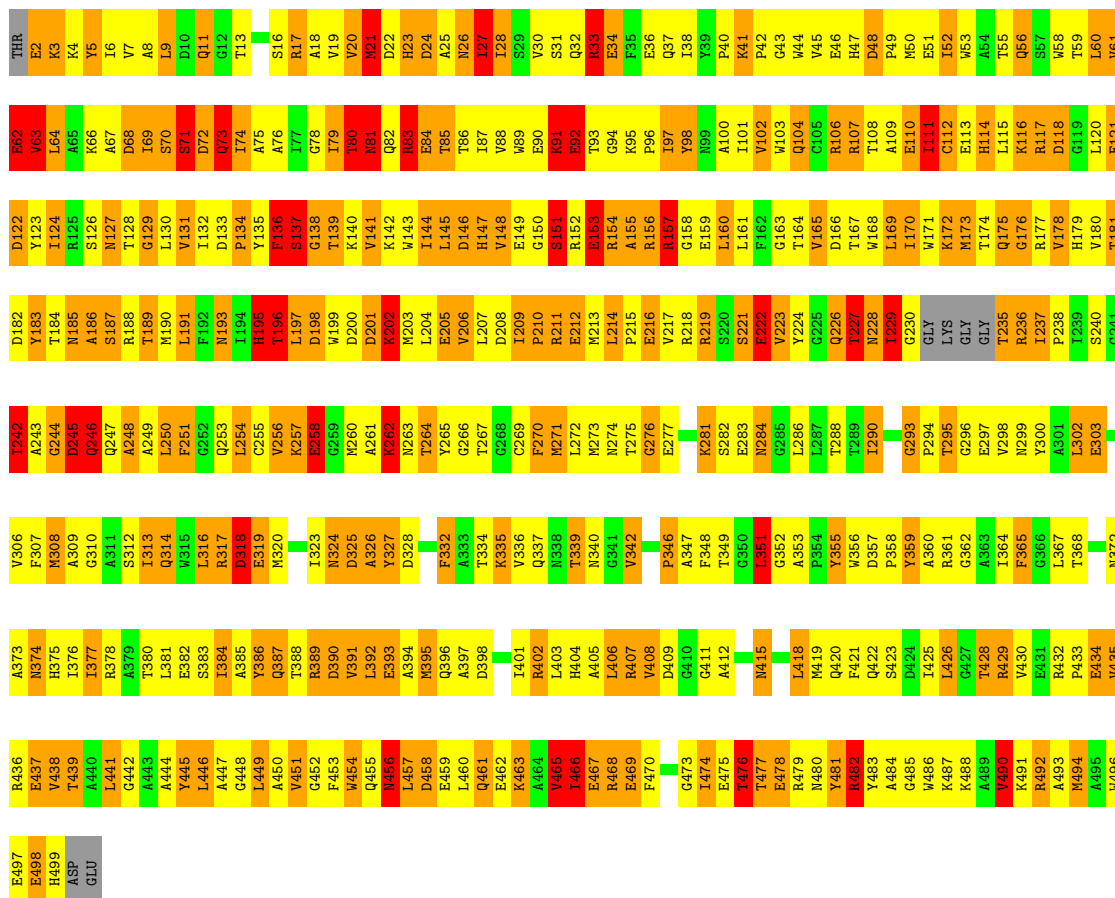
| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | Y     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 4   | O     | 1        | Total C O<br>6 3 3 | 0       | 0       |

### 3 Residue-property plots

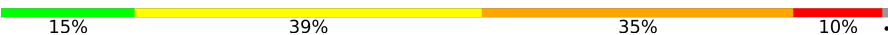
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

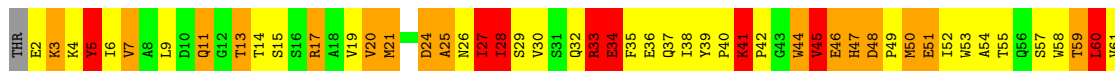
#### • Molecule 1: GLYCEROL KINASE

Chain Y: 



#### • Molecule 1: GLYCEROL KINASE

Chain O: 





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 99.77Å 200.29Å 114.74Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.00<br>20.00 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.0 (20.00-3.00)<br>94.4 (20.00-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 200.72 (at 2.92Å)                                           | Xtriage          |
| Refinement program                                                      | TNT 5F                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.168 , (Not available)<br>0.160 , (Not available)          | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 48.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.104                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 171.4                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 7900                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 49.0                                                        | wwPDB-VP         |

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

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

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

## 5 Model quality [i](#)

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

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

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   | O     | 1.50         | 18/3991 (0.5%) | 2.12        | 166/5412 (3.1%)  |
| 1   | Y     | 1.62         | 32/3991 (0.8%) | 2.20        | 176/5412 (3.3%)  |
| All | All   | 1.56         | 50/7982 (0.6%) | 2.16        | 342/10824 (3.2%) |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | O     | 353 | ALA  | C-O   | 9.64  | 1.35        | 1.23     |
| 1   | Y     | 353 | ALA  | CA-C  | -8.35 | 1.43        | 1.53     |
| 1   | Y     | 359 | TYR  | CA-C  | -7.91 | 1.42        | 1.52     |
| 1   | O     | 357 | ASP  | C-N   | -7.18 | 1.26        | 1.34     |
| 1   | Y     | 481 | TYR  | N-CA  | -6.76 | 1.38        | 1.46     |
| 1   | Y     | 319 | GLU  | CA-C  | -6.64 | 1.46        | 1.52     |
| 1   | Y     | 342 | VAL  | CA-CB | -6.55 | 1.47        | 1.54     |
| 1   | Y     | 332 | PHE  | CA-C  | -6.53 | 1.44        | 1.52     |
| 1   | Y     | 359 | TYR  | CA-CB | -6.38 | 1.44        | 1.54     |
| 1   | Y     | 196 | THR  | CA-C  | -6.32 | 1.44        | 1.52     |
| 1   | Y     | 160 | LEU  | CA-C  | -6.31 | 1.45        | 1.52     |
| 1   | Y     | 33  | ARG  | NE-CZ | 6.31  | 1.40        | 1.33     |
| 1   | O     | 125 | ARG  | NE-CZ | 6.12  | 1.39        | 1.33     |
| 1   | O     | 316 | LEU  | N-CA  | -5.97 | 1.39        | 1.46     |
| 1   | O     | 391 | VAL  | N-CA  | -5.97 | 1.39        | 1.46     |
| 1   | Y     | 111 | ILE  | CA-C  | -5.92 | 1.45        | 1.52     |
| 1   | Y     | 346 | PRO  | CA-C  | -5.91 | 1.47        | 1.53     |
| 1   | Y     | 270 | PHE  | CA-C  | -5.90 | 1.46        | 1.52     |
| 1   | O     | 359 | TYR  | CA-CB | -5.78 | 1.44        | 1.53     |
| 1   | Y     | 96  | PRO  | CA-C  | -5.76 | 1.45        | 1.52     |
| 1   | Y     | 195 | HIS  | CA-C  | -5.76 | 1.46        | 1.53     |
| 1   | Y     | 438 | VAL  | CA-CB | -5.73 | 1.46        | 1.54     |
| 1   | Y     | 263 | ASN  | N-CA  | -5.72 | 1.39        | 1.46     |
| 1   | Y     | 377 | ILE  | CA-CB | -5.67 | 1.47        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | Y     | 34  | GLU  | CD-OE1 | 5.66  | 1.36        | 1.25     |
| 1   | O     | 5   | TYR  | CA-C   | -5.61 | 1.45        | 1.52     |
| 1   | Y     | 223 | VAL  | CA-C   | -5.50 | 1.46        | 1.52     |
| 1   | Y     | 134 | PRO  | C-N    | -5.45 | 1.27        | 1.33     |
| 1   | Y     | 477 | THR  | C-N    | -5.45 | 1.26        | 1.33     |
| 1   | Y     | 68  | ASP  | CG-OD1 | 5.40  | 1.35        | 1.25     |
| 1   | O     | 373 | ALA  | CA-CB  | -5.32 | 1.45        | 1.53     |
| 1   | O     | 490 | VAL  | CA-CB  | -5.28 | 1.48        | 1.54     |
| 1   | O     | 330 | GLU  | CA-C   | 5.26  | 1.59        | 1.52     |
| 1   | Y     | 33  | ARG  | CA-C   | 5.24  | 1.59        | 1.52     |
| 1   | Y     | 112 | CYS  | N-CA   | -5.24 | 1.39        | 1.46     |
| 1   | O     | 300 | TYR  | CA-C   | -5.20 | 1.46        | 1.52     |
| 1   | Y     | 96  | PRO  | C-N    | -5.20 | 1.28        | 1.33     |
| 1   | Y     | 106 | ARG  | CZ-NH1 | 5.17  | 1.40        | 1.32     |
| 1   | O     | 121 | GLU  | CD-OE2 | 5.16  | 1.35        | 1.25     |
| 1   | Y     | 144 | ILE  | CA-CB  | -5.15 | 1.48        | 1.54     |
| 1   | O     | 365 | PHE  | C-N    | 5.14  | 1.39        | 1.33     |
| 1   | Y     | 387 | GLN  | N-CA   | -5.13 | 1.40        | 1.46     |
| 1   | O     | 34  | GLU  | CD-OE2 | 5.09  | 1.35        | 1.25     |
| 1   | O     | 481 | TYR  | N-CA   | -5.08 | 1.40        | 1.46     |
| 1   | Y     | 165 | VAL  | CA-CB  | -5.07 | 1.48        | 1.54     |
| 1   | O     | 363 | ALA  | CA-C   | -5.07 | 1.46        | 1.52     |
| 1   | Y     | 377 | ILE  | C-N    | -5.01 | 1.27        | 1.33     |
| 1   | O     | 84  | GLU  | CD-OE1 | 5.01  | 1.34        | 1.25     |
| 1   | O     | 33  | ARG  | NE-CZ  | 5.00  | 1.38        | 1.33     |
| 1   | Y     | 216 | GLU  | CD-OE2 | 5.00  | 1.34        | 1.25     |

All (342) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | Y     | 83  | ARG  | CA-C-N   | -15.39 | 98.07       | 122.24   |
| 1   | Y     | 83  | ARG  | C-N-CA   | -15.39 | 98.07       | 122.24   |
| 1   | Y     | 229 | ILE  | N-CA-C   | -12.77 | 99.12       | 110.74   |
| 1   | O     | 351 | LEU  | CA-C-N   | -12.05 | 101.51      | 122.00   |
| 1   | O     | 351 | LEU  | C-N-CA   | -12.05 | 101.51      | 122.00   |
| 1   | O     | 83  | ARG  | N-CA-C   | 11.69  | 127.73      | 113.23   |
| 1   | Y     | 351 | LEU  | CA-C-N   | -11.63 | 102.14      | 121.57   |
| 1   | Y     | 351 | LEU  | C-N-CA   | -11.63 | 102.14      | 121.57   |
| 1   | O     | 147 | HIS  | CA-CB-CG | -10.41 | 103.39      | 113.80   |
| 1   | O     | 332 | PHE  | CA-CB-CG | -10.29 | 103.51      | 113.80   |
| 1   | Y     | 137 | SER  | N-CA-C   | 10.23  | 123.71      | 111.33   |
| 1   | O     | 122 | ASP  | CA-CB-CG | -10.04 | 102.56      | 112.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | O     | 83  | ARG  | CA-C-N   | -9.54 | 106.46      | 122.11   |
| 1   | O     | 83  | ARG  | C-N-CA   | -9.54 | 106.46      | 122.11   |
| 1   | O     | 227 | THR  | CA-C-N   | -9.49 | 108.45      | 122.41   |
| 1   | O     | 227 | THR  | C-N-CA   | -9.49 | 108.45      | 122.41   |
| 1   | O     | 453 | PHE  | N-CA-C   | -9.47 | 101.85      | 113.50   |
| 1   | O     | 307 | PHE  | N-CA-C   | 9.36  | 121.48      | 111.28   |
| 1   | Y     | 147 | HIS  | CA-CB-CG | -9.28 | 104.52      | 113.80   |
| 1   | Y     | 406 | LEU  | CA-C-N   | -9.23 | 110.50      | 122.77   |
| 1   | Y     | 406 | LEU  | C-N-CA   | -9.23 | 110.50      | 122.77   |
| 1   | Y     | 83  | ARG  | N-CA-C   | 9.22  | 124.34      | 113.18   |
| 1   | Y     | 228 | ASN  | N-CA-CB  | 9.18  | 124.03      | 110.35   |
| 1   | O     | 229 | ILE  | N-CA-C   | -9.18 | 102.91      | 111.45   |
| 1   | Y     | 104 | GLN  | N-CA-CB  | -9.07 | 96.22       | 110.28   |
| 1   | O     | 456 | ASN  | CA-CB-CG | 8.86  | 121.45      | 112.60   |
| 1   | O     | 359 | TYR  | CA-CB-CG | -8.72 | 98.20       | 113.90   |
| 1   | Y     | 5   | TYR  | N-CA-C   | 8.67  | 121.49      | 109.18   |
| 1   | O     | 27  | ILE  | CB-CA-C  | 8.58  | 120.50      | 111.23   |
| 1   | Y     | 155 | ALA  | CA-C-N   | 8.49  | 131.47      | 120.44   |
| 1   | Y     | 155 | ALA  | C-N-CA   | 8.49  | 131.47      | 120.44   |
| 1   | Y     | 114 | HIS  | CA-CB-CG | -8.48 | 105.32      | 113.80   |
| 1   | O     | 228 | ASN  | N-CA-CB  | 8.16  | 122.51      | 110.35   |
| 1   | O     | 365 | PHE  | N-CA-C   | 8.15  | 122.15      | 109.52   |
| 1   | O     | 245 | ASP  | CA-C-N   | -8.11 | 109.90      | 120.44   |
| 1   | O     | 245 | ASP  | C-N-CA   | -8.11 | 109.90      | 120.44   |
| 1   | O     | 5   | TYR  | N-CA-C   | 8.10  | 120.68      | 109.18   |
| 1   | Y     | 227 | THR  | CA-C-N   | -8.06 | 110.56      | 122.41   |
| 1   | Y     | 227 | THR  | C-N-CA   | -8.06 | 110.56      | 122.41   |
| 1   | Y     | 242 | ILE  | N-CA-CB  | 7.97  | 121.96      | 111.19   |
| 1   | Y     | 245 | ASP  | CA-CB-CG | 7.96  | 120.56      | 112.60   |
| 1   | Y     | 390 | ASP  | CA-CB-CG | 7.91  | 120.51      | 112.60   |
| 1   | Y     | 122 | ASP  | CA-CB-CG | -7.87 | 104.73      | 112.60   |
| 1   | Y     | 374 | ASN  | CA-CB-CG | -7.76 | 104.84      | 112.60   |
| 1   | Y     | 262 | LYS  | CA-C-N   | -7.75 | 112.06      | 122.99   |
| 1   | Y     | 262 | LYS  | C-N-CA   | -7.75 | 112.06      | 122.99   |
| 1   | Y     | 465 | VAL  | CA-C-N   | -7.73 | 112.69      | 122.43   |
| 1   | Y     | 465 | VAL  | C-N-CA   | -7.73 | 112.69      | 122.43   |
| 1   | Y     | 353 | ALA  | N-CA-C   | 7.69  | 120.70      | 110.08   |
| 1   | Y     | 27  | ILE  | CB-CA-C  | 7.66  | 120.98      | 111.25   |
| 1   | O     | 48  | ASP  | N-CA-CB  | 7.66  | 119.89      | 110.17   |
| 1   | Y     | 195 | HIS  | N-CA-C   | -7.65 | 97.98       | 109.83   |
| 1   | O     | 20  | VAL  | N-CA-C   | 7.63  | 119.83      | 108.46   |
| 1   | O     | 352 | GLY  | CA-C-N   | -7.56 | 108.93      | 121.03   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | O     | 352 | GLY  | C-N-CA   | -7.56 | 108.93      | 121.03   |
| 1   | O     | 256 | VAL  | N-CA-CB  | -7.56 | 103.55      | 112.39   |
| 1   | Y     | 228 | ASN  | CA-CB-CG | -7.55 | 105.05      | 112.60   |
| 1   | O     | 144 | ILE  | N-CA-CB  | 7.53  | 118.83      | 110.62   |
| 1   | O     | 122 | ASP  | N-CA-C   | 7.50  | 120.33      | 111.71   |
| 1   | O     | 100 | ALA  | CA-C-N   | -7.47 | 113.12      | 123.13   |
| 1   | O     | 100 | ALA  | C-N-CA   | -7.47 | 113.12      | 123.13   |
| 1   | Y     | 454 | TRP  | CA-C-N   | -7.44 | 109.08      | 123.13   |
| 1   | Y     | 454 | TRP  | C-N-CA   | -7.44 | 109.08      | 123.13   |
| 1   | Y     | 327 | TYR  | CA-CB-CG | -7.30 | 100.76      | 113.90   |
| 1   | Y     | 353 | ALA  | N-CA-CB  | 7.25  | 120.69      | 110.11   |
| 1   | O     | 144 | ILE  | CB-CA-C  | -7.23 | 102.77      | 111.81   |
| 1   | Y     | 412 | ALA  | N-CA-C   | 7.14  | 121.09      | 112.38   |
| 1   | O     | 480 | ASN  | CA-CB-CG | -7.13 | 105.47      | 112.60   |
| 1   | Y     | 79  | ILE  | N-CA-C   | 7.13  | 119.51      | 107.18   |
| 1   | O     | 236 | ARG  | N-CA-C   | 7.12  | 119.70      | 108.67   |
| 1   | Y     | 490 | VAL  | N-CA-C   | 7.06  | 117.20      | 110.42   |
| 1   | O     | 173 | MET  | N-CA-CB  | 7.03  | 120.42      | 109.94   |
| 1   | O     | 404 | HIS  | CA-CB-CG | -7.03 | 106.77      | 113.80   |
| 1   | Y     | 303 | GLU  | N-CA-C   | 7.00  | 120.30      | 108.90   |
| 1   | O     | 154 | ARG  | N-CA-C   | -6.98 | 102.73      | 111.11   |
| 1   | Y     | 318 | ASP  | N-CA-CB  | 6.96  | 121.30      | 110.44   |
| 1   | O     | 86  | THR  | N-CA-C   | 6.89  | 120.17      | 109.07   |
| 1   | Y     | 307 | PHE  | N-CA-C   | 6.89  | 118.58      | 111.14   |
| 1   | Y     | 359 | TYR  | CA-CB-CG | -6.88 | 101.51      | 113.90   |
| 1   | O     | 131 | VAL  | CB-CA-C  | 6.88  | 118.21      | 111.74   |
| 1   | Y     | 210 | PRO  | CA-C-N   | 6.87  | 131.69      | 120.63   |
| 1   | Y     | 210 | PRO  | C-N-CA   | 6.87  | 131.69      | 120.63   |
| 1   | Y     | 390 | ASP  | N-CA-CB  | 6.86  | 122.08      | 110.49   |
| 1   | Y     | 244 | GLY  | N-CA-C   | -6.85 | 100.28      | 112.54   |
| 1   | O     | 490 | VAL  | N-CA-C   | 6.83  | 117.53      | 110.36   |
| 1   | O     | 114 | HIS  | CA-CB-CG | -6.80 | 107.00      | 113.80   |
| 1   | Y     | 80  | THR  | N-CA-CB  | 6.80  | 122.71      | 111.08   |
| 1   | Y     | 21  | MET  | N-CA-C   | 6.79  | 119.65      | 108.99   |
| 1   | Y     | 84  | GLU  | O-C-N    | 6.69  | 129.69      | 122.34   |
| 1   | Y     | 33  | ARG  | CA-C-N   | 6.67  | 130.18      | 120.71   |
| 1   | Y     | 33  | ARG  | C-N-CA   | 6.67  | 130.18      | 120.71   |
| 1   | Y     | 481 | TYR  | CA-CB-CG | -6.67 | 101.89      | 113.90   |
| 1   | Y     | 56  | GLN  | N-CA-CB  | 6.67  | 120.13      | 110.20   |
| 1   | O     | 284 | ASN  | N-CA-C   | 6.67  | 118.44      | 110.44   |
| 1   | O     | 155 | ALA  | CA-C-N   | 6.66  | 129.10      | 120.44   |
| 1   | O     | 155 | ALA  | C-N-CA   | 6.66  | 129.10      | 120.44   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | O     | 44  | TRP  | N-CA-C   | 6.63  | 120.05      | 109.24   |
| 1   | Y     | 353 | ALA  | CB-CA-C  | -6.62 | 98.62       | 109.27   |
| 1   | Y     | 365 | PHE  | N-CA-C   | 6.60  | 119.75      | 109.52   |
| 1   | Y     | 136 | PHE  | CA-CB-CG | -6.58 | 107.22      | 113.80   |
| 1   | Y     | 92  | GLU  | N-CA-C   | -6.56 | 104.05      | 111.07   |
| 1   | Y     | 200 | ASP  | CA-C-O   | 6.55  | 127.41      | 120.33   |
| 1   | Y     | 81  | ASN  | CA-CB-CG | -6.50 | 106.09      | 112.60   |
| 1   | O     | 292 | CYS  | N-CA-C   | 6.50  | 119.00      | 108.41   |
| 1   | Y     | 437 | GLU  | N-CA-CB  | 6.44  | 117.76      | 110.35   |
| 1   | Y     | 458 | ASP  | CA-CB-CG | 6.44  | 119.04      | 112.60   |
| 1   | O     | 453 | PHE  | CA-C-O   | 6.43  | 126.22      | 119.14   |
| 1   | Y     | 76  | ALA  | N-CA-C   | 6.43  | 118.31      | 109.18   |
| 1   | O     | 481 | TYR  | CA-CB-CG | -6.43 | 102.33      | 113.90   |
| 1   | O     | 20  | VAL  | CB-CA-C  | -6.41 | 100.62      | 110.50   |
| 1   | O     | 242 | ILE  | CB-CA-C  | -6.39 | 100.82      | 111.29   |
| 1   | Y     | 404 | HIS  | CA-CB-CG | -6.38 | 107.42      | 113.80   |
| 1   | O     | 73  | GLN  | CA-C-N   | -6.37 | 115.29      | 123.19   |
| 1   | O     | 73  | GLN  | C-N-CA   | -6.37 | 115.29      | 123.19   |
| 1   | Y     | 81  | ASN  | O-C-N    | 6.31  | 130.30      | 122.92   |
| 1   | Y     | 248 | ALA  | N-CA-CB  | 6.29  | 119.32      | 109.94   |
| 1   | O     | 345 | VAL  | CA-C-N   | 6.29  | 127.71      | 119.84   |
| 1   | O     | 345 | VAL  | C-N-CA   | 6.29  | 127.71      | 119.84   |
| 1   | O     | 242 | ILE  | N-CA-CB  | 6.27  | 121.58      | 111.23   |
| 1   | O     | 324 | ASN  | CA-C-N   | 6.27  | 132.39      | 122.74   |
| 1   | O     | 324 | ASN  | C-N-CA   | 6.27  | 132.39      | 122.74   |
| 1   | O     | 494 | MET  | N-CA-C   | 6.26  | 118.86      | 110.35   |
| 1   | Y     | 346 | PRO  | N-CA-CB  | 6.24  | 106.62      | 102.25   |
| 1   | Y     | 134 | PRO  | CA-C-O   | 6.23  | 127.21      | 118.99   |
| 1   | Y     | 277 | GLU  | N-CA-C   | 6.22  | 119.04      | 111.82   |
| 1   | O     | 372 | ASN  | N-CA-C   | 6.22  | 118.02      | 109.18   |
| 1   | Y     | 326 | ALA  | N-CA-C   | -6.19 | 103.84      | 111.33   |
| 1   | O     | 24  | ASP  | N-CA-C   | -6.19 | 105.48      | 113.16   |
| 1   | Y     | 293 | GLY  | N-CA-C   | -6.18 | 104.75      | 112.23   |
| 1   | O     | 301 | ALA  | N-CA-C   | 6.18  | 118.52      | 108.76   |
| 1   | Y     | 144 | ILE  | N-CA-CB  | 6.18  | 117.11      | 110.62   |
| 1   | Y     | 476 | THR  | CA-C-N   | -6.17 | 110.99      | 122.60   |
| 1   | Y     | 476 | THR  | C-N-CA   | -6.17 | 110.99      | 122.60   |
| 1   | Y     | 104 | GLN  | CB-CA-C  | 6.16  | 122.50      | 110.67   |
| 1   | Y     | 100 | ALA  | CA-C-N   | -6.16 | 115.02      | 122.90   |
| 1   | Y     | 100 | ALA  | C-N-CA   | -6.16 | 115.02      | 122.90   |
| 1   | O     | 148 | VAL  | CB-CA-C  | 6.16  | 119.66      | 110.98   |
| 1   | O     | 99  | ASN  | CA-CB-CG | -6.16 | 106.44      | 112.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 293 | GLY  | N-CA-C    | -6.16 | 104.78      | 112.23   |
| 1   | Y     | 296 | GLY  | N-CA-C    | -6.15 | 106.76      | 115.43   |
| 1   | Y     | 283 | GLU  | N-CA-C    | -6.14 | 105.59      | 114.12   |
| 1   | Y     | 73  | GLN  | CA-C-N    | -6.14 | 115.58      | 123.19   |
| 1   | Y     | 73  | GLN  | C-N-CA    | -6.14 | 115.58      | 123.19   |
| 1   | O     | 494 | MET  | N-CA-CB   | 6.13  | 119.05      | 110.04   |
| 1   | Y     | 276 | GLY  | CA-C-N    | 6.11  | 129.60      | 120.31   |
| 1   | Y     | 276 | GLY  | C-N-CA    | 6.11  | 129.60      | 120.31   |
| 1   | O     | 195 | HIS  | N-CA-C    | -6.11 | 97.78       | 110.80   |
| 1   | O     | 270 | PHE  | CA-CB-CG  | -6.11 | 107.69      | 113.80   |
| 1   | O     | 324 | ASN  | O-C-N     | 6.10  | 129.05      | 122.34   |
| 1   | O     | 246 | GLN  | N-CA-CB   | 6.09  | 118.84      | 110.01   |
| 1   | Y     | 247 | GLN  | N-CA-C    | -6.09 | 104.64      | 111.28   |
| 1   | Y     | 84  | GLU  | N-CA-CB   | 6.07  | 118.97      | 110.90   |
| 1   | O     | 13  | THR  | CA-CB-OG1 | 6.05  | 118.68      | 109.60   |
| 1   | Y     | 33  | ARG  | CD-NE-CZ  | 6.04  | 132.86      | 124.40   |
| 1   | Y     | 308 | MET  | N-CA-C    | 6.04  | 118.37      | 108.52   |
| 1   | Y     | 155 | ALA  | O-C-N     | 6.03  | 129.05      | 122.11   |
| 1   | Y     | 136 | PHE  | CA-C-N    | 6.03  | 128.63      | 120.38   |
| 1   | Y     | 136 | PHE  | C-N-CA    | 6.03  | 128.63      | 120.38   |
| 1   | O     | 36  | GLU  | N-CA-C    | 6.02  | 119.33      | 109.76   |
| 1   | Y     | 251 | PHE  | CA-C-N    | 6.01  | 127.70      | 120.13   |
| 1   | Y     | 251 | PHE  | C-N-CA    | 6.01  | 127.70      | 120.13   |
| 1   | Y     | 144 | ILE  | CB-CA-C   | -5.99 | 104.03      | 111.70   |
| 1   | O     | 491 | LYS  | N-CA-CB   | 5.99  | 118.86      | 109.94   |
| 1   | O     | 376 | ILE  | CB-CA-C   | -5.99 | 101.47      | 111.29   |
| 1   | O     | 299 | ASN  | CA-CB-CG  | -5.99 | 106.61      | 112.60   |
| 1   | O     | 474 | ILE  | N-CA-C    | 5.98  | 117.09      | 108.48   |
| 1   | O     | 28  | ILE  | N-CA-C    | 5.98  | 117.52      | 111.00   |
| 1   | O     | 104 | GLN  | O-C-N     | 5.96  | 128.29      | 122.09   |
| 1   | Y     | 68  | ASP  | N-CA-C    | -5.96 | 105.31      | 112.58   |
| 1   | O     | 499 | HIS  | CA-CB-CG  | 5.96  | 119.76      | 113.80   |
| 1   | O     | 118 | ASP  | CA-CB-CG  | -5.96 | 106.64      | 112.60   |
| 1   | Y     | 318 | ASP  | CA-C-N    | -5.95 | 112.68      | 122.79   |
| 1   | Y     | 318 | ASP  | C-N-CA    | -5.95 | 112.68      | 122.79   |
| 1   | O     | 214 | LEU  | N-CA-CB   | 5.94  | 117.98      | 109.78   |
| 1   | Y     | 332 | PHE  | CA-CB-CG  | -5.93 | 107.87      | 113.80   |
| 1   | O     | 173 | MET  | CB-CA-C   | -5.91 | 101.35      | 110.81   |
| 1   | O     | 296 | GLY  | CA-C-O    | 5.91  | 125.18      | 118.86   |
| 1   | O     | 451 | VAL  | N-CA-CB   | -5.89 | 101.51      | 111.23   |
| 1   | O     | 488 | LYS  | CA-C-O    | 5.88  | 127.19      | 120.90   |
| 1   | Y     | 355 | TYR  | N-CA-C    | 5.87  | 117.48      | 111.14   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | Y     | 17  | ARG  | N-CA-CB  | 5.87  | 121.90      | 111.69   |
| 1   | Y     | 91  | LYS  | CA-C-N   | -5.87 | 112.81      | 120.44   |
| 1   | Y     | 91  | LYS  | C-N-CA   | -5.87 | 112.81      | 120.44   |
| 1   | O     | 103 | TRP  | CA-C-N   | 5.87  | 128.46      | 120.54   |
| 1   | O     | 103 | TRP  | C-N-CA   | 5.87  | 128.46      | 120.54   |
| 1   | O     | 209 | ILE  | N-CA-C   | 5.85  | 114.57      | 107.61   |
| 1   | Y     | 122 | ASP  | N-CA-C   | 5.83  | 117.31      | 111.07   |
| 1   | O     | 92  | GLU  | N-CA-C   | -5.83 | 104.56      | 111.03   |
| 1   | O     | 105 | CYS  | CA-C-N   | -5.82 | 113.42      | 122.67   |
| 1   | O     | 105 | CYS  | C-N-CA   | -5.82 | 113.42      | 122.67   |
| 1   | Y     | 48  | ASP  | N-CA-CB  | 5.82  | 118.62      | 110.07   |
| 1   | Y     | 183 | TYR  | N-CA-C   | 5.82  | 117.42      | 111.14   |
| 1   | Y     | 298 | VAL  | N-CA-C   | 5.80  | 116.90      | 109.30   |
| 1   | Y     | 271 | MET  | CA-C-N   | -5.79 | 113.07      | 122.81   |
| 1   | Y     | 271 | MET  | C-N-CA   | -5.79 | 113.07      | 122.81   |
| 1   | Y     | 193 | ASN  | CA-CB-CG | -5.79 | 106.81      | 112.60   |
| 1   | O     | 154 | ARG  | CB-CA-C  | 5.79  | 120.07      | 110.81   |
| 1   | O     | 282 | SER  | N-CA-CB  | 5.79  | 118.48      | 109.85   |
| 1   | Y     | 5   | TYR  | CB-CA-C  | -5.78 | 98.97       | 111.11   |
| 1   | O     | 490 | VAL  | O-C-N    | 5.78  | 127.72      | 121.94   |
| 1   | O     | 198 | ASP  | CA-CB-CG | -5.75 | 106.85      | 112.60   |
| 1   | O     | 390 | ASP  | CA-C-O   | 5.74  | 127.74      | 121.02   |
| 1   | O     | 85  | THR  | N-CA-CB  | -5.74 | 100.79      | 110.49   |
| 1   | O     | 326 | ALA  | N-CA-C   | -5.73 | 105.12      | 111.71   |
| 1   | O     | 386 | TYR  | O-C-N    | 5.71  | 128.03      | 122.09   |
| 1   | O     | 262 | LYS  | CA-C-N   | -5.70 | 114.96      | 122.99   |
| 1   | O     | 262 | LYS  | C-N-CA   | -5.70 | 114.96      | 122.99   |
| 1   | Y     | 377 | ILE  | CA-C-O   | 5.69  | 127.20      | 121.17   |
| 1   | O     | 288 | THR  | CA-C-N   | -5.68 | 113.27      | 122.36   |
| 1   | O     | 288 | THR  | C-N-CA   | -5.68 | 113.27      | 122.36   |
| 1   | Y     | 242 | ILE  | CB-CA-C  | -5.67 | 103.07      | 111.80   |
| 1   | Y     | 109 | ALA  | CA-C-O   | -5.66 | 114.88      | 120.82   |
| 1   | O     | 328 | ASP  | N-CA-C   | 5.65  | 118.98      | 111.75   |
| 1   | O     | 102 | VAL  | N-CA-C   | 5.64  | 118.70      | 109.78   |
| 1   | O     | 47  | HIS  | CA-C-N   | -5.63 | 114.30      | 121.74   |
| 1   | O     | 47  | HIS  | C-N-CA   | -5.63 | 114.30      | 121.74   |
| 1   | O     | 352 | GLY  | CA-C-O   | -5.63 | 115.44      | 122.59   |
| 1   | Y     | 385 | ALA  | N-CA-C   | 5.62  | 117.41      | 111.28   |
| 1   | O     | 76  | ALA  | N-CA-C   | 5.62  | 118.42      | 109.65   |
| 1   | O     | 373 | ALA  | CA-C-N   | -5.61 | 112.81      | 120.44   |
| 1   | O     | 373 | ALA  | C-N-CA   | -5.61 | 112.81      | 120.44   |
| 1   | O     | 91  | LYS  | N-CA-C   | 5.61  | 118.33      | 111.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 345 | VAL  | O-C-N     | 5.60  | 127.48      | 121.10   |
| 1   | Y     | 358 | PRO  | CA-C-N    | -5.59 | 113.38      | 122.26   |
| 1   | Y     | 358 | PRO  | C-N-CA    | -5.59 | 113.38      | 122.26   |
| 1   | O     | 368 | THR  | CA-CB-OG1 | -5.58 | 101.22      | 109.60   |
| 1   | O     | 104 | GLN  | N-CA-C    | 5.58  | 117.81      | 111.11   |
| 1   | O     | 432 | ARG  | CA-C-O    | 5.58  | 125.57      | 119.32   |
| 1   | Y     | 228 | ASN  | CA-C-O    | 5.56  | 126.70      | 120.92   |
| 1   | O     | 457 | LEU  | N-CA-C    | -5.56 | 106.63      | 113.41   |
| 1   | O     | 129 | GLY  | N-CA-C    | -5.55 | 107.58      | 115.30   |
| 1   | Y     | 38  | ILE  | N-CA-C    | 5.55  | 115.85      | 107.75   |
| 1   | O     | 468 | ARG  | N-CA-C    | 5.55  | 118.51      | 108.69   |
| 1   | Y     | 452 | GLY  | N-CA-C    | -5.54 | 108.49      | 115.08   |
| 1   | O     | 41  | LYS  | N-CA-CB   | -5.52 | 105.60      | 111.29   |
| 1   | O     | 45  | VAL  | N-CA-C    | 5.51  | 116.22      | 108.17   |
| 1   | Y     | 24  | ASP  | N-CA-C    | -5.51 | 106.33      | 113.16   |
| 1   | O     | 351 | LEU  | N-CA-C    | 5.50  | 122.52      | 110.80   |
| 1   | O     | 209 | ILE  | CA-C-O    | 5.50  | 122.92      | 119.51   |
| 1   | Y     | 386 | TYR  | O-C-N     | 5.50  | 127.73      | 122.07   |
| 1   | Y     | 441 | LEU  | N-CA-C    | -5.50 | 104.31      | 111.02   |
| 1   | Y     | 246 | GLN  | N-CA-C    | 5.49  | 117.97      | 111.33   |
| 1   | O     | 303 | GLU  | N-CA-C    | 5.48  | 118.33      | 109.40   |
| 1   | Y     | 106 | ARG  | N-CA-C    | 5.48  | 118.96      | 112.72   |
| 1   | Y     | 359 | TYR  | N-CA-CB   | 5.47  | 118.69      | 110.65   |
| 1   | Y     | 193 | ASN  | N-CA-CB   | 5.47  | 118.00      | 109.85   |
| 1   | Y     | 129 | GLY  | N-CA-C    | -5.47 | 108.10      | 115.21   |
| 1   | O     | 78  | GLY  | N-CA-C    | -5.46 | 105.28      | 112.82   |
| 1   | O     | 80  | THR  | N-CA-C    | 5.46  | 117.69      | 109.23   |
| 1   | Y     | 20  | VAL  | N-CA-C    | 5.46  | 116.59      | 108.46   |
| 1   | O     | 131 | VAL  | N-CA-CB   | -5.46 | 102.64      | 109.84   |
| 1   | Y     | 335 | LYS  | N-CA-C    | -5.45 | 105.34      | 111.28   |
| 1   | O     | 296 | GLY  | N-CA-C    | -5.45 | 107.27      | 114.95   |
| 1   | Y     | 80  | THR  | CA-C-N    | -5.44 | 113.46      | 122.11   |
| 1   | Y     | 80  | THR  | C-N-CA    | -5.44 | 113.46      | 122.11   |
| 1   | Y     | 351 | LEU  | O-C-N     | -5.44 | 115.36      | 122.59   |
| 1   | O     | 351 | LEU  | O-C-N     | -5.44 | 115.36      | 122.59   |
| 1   | Y     | 137 | SER  | CB-CA-C   | -5.43 | 101.45      | 110.68   |
| 1   | O     | 13  | THR  | CA-CB-CG2 | -5.43 | 101.27      | 110.50   |
| 1   | O     | 455 | GLN  | CB-CG-CD  | 5.43  | 121.83      | 112.60   |
| 1   | O     | 407 | ARG  | CA-C-O    | 5.43  | 126.19      | 120.54   |
| 1   | O     | 48  | ASP  | O-C-N     | 5.42  | 125.62      | 121.23   |
| 1   | O     | 314 | GLN  | N-CA-CB   | 5.42  | 118.69      | 110.28   |
| 1   | Y     | 36  | GLU  | N-CA-C    | 5.42  | 118.38      | 109.76   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 307 | PHE  | CB-CA-C   | -5.42 | 101.80      | 110.79   |
| 1   | Y     | 334 | THR  | CA-CB-CG2 | -5.41 | 101.31      | 110.50   |
| 1   | O     | 47  | HIS  | CA-CB-CG  | 5.40  | 119.20      | 113.80   |
| 1   | O     | 80  | THR  | N-CA-CB   | 5.40  | 121.57      | 111.53   |
| 1   | O     | 323 | ILE  | CA-CB-CG1 | -5.38 | 101.25      | 110.40   |
| 1   | O     | 195 | HIS  | N-CA-CB   | 5.38  | 119.58      | 110.49   |
| 1   | Y     | 7   | VAL  | N-CA-C    | 5.37  | 115.69      | 108.17   |
| 1   | Y     | 256 | VAL  | N-CA-CB   | -5.37 | 102.37      | 111.23   |
| 1   | Y     | 210 | PRO  | N-CA-CB   | 5.36  | 106.82      | 103.23   |
| 1   | Y     | 136 | PHE  | O-C-N     | 5.36  | 129.01      | 122.96   |
| 1   | Y     | 83  | ARG  | O-C-N     | -5.35 | 114.62      | 122.43   |
| 1   | O     | 191 | LEU  | N-CA-CB   | 5.33  | 120.02      | 110.79   |
| 1   | O     | 312 | SER  | N-CA-C    | -5.33 | 105.37      | 111.07   |
| 1   | Y     | 367 | LEU  | CA-C-O    | 5.33  | 126.76      | 120.69   |
| 1   | O     | 294 | PRO  | CA-C-N    | -5.32 | 113.84      | 121.98   |
| 1   | O     | 294 | PRO  | C-N-CA    | -5.32 | 113.84      | 121.98   |
| 1   | O     | 228 | ASN  | CA-CB-CG  | -5.31 | 107.29      | 112.60   |
| 1   | Y     | 275 | THR  | N-CA-CB   | 5.28  | 118.27      | 110.56   |
| 1   | Y     | 127 | ASN  | CA-CB-CG  | -5.28 | 107.32      | 112.60   |
| 1   | Y     | 157 | ARG  | N-CA-CB   | 5.28  | 119.41      | 110.49   |
| 1   | Y     | 86  | THR  | N-CA-C    | 5.27  | 117.56      | 109.07   |
| 1   | Y     | 72  | ASP  | CA-C-N    | -5.27 | 112.85      | 122.38   |
| 1   | Y     | 72  | ASP  | C-N-CA    | -5.27 | 112.85      | 122.38   |
| 1   | Y     | 482 | ARG  | N-CA-CB   | 5.27  | 117.60      | 109.91   |
| 1   | O     | 486 | TRP  | CA-C-N    | -5.26 | 111.74      | 120.68   |
| 1   | O     | 486 | TRP  | C-N-CA    | -5.26 | 111.74      | 120.68   |
| 1   | O     | 17  | ARG  | N-CA-CB   | 5.25  | 119.78      | 111.43   |
| 1   | Y     | 23  | HIS  | CA-C-N    | -5.25 | 112.88      | 122.38   |
| 1   | Y     | 23  | HIS  | C-N-CA    | -5.25 | 112.88      | 122.38   |
| 1   | Y     | 222 | GLU  | CA-C-N    | -5.25 | 115.81      | 122.37   |
| 1   | Y     | 222 | GLU  | C-N-CA    | -5.25 | 115.81      | 122.37   |
| 1   | Y     | 325 | ASP  | CA-C-O    | -5.25 | 113.83      | 120.28   |
| 1   | Y     | 147 | HIS  | CA-C-O    | 5.25  | 124.58      | 118.97   |
| 1   | Y     | 26  | ASN  | CB-CA-C   | 5.24  | 118.18      | 109.53   |
| 1   | O     | 239 | ILE  | N-CA-CB   | -5.23 | 107.42      | 112.65   |
| 1   | Y     | 189 | THR  | N-CA-C    | 5.22  | 118.81      | 112.23   |
| 1   | O     | 7   | VAL  | N-CA-C    | 5.22  | 115.64      | 108.12   |
| 1   | Y     | 326 | ALA  | CA-C-O    | 5.22  | 126.27      | 120.63   |
| 1   | Y     | 284 | ASN  | N-CA-C    | 5.21  | 117.55      | 110.88   |
| 1   | Y     | 435 | VAL  | CB-CA-C   | -5.19 | 105.88      | 111.59   |
| 1   | Y     | 359 | TYR  | O-C-N     | 5.19  | 128.73      | 122.35   |
| 1   | O     | 44  | TRP  | CA-C-O    | 5.17  | 126.07      | 120.43   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Y     | 85  | THR  | N-CA-CB    | -5.17 | 101.76      | 110.49   |
| 1   | Y     | 63  | VAL  | N-CA-CB    | 5.16  | 119.75      | 111.23   |
| 1   | O     | 432 | ARG  | CA-C-N     | 5.16  | 125.10      | 119.78   |
| 1   | O     | 432 | ARG  | C-N-CA     | 5.16  | 125.10      | 119.78   |
| 1   | O     | 126 | SER  | N-CA-C     | 5.16  | 118.03      | 111.69   |
| 1   | O     | 468 | ARG  | CA-C-N     | -5.16 | 115.89      | 123.00   |
| 1   | O     | 468 | ARG  | C-N-CA     | -5.16 | 115.89      | 123.00   |
| 1   | O     | 164 | THR  | N-CA-C     | -5.15 | 102.84      | 110.46   |
| 1   | Y     | 186 | ALA  | O-C-N      | 5.14  | 127.44      | 122.09   |
| 1   | Y     | 97  | ILE  | N-CA-C     | -5.14 | 107.46      | 112.29   |
| 1   | Y     | 340 | ASN  | N-CA-CB    | -5.13 | 104.50      | 112.30   |
| 1   | Y     | 390 | ASP  | CB-CA-C    | -5.12 | 100.23      | 110.42   |
| 1   | Y     | 118 | ASP  | N-CA-C     | -5.11 | 105.40      | 113.02   |
| 1   | Y     | 74  | ILE  | CA-C-O     | 5.10  | 125.88      | 120.48   |
| 1   | O     | 275 | THR  | CA-C-O     | 5.09  | 125.96      | 119.95   |
| 1   | Y     | 314 | GLN  | O-C-N      | 5.08  | 127.51      | 122.12   |
| 1   | Y     | 96  | PRO  | N-CA-CB    | 5.08  | 107.72      | 103.25   |
| 1   | Y     | 316 | LEU  | O-C-N      | 5.08  | 127.30      | 122.07   |
| 1   | Y     | 334 | THR  | OG1-CB-CG2 | 5.08  | 119.46      | 109.30   |
| 1   | Y     | 314 | GLN  | CA-C-N     | 5.07  | 127.39      | 120.54   |
| 1   | Y     | 314 | GLN  | C-N-CA     | 5.07  | 127.39      | 120.54   |
| 1   | O     | 229 | ILE  | CB-CA-C    | 5.07  | 118.56      | 111.92   |
| 1   | O     | 490 | VAL  | CB-CA-C    | -5.06 | 105.40      | 111.88   |
| 1   | O     | 72  | ASP  | N-CA-C     | 5.06  | 118.61      | 112.23   |
| 1   | Y     | 178 | VAL  | N-CA-C     | 5.06  | 116.25      | 108.71   |
| 1   | O     | 33  | ARG  | CD-NE-CZ   | 5.05  | 131.47      | 124.40   |
| 1   | O     | 318 | ASP  | N-CA-CB    | 5.05  | 118.07      | 110.30   |
| 1   | O     | 332 | PHE  | O-C-N      | 5.03  | 127.53      | 122.09   |
| 1   | O     | 326 | ALA  | CA-C-O     | 5.03  | 125.78      | 120.10   |
| 1   | Y     | 318 | ASP  | CB-CA-C    | -5.03 | 99.35       | 109.55   |
| 1   | Y     | 466 | ILE  | CA-C-N     | -5.00 | 113.64      | 120.44   |
| 1   | Y     | 466 | ILE  | C-N-CA     | -5.00 | 113.64      | 120.44   |
| 1   | O     | 292 | CYS  | CB-CA-C    | -5.00 | 101.85      | 110.16   |
| 1   | O     | 25  | ALA  | CA-C-N     | -5.00 | 114.35      | 121.50   |
| 1   | O     | 25  | ALA  | C-N-CA     | -5.00 | 114.35      | 121.50   |
| 1   | O     | 348 | PHE  | CA-CB-CG   | -5.00 | 108.80      | 113.80   |

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   | O     | 3910  | 0        | 3841     | 684     | 0            |
| 1   | Y     | 3910  | 0        | 3841     | 575     | 1            |
| 2   | O     | 1     | 0        | 0        | 0       | 0            |
| 2   | Y     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 33    | 0        | 12       | 2       | 0            |
| 3   | Y     | 33    | 0        | 12       | 3       | 0            |
| 4   | O     | 6     | 0        | 8        | 2       | 0            |
| 4   | Y     | 6     | 0        | 8        | 1       | 0            |
| All | All   | 7900  | 0        | 7722     | 1254    | 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 80.

All (1254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:458:ASP:HA   | 1:Y:461:GLN:HG3  | 1.24                     | 1.17              |
| 1:Y:74:ILE:HD11  | 1:Y:237:ILE:HG13 | 1.21                     | 1.13              |
| 1:Y:229:ILE:HG21 | 1:Y:237:ILE:HG12 | 1.31                     | 1.11              |
| 1:Y:124:ILE:HD13 | 1:Y:203:MET:HE1  | 1.26                     | 1.09              |
| 1:Y:459:GLU:HB2  | 1:Y:460:LEU:HD12 | 1.32                     | 1.07              |
| 1:O:240:SER:HB2  | 1:O:450:ALA:HB3  | 1.37                     | 1.05              |
| 1:Y:476:THR:O    | 1:Y:480:ASN:ND2  | 1.88                     | 1.04              |
| 1:O:74:ILE:HD11  | 1:O:237:ILE:HG13 | 1.39                     | 1.03              |
| 1:O:313:ILE:HD11 | 1:O:381:LEU:HD23 | 1.40                     | 1.02              |
| 1:O:229:ILE:HG21 | 1:O:237:ILE:HG12 | 1.41                     | 1.00              |
| 1:Y:24:ASP:HB2   | 1:Y:26:ASN:HD21  | 1.27                     | 0.99              |
| 1:Y:250:LEU:HD11 | 1:Y:255:CYS:HB2  | 1.43                     | 0.99              |
| 1:Y:230:GLY:HA2  | 1:Y:235:THR:HB   | 1.43                     | 0.99              |
| 1:O:137:SER:HA   | 1:O:140:LYS:HD2  | 1.44                     | 0.97              |
| 1:Y:104:GLN:HG3  | 1:Y:349:THR:HG21 | 1.45                     | 0.97              |
| 1:O:155:ALA:HB1  | 1:O:210:PRO:HG2  | 1.46                     | 0.96              |
| 1:Y:325:ASP:HB3  | 1:Y:327:TYR:HB3  | 1.47                     | 0.95              |
| 1:O:273:MET:HB2  | 1:O:395:MET:HE3  | 1.49                     | 0.95              |
| 1:Y:124:ILE:HG21 | 1:Y:190:MET:HE2  | 1.48                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:154:ARG:HA   | 1:Y:157:ARG:HG2  | 1.49                     | 0.94              |
| 1:O:476:THR:O    | 1:O:480:ASN:ND2  | 2.01                     | 0.93              |
| 1:O:124:ILE:HG21 | 1:O:190:MET:HE2  | 1.50                     | 0.93              |
| 1:O:114:HIS:HA   | 1:O:117:ARG:NH1  | 1.84                     | 0.92              |
| 1:Y:211:ARG:HG3  | 1:Y:211:ARG:HH11 | 1.34                     | 0.92              |
| 1:O:314:GLN:HG2  | 1:O:317:ARG:HH12 | 1.32                     | 0.92              |
| 1:Y:492:ARG:HG2  | 1:Y:492:ARG:HH11 | 1.34                     | 0.92              |
| 1:O:180:VAL:HG23 | 1:O:216:GLU:HB3  | 1.50                     | 0.91              |
| 1:Y:24:ASP:HB2   | 1:Y:26:ASN:ND2   | 1.85                     | 0.91              |
| 1:O:251:PHE:CE2  | 1:O:446:LEU:HD13 | 2.06                     | 0.90              |
| 1:O:95:LYS:HG3   | 1:O:96:PRO:HD2   | 1.53                     | 0.89              |
| 1:Y:230:GLY:HA2  | 1:Y:235:THR:CB   | 2.03                     | 0.89              |
| 1:Y:419:MET:HE2  | 1:Y:419:MET:HA   | 1.54                     | 0.89              |
| 1:O:278:LYS:HZ2  | 1:O:280:VAL:HB   | 1.38                     | 0.89              |
| 1:O:278:LYS:NZ   | 1:O:280:VAL:HB   | 1.87                     | 0.89              |
| 1:O:314:GLN:HG2  | 1:O:317:ARG:NH1  | 1.88                     | 0.88              |
| 1:O:228:ASN:HD21 | 1:O:235:THR:N    | 1.71                     | 0.88              |
| 1:O:253:GLN:HG3  | 1:O:407:ARG:HD2  | 1.56                     | 0.88              |
| 1:O:5:TYR:HB2    | 1:O:74:ILE:HG22  | 1.53                     | 0.88              |
| 1:O:480:ASN:ND2  | 1:O:480:ASN:H    | 1.64                     | 0.88              |
| 1:Y:69:ILE:HG23  | 1:Y:73:GLN:HG3   | 1.56                     | 0.88              |
| 1:O:193:ASN:HB3  | 1:O:196:THR:HG21 | 1.56                     | 0.88              |
| 1:O:137:SER:O    | 1:O:138:GLY:C    | 2.12                     | 0.88              |
| 1:Y:468:ARG:HD2  | 1:Y:469:GLU:N    | 1.89                     | 0.87              |
| 1:O:273:MET:CB   | 1:O:395:MET:HE3  | 2.04                     | 0.87              |
| 1:O:47:HIS:CB    | 1:O:52:ILE:HD11  | 2.04                     | 0.87              |
| 1:O:17:ARG:HH22  | 1:O:437:GLU:HG2  | 1.39                     | 0.87              |
| 1:Y:250:LEU:CD1  | 1:Y:255:CYS:HB2  | 2.05                     | 0.86              |
| 1:O:193:ASN:HB3  | 1:O:196:THR:CG2  | 2.03                     | 0.86              |
| 1:O:415:ASN:ND2  | 1:O:418:LEU:H    | 1.73                     | 0.86              |
| 1:Y:460:LEU:HD12 | 1:Y:460:LEU:H    | 1.41                     | 0.86              |
| 1:Y:124:ILE:HD13 | 1:Y:203:MET:CE   | 2.03                     | 0.85              |
| 1:Y:229:ILE:HG21 | 1:Y:237:ILE:CG1  | 2.06                     | 0.85              |
| 1:O:183:TYR:HB3  | 1:O:290:ILE:HG21 | 1.57                     | 0.85              |
| 1:Y:293:GLY:HA2  | 1:Y:299:ASN:ND2  | 1.91                     | 0.85              |
| 1:Y:314:GLN:HG2  | 1:Y:317:ARG:HH12 | 1.41                     | 0.84              |
| 1:O:402:ARG:HB3  | 1:O:402:ARG:HH11 | 1.41                     | 0.84              |
| 1:O:120:LEU:O    | 1:O:121:GLU:C    | 2.17                     | 0.84              |
| 1:Y:458:ASP:HA   | 1:Y:461:GLN:CG   | 2.05                     | 0.84              |
| 1:O:115:LEU:HD12 | 1:O:115:LEU:H    | 1.43                     | 0.84              |
| 1:O:419:MET:HE2  | 1:O:419:MET:HA   | 1.56                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:313:ILE:HD11 | 1:O:381:LEU:CD2  | 2.07                     | 0.84              |
| 1:O:47:HIS:HB2   | 1:O:52:ILE:HD11  | 1.60                     | 0.83              |
| 1:O:221:SER:HB3  | 1:O:296:GLY:HA3  | 1.61                     | 0.83              |
| 1:O:240:SER:HB2  | 1:O:450:ALA:CB   | 2.07                     | 0.83              |
| 1:O:155:ALA:CB   | 1:O:210:PRO:HG2  | 2.07                     | 0.83              |
| 1:O:254:LEU:HD11 | 1:O:445:TYR:HE2  | 1.41                     | 0.83              |
| 1:O:389:ARG:HB2  | 1:O:426:LEU:CD1  | 2.08                     | 0.83              |
| 1:Y:61:VAL:O     | 1:Y:62:GLU:C     | 2.20                     | 0.83              |
| 1:O:17:ARG:HA    | 1:O:59:THR:HG21  | 1.59                     | 0.83              |
| 1:O:83:ARG:HB2   | 4:O:600:GOL:H12  | 1.59                     | 0.82              |
| 1:Y:415:ASN:ND2  | 1:Y:418:LEU:H    | 1.78                     | 0.82              |
| 1:O:351:LEU:HD22 | 1:O:360:ALA:CB   | 2.09                     | 0.82              |
| 1:O:455:GLN:O    | 1:O:456:ASN:HB2  | 1.79                     | 0.81              |
| 1:Y:58:TRP:O     | 1:Y:59:THR:C     | 2.24                     | 0.81              |
| 1:Y:74:ILE:CD1   | 1:Y:237:ILE:HG13 | 2.05                     | 0.80              |
| 1:O:33:ARG:CZ    | 1:O:58:TRP:HB3   | 2.11                     | 0.80              |
| 1:Y:434:GLU:HB2  | 1:Y:465:VAL:HB   | 1.63                     | 0.80              |
| 1:Y:17:ARG:HG2   | 1:Y:32:GLN:HG3   | 1.64                     | 0.79              |
| 1:O:59:THR:O     | 1:O:63:VAL:HG23  | 1.82                     | 0.79              |
| 1:O:211:ARG:HG3  | 1:O:211:ARG:HH11 | 1.45                     | 0.79              |
| 1:Y:48:ASP:O     | 1:Y:52:ILE:HD12  | 1.83                     | 0.79              |
| 1:Y:246:GLN:HG3  | 1:Y:262:LYS:NZ   | 1.98                     | 0.79              |
| 1:O:19:VAL:CG1   | 1:O:27:ILE:HD13  | 2.12                     | 0.79              |
| 1:O:206:VAL:HG12 | 1:O:207:LEU:CD2  | 2.12                     | 0.79              |
| 1:O:199:TRP:CE2  | 1:O:214:LEU:HD23 | 2.16                     | 0.79              |
| 1:Y:271:MET:C    | 1:Y:272:LEU:HD12 | 2.07                     | 0.79              |
| 1:O:70:SER:HB2   | 1:O:72:ASP:OD1   | 1.83                     | 0.79              |
| 1:Y:60:LEU:O     | 1:Y:63:VAL:HG23  | 1.84                     | 0.78              |
| 1:O:463:LYS:HE2  | 1:O:463:LYS:HA   | 1.65                     | 0.78              |
| 1:O:199:TRP:CD1  | 1:O:214:LEU:HD23 | 2.17                     | 0.78              |
| 1:O:86:THR:OG1   | 1:O:137:SER:HB3  | 1.84                     | 0.78              |
| 1:O:250:LEU:HD11 | 1:O:255:CYS:HB2  | 1.66                     | 0.78              |
| 1:Y:463:LYS:HA   | 1:Y:463:LYS:CE   | 2.13                     | 0.78              |
| 1:O:271:MET:C    | 1:O:272:LEU:HD12 | 2.09                     | 0.78              |
| 1:Y:137:SER:O    | 1:Y:141:VAL:HG23 | 1.83                     | 0.77              |
| 1:Y:31:SER:OG    | 1:Y:59:THR:HA    | 1.84                     | 0.77              |
| 1:Y:261:ALA:HB2  | 1:Y:273:MET:HB2  | 1.66                     | 0.77              |
| 1:O:253:GLN:CG   | 1:O:407:ARG:HD2  | 2.14                     | 0.77              |
| 1:O:360:ALA:O    | 1:O:361:ARG:HD3  | 1.84                     | 0.77              |
| 1:O:463:LYS:HA   | 1:O:463:LYS:CE   | 2.12                     | 0.77              |
| 1:O:183:TYR:CE1  | 1:O:217:VAL:HG12 | 2.19                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:3:LYS:HA     | 1:O:73:GLN:HA    | 1.65                     | 0.77              |
| 1:Y:84:GLU:HB2   | 1:Y:103:TRP:HB3  | 1.66                     | 0.76              |
| 1:O:55:THR:HA    | 1:O:58:TRP:CD1   | 2.19                     | 0.76              |
| 1:Y:69:ILE:HG23  | 1:Y:73:GLN:CG    | 2.15                     | 0.76              |
| 1:Y:246:GLN:HG2  | 1:Y:270:PHE:HB2  | 1.68                     | 0.76              |
| 1:Y:229:ILE:HG23 | 1:Y:235:THR:O    | 1.85                     | 0.76              |
| 1:O:186:ALA:O    | 1:O:189:THR:HG23 | 1.85                     | 0.76              |
| 1:Y:154:ARG:CB   | 1:Y:159:GLU:HB3  | 2.16                     | 0.76              |
| 1:Y:432:ARG:HG2  | 1:Y:436:ARG:HH12 | 1.51                     | 0.75              |
| 1:O:226:GLN:NE2  | 1:O:236:ARG:HB3  | 2.02                     | 0.75              |
| 1:Y:185:ASN:HD21 | 1:Y:244:GLY:N    | 1.83                     | 0.75              |
| 1:O:184:THR:HG22 | 1:O:290:ILE:O    | 1.87                     | 0.75              |
| 1:Y:117:ARG:CB   | 1:Y:117:ARG:HH11 | 2.00                     | 0.75              |
| 1:Y:70:SER:HB2   | 1:Y:72:ASP:OD1   | 1.87                     | 0.74              |
| 1:Y:104:GLN:CG   | 1:Y:349:THR:HG21 | 2.16                     | 0.74              |
| 1:Y:193:ASN:HB3  | 1:Y:196:THR:HG21 | 1.69                     | 0.74              |
| 1:O:24:ASP:HB2   | 1:O:26:ASN:ND2   | 2.02                     | 0.74              |
| 1:O:373:ALA:O    | 1:O:377:ILE:HG13 | 1.87                     | 0.74              |
| 1:O:17:ARG:CA    | 1:O:59:THR:HG21  | 2.16                     | 0.74              |
| 1:O:185:ASN:O    | 1:O:188:ARG:HB2  | 1.88                     | 0.74              |
| 1:O:196:THR:O    | 1:O:197:LEU:C    | 2.27                     | 0.74              |
| 1:Y:186:ALA:O    | 1:Y:189:THR:HG23 | 1.87                     | 0.74              |
| 1:Y:221:SER:HB3  | 1:Y:446:LEU:HD12 | 1.69                     | 0.74              |
| 1:O:206:VAL:HG12 | 1:O:207:LEU:HD22 | 1.68                     | 0.73              |
| 1:Y:392:LEU:HD23 | 1:Y:393:GLU:N    | 2.02                     | 0.73              |
| 1:O:219:ARG:HG2  | 1:O:222:GLU:HB3  | 1.69                     | 0.73              |
| 1:O:279:ALA:HB2  | 1:O:300:TYR:CD1  | 2.23                     | 0.73              |
| 1:O:24:ASP:HB2   | 1:O:26:ASN:HD21  | 1.53                     | 0.73              |
| 1:O:181:THR:HG23 | 1:O:182:ASP:O    | 1.89                     | 0.73              |
| 1:Y:48:ASP:C     | 1:Y:52:ILE:HD12  | 2.13                     | 0.73              |
| 1:Y:183:TYR:CD1  | 1:Y:217:VAL:HG12 | 2.24                     | 0.73              |
| 1:Y:183:TYR:CE1  | 1:Y:217:VAL:HG12 | 2.24                     | 0.73              |
| 1:Y:273:MET:HB2  | 1:Y:395:MET:HE3  | 1.70                     | 0.72              |
| 1:O:102:VAL:HG12 | 1:O:103:TRP:CD1  | 2.23                     | 0.72              |
| 1:Y:273:MET:CB   | 1:Y:395:MET:HE3  | 2.19                     | 0.72              |
| 1:O:325:ASP:HB3  | 1:O:327:TYR:HB3  | 1.71                     | 0.72              |
| 1:O:44:TRP:CE2   | 1:O:107:ARG:HB2  | 2.24                     | 0.72              |
| 1:Y:145:LEU:HD12 | 1:Y:151:SER:HB2  | 1.71                     | 0.72              |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CD1  | 2.25                     | 0.72              |
| 1:O:250:LEU:CD1  | 1:O:255:CYS:HB2  | 2.18                     | 0.72              |
| 1:O:144:ILE:HD12 | 1:O:144:ILE:H    | 1.55                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:478:GLU:O    | 1:Y:481:TYR:HB3  | 1.90                     | 0.72              |
| 1:O:152:ARG:O    | 1:O:155:ALA:HB3  | 1.91                     | 0.71              |
| 1:Y:106:ARG:HD2  | 1:Y:349:THR:O    | 1.91                     | 0.71              |
| 1:O:434:GLU:HB2  | 1:O:465:VAL:HB   | 1.72                     | 0.71              |
| 1:Y:180:VAL:HG23 | 1:Y:216:GLU:HB3  | 1.72                     | 0.71              |
| 1:Y:451:VAL:HG13 | 1:Y:453:PHE:H    | 1.55                     | 0.71              |
| 1:Y:324:ASN:N    | 1:Y:324:ASN:ND2  | 2.38                     | 0.71              |
| 1:Y:456:ASN:OD1  | 1:Y:459:GLU:HG3  | 1.90                     | 0.71              |
| 1:O:332:PHE:O    | 1:O:335:LYS:HB2  | 1.90                     | 0.71              |
| 1:Y:458:ASP:CA   | 1:Y:461:GLN:HG3  | 2.14                     | 0.71              |
| 1:O:87:ILE:HD13  | 1:O:168:TRP:HB2  | 1.73                     | 0.71              |
| 1:Y:193:ASN:HB3  | 1:Y:196:THR:CG2  | 2.20                     | 0.71              |
| 1:O:254:LEU:HD11 | 1:O:445:TYR:CE2  | 2.25                     | 0.71              |
| 1:O:435:VAL:HG22 | 1:O:436:ARG:H    | 1.56                     | 0.71              |
| 1:Y:180:VAL:CG2  | 1:Y:218:ARG:HG2  | 2.21                     | 0.70              |
| 1:Y:459:GLU:HB2  | 1:Y:460:LEU:CD1  | 2.18                     | 0.70              |
| 1:O:179:HIS:CE1  | 1:O:215:PRO:HB3  | 2.26                     | 0.70              |
| 1:O:476:THR:O    | 1:O:477:THR:C    | 2.31                     | 0.70              |
| 1:O:286:LEU:C    | 1:O:287:LEU:HD23 | 2.15                     | 0.70              |
| 1:Y:51:GLU:O     | 1:Y:55:THR:HG23  | 1.90                     | 0.70              |
| 1:O:158:GLY:HA2  | 1:O:212:GLU:HB3  | 1.71                     | 0.70              |
| 1:O:80:THR:HG21  | 1:O:248:ALA:CB   | 2.22                     | 0.70              |
| 1:O:354:PRO:HD2  | 1:O:355:TYR:CD2  | 2.27                     | 0.70              |
| 1:Y:2:GLU:O      | 1:Y:73:GLN:HA    | 1.90                     | 0.70              |
| 1:O:200:ASP:OD1  | 1:O:202:LYS:HB2  | 1.91                     | 0.70              |
| 1:Y:45:VAL:O     | 1:Y:102:VAL:HG23 | 1.92                     | 0.70              |
| 1:Y:74:ILE:HD12  | 1:Y:74:ILE:O     | 1.91                     | 0.70              |
| 1:Y:140:LYS:O    | 1:Y:144:ILE:HD12 | 1.92                     | 0.70              |
| 1:Y:269:CYS:HB2  | 1:Y:306:VAL:HB   | 1.74                     | 0.70              |
| 1:O:227:THR:O    | 1:O:229:ILE:HG22 | 1.92                     | 0.70              |
| 1:Y:27:ILE:HD11  | 1:Y:30:VAL:HG23  | 1.73                     | 0.70              |
| 1:O:95:LYS:HG3   | 1:O:96:PRO:CD    | 2.20                     | 0.70              |
| 1:O:199:TRP:CD2  | 1:O:214:LEU:HD23 | 2.25                     | 0.70              |
| 1:Y:253:GLN:HG3  | 1:Y:407:ARG:HD2  | 1.73                     | 0.70              |
| 1:O:47:HIS:HB3   | 1:O:52:ILE:HD11  | 1.72                     | 0.70              |
| 1:O:87:ILE:HD13  | 1:O:168:TRP:CB   | 2.22                     | 0.69              |
| 1:Y:22:ASP:OD2   | 1:Y:26:ASN:HB2   | 1.90                     | 0.69              |
| 1:Y:180:VAL:HG21 | 1:Y:218:ARG:HG2  | 1.73                     | 0.69              |
| 1:Y:415:ASN:HD22 | 1:Y:418:LEU:H    | 1.40                     | 0.69              |
| 1:O:170:ILE:O    | 1:O:171:TRP:C    | 2.35                     | 0.69              |
| 1:O:211:ARG:HG3  | 1:O:211:ARG:NH1  | 2.03                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:415:ASN:HD21 | 1:O:417:PHE:HB3  | 1.58                     | 0.69              |
| 1:O:251:PHE:CE1  | 1:O:256:VAL:HG21 | 2.26                     | 0.69              |
| 1:O:17:ARG:HH22  | 1:O:437:GLU:CG   | 2.05                     | 0.69              |
| 1:O:84:GLU:HB2   | 1:O:103:TRP:HB3  | 1.75                     | 0.69              |
| 1:O:210:PRO:O    | 1:O:213:MET:HG2  | 1.91                     | 0.69              |
| 1:Y:124:ILE:CD1  | 1:Y:203:MET:HE1  | 2.15                     | 0.69              |
| 1:O:222:GLU:O    | 1:O:240:SER:HA   | 1.93                     | 0.69              |
| 1:O:20:VAL:CG2   | 1:O:63:VAL:HG11  | 2.23                     | 0.69              |
| 1:O:89:TRP:HB2   | 1:O:95:LYS:C     | 2.17                     | 0.69              |
| 1:O:293:GLY:HA2  | 1:O:299:ASN:ND2  | 2.08                     | 0.69              |
| 1:O:389:ARG:HB2  | 1:O:426:LEU:HD11 | 1.75                     | 0.69              |
| 1:Y:68:ASP:C     | 1:Y:69:ILE:HD13  | 2.17                     | 0.69              |
| 1:Y:111:ILE:HG22 | 1:Y:115:LEU:CD1  | 2.23                     | 0.69              |
| 1:O:441:LEU:HD22 | 1:O:445:TYR:OH   | 1.92                     | 0.69              |
| 1:Y:250:LEU:O    | 1:Y:250:LEU:HD12 | 1.93                     | 0.69              |
| 1:O:179:HIS:CD2  | 1:O:215:PRO:HB3  | 2.28                     | 0.68              |
| 1:O:391:VAL:O    | 1:O:392:LEU:C    | 2.33                     | 0.68              |
| 1:Y:271:MET:HE1  | 1:Y:392:LEU:HB2  | 1.73                     | 0.68              |
| 1:Y:123:TYR:HD2  | 1:Y:203:MET:HE2  | 1.58                     | 0.68              |
| 1:O:435:VAL:HG22 | 1:O:436:ARG:N    | 2.07                     | 0.68              |
| 1:Y:20:VAL:C     | 1:Y:21:MET:HG3   | 2.17                     | 0.68              |
| 1:Y:127:ASN:HB3  | 1:Y:193:ASN:ND2  | 2.07                     | 0.68              |
| 1:Y:210:PRO:O    | 1:Y:213:MET:HG2  | 1.94                     | 0.68              |
| 1:O:26:ASN:O     | 1:O:28:ILE:HD13  | 1.93                     | 0.68              |
| 1:O:227:THR:OG1  | 1:O:239:ILE:HD11 | 1.94                     | 0.68              |
| 1:O:340:ASN:ND2  | 1:O:371:VAL:HG22 | 2.09                     | 0.68              |
| 1:Y:253:GLN:CG   | 1:Y:407:ARG:HD2  | 2.24                     | 0.68              |
| 1:Y:448:GLY:O    | 1:Y:451:VAL:HG12 | 1.93                     | 0.68              |
| 1:Y:115:LEU:HD12 | 1:Y:115:LEU:H    | 1.59                     | 0.68              |
| 1:Y:5:TYR:HB2    | 1:Y:74:ILE:HG22  | 1.75                     | 0.67              |
| 1:Y:155:ALA:HA   | 1:Y:160:LEU:HB2  | 1.76                     | 0.67              |
| 1:Y:180:VAL:HG22 | 1:Y:181:THR:H    | 1.58                     | 0.67              |
| 1:O:20:VAL:HG12  | 1:O:21:MET:N     | 2.09                     | 0.67              |
| 1:Y:202:LYS:O    | 1:Y:205:GLU:HG3  | 1.93                     | 0.67              |
| 1:Y:468:ARG:HD2  | 1:Y:469:GLU:H    | 1.60                     | 0.67              |
| 1:Y:144:ILE:O    | 1:Y:148:VAL:HG23 | 1.95                     | 0.67              |
| 1:O:230:GLY:HA2  | 1:O:235:THR:OG1  | 1.95                     | 0.67              |
| 1:Y:47:HIS:HB3   | 1:Y:52:ILE:HD11  | 1.77                     | 0.67              |
| 1:Y:390:ASP:HA   | 1:Y:483:TYR:OH   | 1.94                     | 0.67              |
| 1:O:140:LYS:O    | 1:O:144:ILE:HD12 | 1.95                     | 0.67              |
| 1:O:47:HIS:O     | 1:O:49:PRO:HD3   | 1.94                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:88:VAL:O     | 1:O:97:ILE:HG12  | 1.94                     | 0.67              |
| 1:Y:130:LEU:HD23 | 1:Y:130:LEU:N    | 2.07                     | 0.67              |
| 1:O:5:TYR:HE2    | 1:O:73:GLN:HG3   | 1.60                     | 0.67              |
| 1:Y:422:GLN:NE2  | 1:Y:426:LEU:HD22 | 2.10                     | 0.66              |
| 1:Y:170:ILE:HA   | 1:Y:173:MET:HG3  | 1.76                     | 0.66              |
| 1:Y:463:LYS:HA   | 1:Y:463:LYS:HE2  | 1.75                     | 0.66              |
| 1:Y:480:ASN:ND2  | 1:Y:480:ASN:H    | 1.94                     | 0.66              |
| 1:Y:221:SER:CB   | 1:Y:450:ALA:HB2  | 2.25                     | 0.66              |
| 1:O:90:GLU:N     | 1:O:95:LYS:O     | 2.29                     | 0.66              |
| 1:O:154:ARG:HA   | 1:O:157:ARG:CG   | 2.25                     | 0.66              |
| 1:O:435:VAL:HG11 | 1:O:441:LEU:HD11 | 1.76                     | 0.66              |
| 1:Y:154:ARG:O    | 1:Y:155:ALA:C    | 2.33                     | 0.66              |
| 1:Y:388:THR:O    | 1:Y:391:VAL:HG13 | 1.95                     | 0.66              |
| 1:O:169:LEU:O    | 1:O:172:LYS:HB2  | 1.94                     | 0.66              |
| 1:O:199:TRP:CG   | 1:O:214:LEU:HD23 | 2.30                     | 0.66              |
| 1:Y:9:LEU:HG     | 1:Y:56:GLN:HE21  | 1.60                     | 0.66              |
| 1:Y:222:GLU:O    | 1:Y:240:SER:HA   | 1.95                     | 0.66              |
| 1:Y:127:ASN:HB3  | 1:Y:193:ASN:HD22 | 1.58                     | 0.66              |
| 1:Y:84:GLU:OE2   | 1:Y:188:ARG:HD2  | 1.96                     | 0.66              |
| 1:Y:449:LEU:HD12 | 1:Y:449:LEU:O    | 1.95                     | 0.66              |
| 1:O:113:GLU:O    | 1:O:114:HIS:C    | 2.38                     | 0.66              |
| 1:O:279:ALA:HB2  | 1:O:300:TYR:CE1  | 2.31                     | 0.66              |
| 1:Y:314:GLN:HG2  | 1:Y:317:ARG:NH1  | 2.11                     | 0.66              |
| 1:O:74:ILE:HD12  | 1:O:74:ILE:O     | 1.96                     | 0.66              |
| 1:Y:197:LEU:HD13 | 1:Y:197:LEU:H    | 1.60                     | 0.66              |
| 1:O:20:VAL:C     | 1:O:21:MET:HG3   | 2.20                     | 0.66              |
| 1:O:460:LEU:HD12 | 1:O:460:LEU:N    | 2.11                     | 0.66              |
| 1:O:463:LYS:NZ   | 1:O:465:VAL:HG23 | 2.10                     | 0.66              |
| 1:Y:123:TYR:CD2  | 1:Y:203:MET:HE2  | 2.30                     | 0.65              |
| 1:Y:81:ASN:N     | 1:Y:81:ASN:HD22  | 1.94                     | 0.65              |
| 1:O:396:GLN:O    | 1:O:400:GLY:N    | 2.29                     | 0.65              |
| 1:O:480:ASN:ND2  | 1:O:480:ASN:N    | 2.40                     | 0.65              |
| 1:Y:19:VAL:HG12  | 1:Y:21:MET:HE2   | 1.77                     | 0.65              |
| 1:Y:33:ARG:HG3   | 1:Y:33:ARG:HH11  | 1.60                     | 0.65              |
| 1:O:21:MET:HE1   | 1:O:444:ALA:HB2  | 1.78                     | 0.65              |
| 1:O:48:ASP:HB3   | 1:O:51:GLU:HB3   | 1.78                     | 0.65              |
| 1:O:106:ARG:NH2  | 1:O:133:ASP:OD1  | 2.30                     | 0.65              |
| 1:O:229:ILE:CG2  | 1:O:237:ILE:HG12 | 2.22                     | 0.65              |
| 1:Y:184:THR:O    | 1:Y:187:SER:HB3  | 1.97                     | 0.65              |
| 1:Y:196:THR:O    | 1:Y:197:LEU:C    | 2.38                     | 0.65              |
| 1:Y:212:GLU:N    | 1:Y:212:GLU:OE1  | 2.29                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:373:ALA:O    | 1:Y:377:ILE:HG13 | 1.96                     | 0.65              |
| 1:Y:482:ARG:O    | 1:Y:483:TYR:C    | 2.39                     | 0.65              |
| 1:O:146:ASP:OD1  | 1:O:146:ASP:N    | 2.29                     | 0.65              |
| 1:O:275:THR:HG21 | 1:O:280:VAL:CG1  | 2.27                     | 0.65              |
| 1:Y:496:TRP:HZ3  | 1:O:492:ARG:HD3  | 1.62                     | 0.65              |
| 1:O:144:ILE:O    | 1:O:148:VAL:HG23 | 1.97                     | 0.65              |
| 1:Y:142:LYS:NZ   | 1:Y:146:ASP:OD2  | 2.30                     | 0.65              |
| 1:Y:152:ARG:O    | 1:Y:155:ALA:HB3  | 1.97                     | 0.65              |
| 1:O:487:LYS:HA   | 1:O:490:VAL:HG23 | 1.79                     | 0.65              |
| 1:O:177:ARG:NH1  | 1:O:226:GLN:O    | 2.29                     | 0.65              |
| 1:O:415:ASN:O    | 1:O:419:MET:HG2  | 1.97                     | 0.65              |
| 1:Y:180:VAL:HG21 | 1:Y:218:ARG:CG   | 2.27                     | 0.65              |
| 1:O:69:ILE:HD13  | 1:O:69:ILE:N     | 2.12                     | 0.65              |
| 1:O:124:ILE:HD13 | 1:O:203:MET:CE   | 2.27                     | 0.65              |
| 1:O:476:THR:HG22 | 1:O:477:THR:H    | 1.60                     | 0.65              |
| 1:Y:435:VAL:HG22 | 1:Y:436:ARG:N    | 2.11                     | 0.65              |
| 1:O:35:PHE:HB2   | 1:O:51:GLU:CG    | 2.26                     | 0.65              |
| 1:O:161:LEU:HD21 | 1:O:179:HIS:NE2  | 2.12                     | 0.64              |
| 1:O:429:ARG:HD3  | 1:O:469:GLU:OE1  | 1.97                     | 0.64              |
| 1:Y:161:LEU:HD22 | 1:Y:179:HIS:CE1  | 2.32                     | 0.64              |
| 1:Y:262:LYS:HE3  | 1:Y:270:PHE:O    | 1.96                     | 0.64              |
| 1:Y:460:LEU:H    | 1:Y:460:LEU:CD1  | 2.11                     | 0.64              |
| 1:O:40:PRO:HG2   | 1:O:44:TRP:CB    | 2.27                     | 0.64              |
| 1:Y:111:ILE:HG21 | 1:Y:139:THR:HG22 | 1.77                     | 0.64              |
| 1:Y:460:LEU:HD12 | 1:Y:460:LEU:N    | 2.11                     | 0.64              |
| 1:Y:19:VAL:HG13  | 1:Y:27:ILE:HD13  | 1.78                     | 0.64              |
| 1:O:201:ASP:O    | 1:O:205:GLU:HG2  | 1.96                     | 0.64              |
| 1:Y:227:THR:O    | 1:Y:229:ILE:HG22 | 1.96                     | 0.64              |
| 1:Y:467:GLU:HG2  | 1:Y:468:ARG:N    | 2.07                     | 0.64              |
| 1:O:193:ASN:N    | 1:O:198:ASP:O    | 2.29                     | 0.64              |
| 1:O:439:THR:HG22 | 1:O:440:ALA:N    | 2.12                     | 0.64              |
| 1:Y:246:GLN:HG3  | 1:Y:262:LYS:HZ3  | 1.61                     | 0.64              |
| 1:O:61:VAL:HA    | 1:O:64:LEU:HD13  | 1.80                     | 0.64              |
| 1:O:84:GLU:N     | 1:O:84:GLU:OE1   | 2.31                     | 0.64              |
| 1:O:228:ASN:HB2  | 1:O:236:ARG:HE   | 1.62                     | 0.64              |
| 1:O:68:ASP:C     | 1:O:69:ILE:HD13  | 2.22                     | 0.64              |
| 1:O:474:ILE:HG23 | 1:O:478:GLU:HB3  | 1.79                     | 0.64              |
| 1:Y:61:VAL:HG12  | 1:Y:62:GLU:N     | 2.13                     | 0.64              |
| 1:Y:262:LYS:NZ   | 1:Y:264:THR:HB   | 2.13                     | 0.64              |
| 1:Y:382:GLU:HG2  | 1:Y:421:PHE:CE2  | 2.32                     | 0.64              |
| 1:Y:432:ARG:HD2  | 1:Y:436:ARG:NH2  | 2.13                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:156:ARG:HB2  | 1:O:156:ARG:CZ   | 2.27                     | 0.64              |
| 1:O:354:PRO:HD2  | 1:O:355:TYR:CE2  | 2.33                     | 0.64              |
| 1:O:432:ARG:O    | 1:O:467:GLU:N    | 2.31                     | 0.64              |
| 1:O:455:GLN:O    | 1:O:456:ASN:CB   | 2.45                     | 0.64              |
| 1:O:63:VAL:O     | 1:O:66:LYS:HG2   | 1.99                     | 0.63              |
| 1:O:386:TYR:HB3  | 1:O:486:TRP:CE2  | 2.33                     | 0.63              |
| 1:Y:498:GLU:OE1  | 1:Y:498:GLU:HA   | 1.99                     | 0.63              |
| 1:O:497:GLU:HA   | 1:O:497:GLU:OE1  | 1.98                     | 0.63              |
| 1:Y:31:SER:HB2   | 1:Y:62:GLU:HB3   | 1.80                     | 0.63              |
| 1:O:183:TYR:CD1  | 1:O:217:VAL:HG12 | 2.33                     | 0.63              |
| 1:Y:4:LYS:N      | 1:Y:73:GLN:O     | 2.31                     | 0.63              |
| 1:O:5:TYR:O      | 1:O:75:ALA:N     | 2.29                     | 0.63              |
| 1:O:310:GLY:HA3  | 3:O:601:ATF:O3'  | 1.99                     | 0.63              |
| 1:O:477:THR:O    | 1:O:478:GLU:C    | 2.41                     | 0.63              |
| 1:Y:85:THR:HA    | 1:Y:101:ILE:O    | 1.98                     | 0.63              |
| 1:Y:157:ARG:HG3  | 1:Y:159:GLU:OE1  | 1.98                     | 0.63              |
| 1:O:166:ASP:O    | 1:O:167:THR:C    | 2.42                     | 0.63              |
| 1:O:199:TRP:NE1  | 1:O:214:LEU:HD23 | 2.13                     | 0.63              |
| 1:O:390:ASP:HA   | 1:O:483:TYR:OH   | 1.98                     | 0.63              |
| 1:Y:170:ILE:HA   | 1:Y:173:MET:CG   | 2.29                     | 0.63              |
| 1:O:50:MET:O     | 1:O:54:ALA:N     | 2.28                     | 0.63              |
| 1:Y:80:THR:HG21  | 1:Y:248:ALA:CB   | 2.28                     | 0.63              |
| 1:Y:197:LEU:HD13 | 1:Y:197:LEU:N    | 2.11                     | 0.63              |
| 1:Y:207:LEU:HB3  | 1:Y:209:ILE:HD12 | 1.80                     | 0.63              |
| 1:Y:419:MET:HE2  | 1:Y:419:MET:CA   | 2.28                     | 0.63              |
| 1:O:123:TYR:CD2  | 1:O:203:MET:HE2  | 2.33                     | 0.63              |
| 1:Y:196:THR:HG22 | 1:Y:198:ASP:H    | 1.64                     | 0.62              |
| 1:Y:205:GLU:O    | 1:Y:208:ASP:N    | 2.31                     | 0.62              |
| 1:O:113:GLU:O    | 1:O:116:LYS:HB2  | 1.98                     | 0.62              |
| 1:O:184:THR:HA   | 1:O:290:ILE:HG22 | 1.81                     | 0.62              |
| 1:O:456:ASN:OD1  | 1:O:458:ASP:HB2  | 2.00                     | 0.62              |
| 1:Y:69:ILE:HD13  | 1:Y:69:ILE:N     | 2.11                     | 0.62              |
| 1:Y:146:ASP:OD1  | 1:Y:146:ASP:N    | 2.29                     | 0.62              |
| 1:Y:463:LYS:HZ1  | 1:Y:465:VAL:CG2  | 2.12                     | 0.62              |
| 1:O:84:GLU:HB2   | 1:O:103:TRP:CB   | 2.29                     | 0.62              |
| 1:O:32:GLN:HA    | 1:O:59:THR:HG23  | 1.82                     | 0.62              |
| 1:O:183:TYR:CB   | 1:O:290:ILE:HG21 | 2.29                     | 0.62              |
| 1:O:272:LEU:HD21 | 1:O:303:GLU:OE1  | 1.99                     | 0.62              |
| 1:O:53:TRP:HZ3   | 1:O:173:MET:HE3  | 1.65                     | 0.62              |
| 1:O:133:ASP:OD1  | 1:O:135:TYR:N    | 2.31                     | 0.62              |
| 1:Y:22:ASP:O     | 1:Y:25:ALA:N     | 2.31                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:433:PRO:HA   | 1:Y:466:ILE:HD13 | 1.80                     | 0.62              |
| 1:Y:451:VAL:CG1  | 1:Y:453:PHE:H    | 2.12                     | 0.62              |
| 1:Y:156:ARG:CZ   | 1:Y:156:ARG:HB2  | 2.28                     | 0.62              |
| 1:Y:179:HIS:CD2  | 1:Y:215:PRO:HA   | 2.35                     | 0.62              |
| 1:O:19:VAL:HG13  | 1:O:27:ILE:HD13  | 1.82                     | 0.62              |
| 1:O:202:LYS:O    | 1:O:205:GLU:HG3  | 2.00                     | 0.62              |
| 1:O:3:LYS:HA     | 1:O:73:GLN:CA    | 2.29                     | 0.62              |
| 1:O:114:HIS:O    | 1:O:117:ARG:N    | 2.32                     | 0.62              |
| 1:O:124:ILE:HD13 | 1:O:203:MET:HE1  | 1.81                     | 0.62              |
| 1:O:351:LEU:HD22 | 1:O:360:ALA:HB1  | 1.82                     | 0.62              |
| 1:Y:47:HIS:O     | 1:Y:49:PRO:HD3   | 2.00                     | 0.61              |
| 1:O:81:ASN:N     | 1:O:81:ASN:HD22  | 1.97                     | 0.61              |
| 1:O:287:LEU:O    | 1:O:302:LEU:HD23 | 2.00                     | 0.61              |
| 1:O:395:MET:O    | 1:O:396:GLN:C    | 2.43                     | 0.61              |
| 1:O:473:GLY:C    | 1:O:474:ILE:HD13 | 2.25                     | 0.61              |
| 1:Y:67:ALA:CB    | 1:Y:69:ILE:HG12  | 2.30                     | 0.61              |
| 1:Y:174:THR:O    | 1:Y:176:GLY:N    | 2.30                     | 0.61              |
| 1:O:69:ILE:HG23  | 1:O:73:GLN:HG3   | 1.81                     | 0.61              |
| 1:O:110:GLU:O    | 1:O:113:GLU:HB2  | 2.00                     | 0.61              |
| 1:O:17:ARG:NH2   | 1:O:437:GLU:HG2  | 2.13                     | 0.61              |
| 1:O:207:LEU:HB3  | 1:O:209:ILE:CD1  | 2.30                     | 0.61              |
| 1:Y:181:THR:HG23 | 1:Y:182:ASP:O    | 2.00                     | 0.61              |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:CA   | 2.12                     | 0.61              |
| 1:O:322:LEU:N    | 1:O:322:LEU:HD23 | 2.14                     | 0.61              |
| 1:O:478:GLU:HA   | 1:O:478:GLU:OE1  | 2.00                     | 0.61              |
| 1:O:47:HIS:CD2   | 1:O:82:GLN:HE22  | 2.18                     | 0.61              |
| 1:Y:81:ASN:N     | 1:Y:81:ASN:ND2   | 2.46                     | 0.61              |
| 1:Y:478:GLU:HA   | 1:Y:478:GLU:OE1  | 1.98                     | 0.61              |
| 1:O:297:GLU:OE1  | 1:O:297:GLU:N    | 2.30                     | 0.61              |
| 1:O:498:GLU:OE1  | 1:O:498:GLU:HA   | 2.00                     | 0.61              |
| 1:Y:71:SER:HB2   | 1:Y:235:THR:HG21 | 1.83                     | 0.61              |
| 1:Y:211:ARG:HG3  | 1:Y:211:ARG:NH1  | 2.10                     | 0.61              |
| 1:O:74:ILE:CD1   | 1:O:237:ILE:HG13 | 2.25                     | 0.61              |
| 1:Y:222:GLU:HG3  | 1:Y:223:VAL:N    | 2.15                     | 0.61              |
| 1:Y:402:ARG:HB3  | 1:Y:402:ARG:HH11 | 1.66                     | 0.61              |
| 1:O:90:GLU:HB3   | 1:O:93:THR:HG23  | 1.83                     | 0.61              |
| 1:Y:27:ILE:HD12  | 1:Y:27:ILE:C     | 2.27                     | 0.60              |
| 1:Y:149:GLU:HA   | 1:Y:149:GLU:OE1  | 2.00                     | 0.60              |
| 1:Y:310:GLY:O    | 1:Y:313:ILE:HB   | 2.01                     | 0.60              |
| 1:O:41:LYS:CG    | 1:O:42:PRO:HD2   | 2.31                     | 0.60              |
| 1:O:143:TRP:CE3  | 1:O:144:ILE:HA   | 2.36                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:359:TYR:HB2  | 1:O:495:ALA:HA   | 1.83                     | 0.60              |
| 1:Y:425:ILE:O    | 1:Y:479:ARG:HD2  | 2.02                     | 0.60              |
| 1:Y:432:ARG:HG2  | 1:Y:436:ARG:NH1  | 2.16                     | 0.60              |
| 1:O:108:THR:HB   | 1:O:139:THR:HB   | 1.83                     | 0.60              |
| 1:O:193:ASN:OD1  | 1:O:196:THR:HB   | 2.00                     | 0.60              |
| 1:Y:196:THR:HG22 | 1:Y:198:ASP:N    | 2.16                     | 0.60              |
| 1:Y:237:ILE:HG23 | 1:Y:238:PRO:HD2  | 1.83                     | 0.60              |
| 1:Y:362:GLY:HA3  | 1:O:367:LEU:HB2  | 1.83                     | 0.60              |
| 1:O:142:LYS:O    | 1:O:143:TRP:C    | 2.44                     | 0.60              |
| 1:O:154:ARG:HA   | 1:O:157:ARG:HG2  | 1.84                     | 0.60              |
| 1:Y:456:ASN:N    | 1:Y:459:GLU:OE2  | 2.35                     | 0.60              |
| 1:O:90:GLU:HB3   | 1:O:93:THR:CG2   | 2.30                     | 0.60              |
| 1:O:353:ALA:HB2  | 1:O:356:TRP:CZ2  | 2.37                     | 0.60              |
| 1:O:88:VAL:HA    | 1:O:161:LEU:O    | 2.02                     | 0.60              |
| 1:Y:188:ARG:HH22 | 1:Y:303:GLU:CD   | 2.10                     | 0.60              |
| 1:Y:432:ARG:NE   | 1:Y:467:GLU:OE2  | 2.34                     | 0.60              |
| 1:Y:463:LYS:HZ1  | 1:Y:465:VAL:HG23 | 1.67                     | 0.60              |
| 1:O:78:GLY:HA2   | 1:O:447:ALA:HB2  | 1.83                     | 0.60              |
| 1:Y:271:MET:HE1  | 1:Y:392:LEU:HA   | 1.84                     | 0.60              |
| 1:Y:396:GLN:O    | 1:Y:397:ALA:C    | 2.45                     | 0.60              |
| 1:Y:154:ARG:HB2  | 1:Y:159:GLU:HB3  | 1.83                     | 0.59              |
| 1:Y:422:GLN:HE21 | 1:Y:426:LEU:HD22 | 1.66                     | 0.59              |
| 1:O:144:ILE:O    | 1:O:145:LEU:C    | 2.44                     | 0.59              |
| 1:O:251:PHE:O    | 1:O:254:LEU:N    | 2.32                     | 0.59              |
| 1:Y:325:ASP:O    | 1:Y:326:ALA:C    | 2.42                     | 0.59              |
| 1:Y:430:VAL:HB   | 1:Y:470:PHE:HB2  | 1.84                     | 0.59              |
| 1:O:69:ILE:HG23  | 1:O:73:GLN:CG    | 2.32                     | 0.59              |
| 1:Y:94:GLY:HA2   | 1:Y:171:TRP:CH2  | 2.38                     | 0.59              |
| 1:Y:246:GLN:HG3  | 1:Y:262:LYS:HZ1  | 1.67                     | 0.59              |
| 1:Y:433:PRO:O    | 1:Y:436:ARG:NH1  | 2.35                     | 0.59              |
| 1:Y:246:GLN:H    | 1:Y:246:GLN:NE2  | 1.99                     | 0.59              |
| 1:O:222:GLU:HG3  | 1:O:223:VAL:N    | 2.17                     | 0.59              |
| 1:Y:101:ILE:HD12 | 1:Y:144:ILE:HD11 | 1.85                     | 0.59              |
| 1:O:179:HIS:NE2  | 1:O:215:PRO:HB3  | 2.17                     | 0.59              |
| 1:O:179:HIS:CG   | 1:O:215:PRO:HB3  | 2.38                     | 0.59              |
| 1:Y:80:THR:HG22  | 1:Y:243:ALA:O    | 2.03                     | 0.59              |
| 1:Y:237:ILE:HG22 | 1:Y:238:PRO:N    | 2.18                     | 0.59              |
| 1:O:103:TRP:HB2  | 1:O:135:TYR:HE1  | 1.67                     | 0.59              |
| 1:O:108:THR:OG1  | 1:O:134:PRO:HB3  | 2.02                     | 0.59              |
| 1:O:147:HIS:ND1  | 1:O:147:HIS:N    | 2.46                     | 0.59              |
| 1:O:170:ILE:HG22 | 1:O:171:TRP:N    | 2.16                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:237:ILE:HG23 | 1:O:238:PRO:HD2  | 1.85                     | 0.59              |
| 1:O:251:PHE:HE1  | 1:O:256:VAL:HG21 | 1.68                     | 0.59              |
| 1:O:61:VAL:HA    | 1:O:64:LEU:CD1   | 2.33                     | 0.59              |
| 1:Y:87:ILE:HG22  | 1:Y:88:VAL:N     | 2.18                     | 0.58              |
| 1:Y:111:ILE:O    | 1:Y:115:LEU:HD12 | 2.03                     | 0.58              |
| 1:Y:480:ASN:O    | 1:Y:481:TYR:C    | 2.44                     | 0.58              |
| 1:O:88:VAL:HG22  | 1:O:162:PHE:HB2  | 1.85                     | 0.58              |
| 1:Y:87:ILE:HD12  | 1:Y:163:GLY:O    | 2.03                     | 0.58              |
| 1:Y:201:ASP:O    | 1:Y:202:LYS:C    | 2.46                     | 0.58              |
| 1:O:422:GLN:HE21 | 1:O:426:LEU:HD22 | 1.67                     | 0.58              |
| 1:O:132:ILE:HA   | 1:O:190:MET:HE1  | 1.86                     | 0.58              |
| 1:O:149:GLU:OE1  | 1:O:149:GLU:HA   | 2.03                     | 0.58              |
| 1:O:387:GLN:O    | 1:O:390:ASP:HB2  | 2.04                     | 0.58              |
| 1:O:410:GLY:O    | 1:O:413:VAL:HG13 | 2.03                     | 0.58              |
| 1:O:475:GLU:O    | 1:O:478:GLU:HB2  | 2.04                     | 0.58              |
| 1:Y:221:SER:OG   | 1:Y:450:ALA:HB2  | 2.03                     | 0.58              |
| 1:Y:435:VAL:HG22 | 1:Y:436:ARG:H    | 1.68                     | 0.58              |
| 1:O:81:ASN:N     | 1:O:81:ASN:ND2   | 2.51                     | 0.58              |
| 1:O:229:ILE:O    | 1:O:230:GLY:C    | 2.46                     | 0.58              |
| 1:O:281:LYS:HB2  | 1:O:281:LYS:NZ   | 2.19                     | 0.58              |
| 1:O:445:TYR:O    | 1:O:447:ALA:N    | 2.37                     | 0.58              |
| 1:Y:63:VAL:O     | 1:Y:64:LEU:C     | 2.46                     | 0.58              |
| 1:O:41:LYS:CB    | 1:O:42:PRO:HD2   | 2.34                     | 0.58              |
| 1:O:153:GLU:O    | 1:O:157:ARG:HG2  | 2.03                     | 0.58              |
| 1:O:401:ILE:HG22 | 1:O:402:ARG:N    | 2.19                     | 0.58              |
| 1:Y:31:SER:H     | 1:Y:63:VAL:HG13  | 1.68                     | 0.58              |
| 1:O:140:LYS:O    | 1:O:143:TRP:HB3  | 2.04                     | 0.58              |
| 1:O:207:LEU:CB   | 1:O:209:ILE:HD12 | 2.34                     | 0.58              |
| 1:O:244:GLY:O    | 1:O:245:ASP:C    | 2.41                     | 0.58              |
| 1:O:389:ARG:HB2  | 1:O:426:LEU:HD13 | 1.84                     | 0.58              |
| 1:O:476:THR:CG2  | 1:O:477:THR:N    | 2.67                     | 0.58              |
| 1:Y:206:VAL:HG12 | 1:Y:207:LEU:N    | 2.19                     | 0.58              |
| 1:Y:310:GLY:HA3  | 3:Y:601:ATF:O3'  | 2.04                     | 0.58              |
| 1:O:5:TYR:CE2    | 1:O:73:GLN:HG3   | 2.38                     | 0.58              |
| 1:O:41:LYS:HG3   | 1:O:42:PRO:HD2   | 1.84                     | 0.58              |
| 1:Y:3:LYS:HA     | 1:Y:73:GLN:HA    | 1.84                     | 0.57              |
| 1:Y:22:ASP:OD1   | 1:Y:24:ASP:N     | 2.36                     | 0.57              |
| 1:Y:67:ALA:HB3   | 1:Y:69:ILE:HG12  | 1.86                     | 0.57              |
| 1:Y:250:LEU:HD12 | 1:Y:250:LEU:C    | 2.28                     | 0.57              |
| 1:Y:497:GLU:HA   | 1:Y:497:GLU:OE1  | 2.03                     | 0.57              |
| 1:O:398:ASP:O    | 1:O:399:SER:C    | 2.44                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:18:ALA:HB1   | 1:Y:63:VAL:HG21  | 1.85                     | 0.57              |
| 1:Y:226:GLN:NE2  | 1:Y:236:ARG:HB3  | 2.19                     | 0.57              |
| 1:O:207:LEU:HB3  | 1:O:209:ILE:HD12 | 1.85                     | 0.57              |
| 1:Y:114:HIS:O    | 1:Y:115:LEU:C    | 2.47                     | 0.57              |
| 1:O:40:PRO:HD2   | 1:O:44:TRP:O     | 2.05                     | 0.57              |
| 1:O:230:GLY:HA2  | 1:O:235:THR:CB   | 2.33                     | 0.57              |
| 1:O:402:ARG:HB3  | 1:O:402:ARG:NH1  | 2.15                     | 0.57              |
| 1:O:44:TRP:HA    | 1:O:105:CYS:SG   | 2.44                     | 0.57              |
| 1:Y:133:ASP:OD1  | 1:Y:135:TYR:HB2  | 2.04                     | 0.57              |
| 1:O:27:ILE:HD11  | 1:O:30:VAL:HG23  | 1.87                     | 0.57              |
| 1:Y:482:ARG:NH1  | 1:Y:482:ARG:HG3  | 2.20                     | 0.57              |
| 1:O:480:ASN:H    | 1:O:480:ASN:HD22 | 1.49                     | 0.57              |
| 1:O:188:ARG:HH22 | 1:O:303:GLU:CD   | 2.12                     | 0.57              |
| 1:O:490:VAL:O    | 1:O:494:MET:HG2  | 2.05                     | 0.57              |
| 1:Y:193:ASN:OD1  | 1:Y:196:THR:HB   | 2.04                     | 0.57              |
| 1:Y:117:ARG:HH11 | 1:Y:117:ARG:CG   | 2.16                     | 0.57              |
| 1:Y:153:GLU:HA   | 1:Y:153:GLU:OE1  | 2.04                     | 0.57              |
| 1:Y:236:ARG:C    | 1:Y:237:ILE:HD13 | 2.29                     | 0.57              |
| 1:O:120:LEU:O    | 1:O:124:ILE:HG12 | 2.05                     | 0.57              |
| 1:O:143:TRP:O    | 1:O:147:HIS:ND1  | 2.38                     | 0.57              |
| 1:O:85:THR:HG23  | 1:O:102:VAL:HA   | 1.86                     | 0.57              |
| 1:Y:190:MET:HG2  | 1:Y:190:MET:O    | 2.05                     | 0.56              |
| 1:Y:483:TYR:O    | 1:Y:486:TRP:HB3  | 2.04                     | 0.56              |
| 1:O:137:SER:O    | 1:O:141:VAL:HG23 | 2.04                     | 0.56              |
| 1:O:153:GLU:O    | 1:O:156:ARG:HB3  | 2.05                     | 0.56              |
| 1:O:348:PHE:HD1  | 1:O:348:PHE:H    | 1.52                     | 0.56              |
| 1:Y:182:ASP:HB3  | 1:Y:242:ILE:HB   | 1.87                     | 0.56              |
| 1:Y:103:TRP:H    | 1:Y:103:TRP:CD1  | 2.21                     | 0.56              |
| 1:Y:129:GLY:C    | 1:Y:130:LEU:HD23 | 2.29                     | 0.56              |
| 1:Y:237:ILE:HD13 | 1:Y:237:ILE:N    | 2.20                     | 0.56              |
| 1:O:173:MET:O    | 1:O:227:THR:HG23 | 2.06                     | 0.56              |
| 1:O:218:ARG:HG3  | 1:O:218:ARG:NH1  | 2.20                     | 0.56              |
| 1:Y:5:TYR:O      | 1:Y:74:ILE:HA    | 2.05                     | 0.56              |
| 1:Y:74:ILE:HD12  | 1:Y:74:ILE:C     | 2.30                     | 0.56              |
| 1:Y:419:MET:HA   | 1:Y:419:MET:CE   | 2.28                     | 0.56              |
| 1:Y:444:ALA:O    | 1:Y:447:ALA:N    | 2.38                     | 0.56              |
| 1:O:17:ARG:HG2   | 1:O:32:GLN:HG3   | 1.88                     | 0.56              |
| 1:O:40:PRO:HG2   | 1:O:44:TRP:HB3   | 1.87                     | 0.56              |
| 1:O:90:GLU:O     | 1:O:94:GLY:N     | 2.38                     | 0.56              |
| 1:O:487:LYS:HA   | 1:O:490:VAL:CG2  | 2.35                     | 0.56              |
| 1:Y:108:THR:OG1  | 1:Y:134:PRO:HB3  | 2.05                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:293:GLY:HA3  | 1:Y:297:GLU:CD   | 2.30                     | 0.56              |
| 1:O:123:TYR:CE2  | 1:O:203:MET:HE2  | 2.41                     | 0.56              |
| 1:O:340:ASN:HD22 | 1:O:371:VAL:HG22 | 1.70                     | 0.56              |
| 1:O:154:ARG:HA   | 1:O:157:ARG:HG3  | 1.87                     | 0.56              |
| 1:Y:250:LEU:HD11 | 1:Y:255:CYS:CB   | 2.27                     | 0.56              |
| 1:O:240:SER:O    | 1:O:447:ALA:HA   | 2.06                     | 0.56              |
| 1:O:254:LEU:CD1  | 1:O:445:TYR:HE2  | 2.14                     | 0.56              |
| 1:O:445:TYR:O    | 1:O:446:LEU:C    | 2.48                     | 0.56              |
| 1:Y:246:GLN:NE2  | 1:Y:246:GLN:N    | 2.54                     | 0.56              |
| 1:O:433:PRO:O    | 1:O:436:ARG:NH1  | 2.38                     | 0.56              |
| 1:O:476:THR:HG22 | 1:O:477:THR:N    | 2.21                     | 0.56              |
| 1:Y:43:GLY:C     | 1:Y:44:TRP:HD1   | 2.14                     | 0.56              |
| 1:Y:359:TYR:HD2  | 1:Y:497:GLU:HB3  | 1.70                     | 0.56              |
| 1:Y:445:TYR:O    | 1:Y:449:LEU:HB2  | 2.05                     | 0.56              |
| 1:O:80:THR:HG21  | 1:O:248:ALA:HB2  | 1.87                     | 0.56              |
| 1:O:154:ARG:CA   | 1:O:157:ARG:HG2  | 2.36                     | 0.56              |
| 1:Y:20:VAL:HG12  | 1:Y:21:MET:N     | 2.20                     | 0.55              |
| 1:Y:395:MET:O    | 1:Y:396:GLN:C    | 2.48                     | 0.55              |
| 1:O:245:ASP:OD1  | 1:O:246:GLN:N    | 2.39                     | 0.55              |
| 1:O:408:VAL:HG23 | 1:O:409:ASP:N    | 2.21                     | 0.55              |
| 1:O:463:LYS:HZ1  | 1:O:465:VAL:CG2  | 2.17                     | 0.55              |
| 1:Y:70:SER:O     | 1:Y:72:ASP:N     | 2.40                     | 0.55              |
| 1:Y:153:GLU:O    | 1:Y:156:ARG:N    | 2.39                     | 0.55              |
| 1:O:114:HIS:O    | 1:O:117:ARG:HB2  | 2.06                     | 0.55              |
| 1:Y:83:ARG:HB2   | 4:Y:600:GOL:O2   | 2.05                     | 0.55              |
| 1:Y:137:SER:O    | 1:Y:138:GLY:C    | 2.49                     | 0.55              |
| 1:Y:492:ARG:HG2  | 1:Y:492:ARG:NH1  | 2.11                     | 0.55              |
| 1:O:55:THR:HA    | 1:O:58:TRP:HD1   | 1.68                     | 0.55              |
| 1:O:64:LEU:HD12  | 1:O:64:LEU:H     | 1.70                     | 0.55              |
| 1:O:115:LEU:H    | 1:O:115:LEU:CD1  | 2.16                     | 0.55              |
| 1:O:219:ARG:HD3  | 1:O:222:GLU:HB2  | 1.88                     | 0.55              |
| 1:O:179:HIS:CD2  | 1:O:215:PRO:HA   | 2.42                     | 0.55              |
| 1:Y:308:MET:HE3  | 1:Y:349:THR:HG23 | 1.87                     | 0.55              |
| 1:Y:389:ARG:O    | 1:Y:390:ASP:C    | 2.48                     | 0.55              |
| 1:Y:463:LYS:NZ   | 1:Y:465:VAL:HG23 | 2.22                     | 0.55              |
| 1:Y:488:LYS:HD2  | 1:O:496:TRP:CH2  | 2.41                     | 0.55              |
| 1:O:63:VAL:O     | 1:O:66:LYS:N     | 2.40                     | 0.55              |
| 1:O:275:THR:HB   | 1:O:278:LYS:O    | 2.07                     | 0.55              |
| 1:O:441:LEU:HD23 | 1:O:445:TYR:HE1  | 1.71                     | 0.55              |
| 1:Y:40:PRO:HG3   | 1:Y:46:GLU:CD    | 2.32                     | 0.55              |
| 1:Y:150:GLY:O    | 1:Y:153:GLU:N    | 2.39                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:272:LEU:HD21 | 1:Y:303:GLU:OE1  | 2.07                     | 0.55              |
| 1:O:103:TRP:HB2  | 1:O:135:TYR:CE1  | 2.41                     | 0.55              |
| 1:Y:420:GLN:O    | 1:Y:420:GLN:NE2  | 2.39                     | 0.55              |
| 1:O:482:ARG:NH1  | 1:O:482:ARG:HG3  | 2.21                     | 0.55              |
| 1:Y:308:MET:HB2  | 1:Y:346:PRO:HB2  | 1.88                     | 0.55              |
| 1:Y:405:ALA:HB2  | 1:Y:429:ARG:HD2  | 1.88                     | 0.55              |
| 1:O:14:THR:O     | 1:O:34:GLU:HG2   | 2.07                     | 0.55              |
| 1:O:35:PHE:HB2   | 1:O:51:GLU:CD    | 2.32                     | 0.55              |
| 1:O:180:VAL:CG2  | 1:O:218:ARG:HG2  | 2.37                     | 0.55              |
| 1:O:340:ASN:HB2  | 1:O:375:HIS:CD2  | 2.40                     | 0.55              |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CE1  | 2.41                     | 0.54              |
| 1:Y:282:SER:HA   | 1:Y:398:ASP:OD2  | 2.06                     | 0.54              |
| 1:Y:325:ASP:HB3  | 1:Y:327:TYR:CB   | 2.29                     | 0.54              |
| 1:O:206:VAL:HG12 | 1:O:207:LEU:HD23 | 1.89                     | 0.54              |
| 1:Y:80:THR:HG21  | 1:Y:248:ALA:HB3  | 1.89                     | 0.54              |
| 1:Y:219:ARG:HG2  | 1:Y:222:GLU:HB3  | 1.89                     | 0.54              |
| 1:Y:393:GLU:O    | 1:Y:394:ALA:C    | 2.50                     | 0.54              |
| 1:O:41:LYS:HG3   | 1:O:42:PRO:CD    | 2.38                     | 0.54              |
| 1:O:129:GLY:C    | 1:O:130:LEU:HD23 | 2.32                     | 0.54              |
| 1:O:418:LEU:O    | 1:O:419:MET:C    | 2.50                     | 0.54              |
| 1:Y:271:MET:HE1  | 1:Y:392:LEU:CB   | 2.36                     | 0.54              |
| 1:O:3:LYS:HG2    | 1:O:72:ASP:O     | 2.07                     | 0.54              |
| 1:O:6:ILE:HG13   | 1:O:7:VAL:H      | 1.71                     | 0.54              |
| 1:O:473:GLY:O    | 1:O:474:ILE:HD13 | 2.08                     | 0.54              |
| 1:O:164:THR:H    | 1:O:167:THR:HB   | 1.72                     | 0.54              |
| 1:O:201:ASP:O    | 1:O:202:LYS:C    | 2.48                     | 0.54              |
| 1:O:219:ARG:NH2  | 1:O:295:THR:OG1  | 2.40                     | 0.54              |
| 1:O:424:ASP:OD1  | 1:O:473:GLY:N    | 2.36                     | 0.54              |
| 1:O:4:LYS:N      | 1:O:73:GLN:O     | 2.40                     | 0.54              |
| 1:Y:156:ARG:C    | 1:Y:158:GLY:H    | 2.15                     | 0.54              |
| 1:O:166:ASP:CG   | 1:O:167:THR:H    | 2.14                     | 0.54              |
| 1:Y:20:VAL:O     | 1:Y:28:ILE:N     | 2.30                     | 0.54              |
| 1:Y:120:LEU:O    | 1:Y:124:ILE:HG12 | 2.06                     | 0.54              |
| 1:Y:251:PHE:CE2  | 1:Y:446:LEU:HD22 | 2.43                     | 0.54              |
| 1:O:166:ASP:OD1  | 1:O:166:ASP:N    | 2.38                     | 0.54              |
| 1:Y:113:GLU:O    | 1:Y:116:LYS:HB2  | 2.08                     | 0.54              |
| 1:Y:227:THR:N    | 1:Y:237:ILE:O    | 2.29                     | 0.54              |
| 1:O:3:LYS:HA     | 1:O:73:GLN:C     | 2.32                     | 0.54              |
| 1:O:80:THR:CG2   | 1:O:248:ALA:HB2  | 2.38                     | 0.54              |
| 1:O:154:ARG:O    | 1:O:155:ALA:C    | 2.51                     | 0.54              |
| 1:O:180:VAL:HG21 | 1:O:218:ARG:HG3  | 1.90                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:31:SER:N     | 1:Y:63:VAL:HG13  | 2.23                     | 0.54              |
| 1:Y:253:GLN:CD   | 1:Y:407:ARG:HD2  | 2.33                     | 0.54              |
| 1:O:111:ILE:O    | 1:O:112:CYS:C    | 2.51                     | 0.54              |
| 1:O:415:ASN:C    | 1:O:415:ASN:HD22 | 2.15                     | 0.54              |
| 1:O:468:ARG:HG3  | 1:O:468:ARG:HH11 | 1.73                     | 0.54              |
| 1:Y:132:ILE:HA   | 1:Y:190:MET:HE1  | 1.91                     | 0.53              |
| 1:Y:221:SER:HB3  | 1:Y:446:LEU:CD1  | 2.36                     | 0.53              |
| 1:Y:271:MET:HE1  | 1:Y:392:LEU:CA   | 2.37                     | 0.53              |
| 1:O:90:GLU:OE1   | 1:O:95:LYS:NZ    | 2.38                     | 0.53              |
| 1:O:193:ASN:HB3  | 1:O:196:THR:CB   | 2.38                     | 0.53              |
| 1:O:422:GLN:NE2  | 1:O:426:LEU:HD22 | 2.23                     | 0.53              |
| 1:Y:18:ALA:HB1   | 1:Y:63:VAL:CG2   | 2.38                     | 0.53              |
| 1:Y:117:ARG:HH11 | 1:Y:117:ARG:CA   | 2.21                     | 0.53              |
| 1:O:402:ARG:HH12 | 1:O:403:LEU:C    | 2.15                     | 0.53              |
| 1:Y:40:PRO:HG3   | 1:Y:46:GLU:OE2   | 2.09                     | 0.53              |
| 1:Y:445:TYR:O    | 1:Y:446:LEU:C    | 2.49                     | 0.53              |
| 1:Y:468:ARG:HH11 | 1:Y:468:ARG:CG   | 2.21                     | 0.53              |
| 1:O:20:VAL:HG23  | 1:O:63:VAL:HG11  | 1.90                     | 0.53              |
| 1:O:40:PRO:HD2   | 1:O:44:TRP:HB2   | 1.91                     | 0.53              |
| 1:Y:31:SER:CB    | 1:Y:62:GLU:HB3   | 2.39                     | 0.53              |
| 1:Y:174:THR:C    | 1:Y:176:GLY:H    | 2.16                     | 0.53              |
| 1:Y:360:ALA:HB2  | 1:Y:494:MET:HA   | 1.91                     | 0.53              |
| 1:O:61:VAL:O     | 1:O:62:GLU:C     | 2.52                     | 0.53              |
| 1:O:118:ASP:N    | 1:O:118:ASP:OD1  | 2.40                     | 0.53              |
| 1:Y:74:ILE:CD1   | 1:Y:237:ILE:HG21 | 2.39                     | 0.53              |
| 1:Y:272:LEU:HD12 | 1:Y:272:LEU:N    | 2.24                     | 0.53              |
| 1:O:103:TRP:CD1  | 1:O:103:TRP:H    | 2.27                     | 0.53              |
| 1:O:415:ASN:HD22 | 1:O:418:LEU:H    | 1.50                     | 0.53              |
| 1:O:17:ARG:C     | 1:O:59:THR:HG21  | 2.34                     | 0.53              |
| 1:O:71:SER:O     | 1:O:237:ILE:HD11 | 2.09                     | 0.53              |
| 1:O:440:ALA:O    | 1:O:441:LEU:C    | 2.51                     | 0.53              |
| 1:O:451:VAL:O    | 1:O:451:VAL:HG13 | 2.09                     | 0.53              |
| 1:Y:473:GLY:O    | 1:Y:474:ILE:HD13 | 2.09                     | 0.53              |
| 1:O:457:LEU:C    | 1:O:459:GLU:H    | 2.17                     | 0.53              |
| 1:Y:481:TYR:O    | 1:Y:484:ALA:HB3  | 2.09                     | 0.53              |
| 1:O:156:ARG:C    | 1:O:158:GLY:H    | 2.17                     | 0.53              |
| 1:O:419:MET:HE2  | 1:O:419:MET:CA   | 2.32                     | 0.53              |
| 1:Y:91:LYS:O     | 1:Y:92:GLU:C     | 2.51                     | 0.53              |
| 1:Y:153:GLU:O    | 1:Y:154:ARG:C    | 2.49                     | 0.53              |
| 1:O:192:PHE:CE2  | 1:O:217:VAL:HG11 | 2.44                     | 0.53              |
| 1:O:249:ALA:HB2  | 1:O:439:THR:OG1  | 2.09                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:346:PRO:HA   | 1:O:348:PHE:CE1  | 2.44                     | 0.53              |
| 1:Y:3:LYS:HA     | 1:Y:73:GLN:C     | 2.33                     | 0.52              |
| 1:O:180:VAL:HG21 | 1:O:218:ARG:CG   | 2.39                     | 0.52              |
| 1:Y:61:VAL:O     | 1:Y:63:VAL:N     | 2.43                     | 0.52              |
| 1:Y:205:GLU:O    | 1:Y:206:VAL:C    | 2.50                     | 0.52              |
| 1:Y:387:GLN:O    | 1:Y:391:VAL:HG12 | 2.09                     | 0.52              |
| 1:Y:463:LYS:HA   | 1:Y:463:LYS:NZ   | 2.25                     | 0.52              |
| 1:O:21:MET:HB3   | 1:O:26:ASN:O     | 2.09                     | 0.52              |
| 1:O:60:LEU:C     | 1:O:60:LEU:HD12  | 2.33                     | 0.52              |
| 1:O:186:ALA:C    | 1:O:188:ARG:H    | 2.17                     | 0.52              |
| 1:O:488:LYS:O    | 1:O:492:ARG:HD2  | 2.09                     | 0.52              |
| 1:Y:152:ARG:O    | 1:Y:153:GLU:C    | 2.53                     | 0.52              |
| 1:O:35:PHE:HB2   | 1:O:51:GLU:HG3   | 1.91                     | 0.52              |
| 1:O:123:TYR:HD2  | 1:O:203:MET:CE   | 2.23                     | 0.52              |
| 1:O:330:GLU:O    | 1:O:334:THR:HG23 | 2.10                     | 0.52              |
| 1:O:108:THR:HG21 | 1:O:140:LYS:N    | 2.25                     | 0.52              |
| 1:O:181:THR:HG23 | 1:O:182:ASP:N    | 2.25                     | 0.52              |
| 1:Y:364:ILE:O    | 1:O:363:ALA:HB1  | 2.09                     | 0.52              |
| 1:O:141:VAL:O    | 1:O:142:LYS:C    | 2.53                     | 0.52              |
| 1:Y:8:ALA:O      | 1:Y:9:LEU:HD12   | 2.09                     | 0.52              |
| 1:Y:80:THR:CG2   | 1:Y:248:ALA:HB2  | 2.39                     | 0.52              |
| 1:Y:18:ALA:CB    | 1:Y:59:THR:HB    | 2.40                     | 0.52              |
| 1:O:33:ARG:NH1   | 1:O:62:GLU:OE1   | 2.43                     | 0.52              |
| 1:Y:143:TRP:CD2  | 1:Y:147:HIS:HD2  | 2.27                     | 0.52              |
| 1:Y:144:ILE:O    | 1:Y:145:LEU:C    | 2.52                     | 0.52              |
| 1:Y:177:ARG:NH1  | 1:Y:226:GLN:O    | 2.43                     | 0.52              |
| 1:Y:477:THR:O    | 1:Y:478:GLU:C    | 2.52                     | 0.52              |
| 1:O:39:TYR:HA    | 1:O:44:TRP:O     | 2.10                     | 0.52              |
| 1:O:420:GLN:HE21 | 1:O:424:ASP:CG   | 2.18                     | 0.52              |
| 1:O:97:ILE:O     | 1:O:98:TYR:HB2   | 2.08                     | 0.52              |
| 1:O:445:TYR:O    | 1:O:448:GLY:N    | 2.43                     | 0.52              |
| 1:Y:246:GLN:HG2  | 1:Y:270:PHE:CB   | 2.40                     | 0.51              |
| 1:Y:44:TRP:CE2   | 1:Y:107:ARG:HB2  | 2.45                     | 0.51              |
| 1:Y:240:SER:HB2  | 1:Y:450:ALA:HB3  | 1.92                     | 0.51              |
| 1:O:193:ASN:CG   | 1:O:196:THR:HB   | 2.35                     | 0.51              |
| 1:O:237:ILE:CG2  | 1:O:238:PRO:HD2  | 2.40                     | 0.51              |
| 1:O:351:LEU:HD22 | 1:O:360:ALA:HB2  | 1.92                     | 0.51              |
| 1:Y:480:ASN:H    | 1:Y:480:ASN:HD22 | 1.57                     | 0.51              |
| 1:Y:59:THR:O     | 1:Y:63:VAL:HG22  | 2.10                     | 0.51              |
| 1:Y:49:PRO:HA    | 1:Y:52:ILE:HD13  | 1.93                     | 0.51              |
| 1:Y:78:GLY:HA2   | 1:Y:447:ALA:HB2  | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:401:ILE:HG22 | 1:Y:402:ARG:N    | 2.24                     | 0.51              |
| 1:O:173:MET:HB3  | 1:O:227:THR:HG21 | 1.93                     | 0.51              |
| 1:Y:142:LYS:O    | 1:Y:145:LEU:N    | 2.44                     | 0.51              |
| 1:Y:143:TRP:CE2  | 1:Y:147:HIS:CD2  | 2.99                     | 0.51              |
| 1:O:154:ARG:CA   | 1:O:159:GLU:HB3  | 2.41                     | 0.51              |
| 1:Y:26:ASN:O     | 1:Y:28:ILE:HD13  | 2.10                     | 0.51              |
| 1:O:125:ARG:HG2  | 1:O:130:LEU:O    | 2.11                     | 0.51              |
| 1:O:183:TYR:O    | 1:O:187:SER:HB3  | 2.11                     | 0.51              |
| 1:O:278:LYS:HG2  | 1:O:279:ALA:N    | 2.25                     | 0.51              |
| 1:O:286:LEU:O    | 1:O:287:LEU:HD23 | 2.11                     | 0.51              |
| 1:O:273:MET:HB3  | 1:O:395:MET:HE3  | 1.89                     | 0.51              |
| 1:O:281:LYS:HB2  | 1:O:281:LYS:HZ2  | 1.75                     | 0.51              |
| 1:O:406:LEU:HD23 | 1:O:407:ARG:N    | 2.25                     | 0.51              |
| 1:O:476:THR:O    | 1:O:477:THR:O    | 2.28                     | 0.51              |
| 1:Y:56:GLN:HG3   | 1:Y:56:GLN:O     | 2.11                     | 0.51              |
| 1:Y:75:ALA:O     | 1:Y:238:PRO:HD2  | 2.11                     | 0.51              |
| 1:Y:185:ASN:ND2  | 1:Y:244:GLY:N    | 2.55                     | 0.51              |
| 1:O:53:TRP:HE3   | 1:O:169:LEU:CD1  | 2.24                     | 0.51              |
| 1:O:220:SER:O    | 1:O:224:TYR:OH   | 2.29                     | 0.51              |
| 1:O:251:PHE:CZ   | 1:O:446:LEU:HD13 | 2.46                     | 0.51              |
| 1:O:346:PRO:HA   | 1:O:348:PHE:HE1  | 1.75                     | 0.51              |
| 1:Y:71:SER:HB2   | 1:Y:235:THR:CG2  | 2.40                     | 0.50              |
| 1:Y:124:ILE:CG2  | 1:Y:190:MET:HE2  | 2.32                     | 0.50              |
| 1:O:352:GLY:O    | 1:O:356:TRP:N    | 2.34                     | 0.50              |
| 1:Y:117:ARG:HH11 | 1:Y:117:ARG:HB2  | 1.77                     | 0.50              |
| 1:Y:466:ILE:O    | 1:Y:466:ILE:HG22 | 2.11                     | 0.50              |
| 1:O:158:GLY:CA   | 1:O:212:GLU:HB3  | 2.39                     | 0.50              |
| 1:O:395:MET:O    | 1:O:399:SER:N    | 2.44                     | 0.50              |
| 1:Y:150:GLY:O    | 1:Y:151:SER:C    | 2.54                     | 0.50              |
| 1:O:196:THR:HG22 | 1:O:198:ASP:H    | 1.77                     | 0.50              |
| 1:Y:314:GLN:O    | 1:Y:318:ASP:N    | 2.35                     | 0.50              |
| 1:O:228:ASN:HB2  | 1:O:236:ARG:NE   | 2.26                     | 0.50              |
| 1:O:477:THR:O    | 1:O:480:ASN:N    | 2.44                     | 0.50              |
| 1:Y:47:HIS:CD2   | 1:Y:82:GLN:HE22  | 2.30                     | 0.50              |
| 1:O:144:ILE:CG2  | 1:O:148:VAL:HG21 | 2.41                     | 0.50              |
| 1:O:174:THR:HB   | 1:O:177:ARG:HB2  | 1.93                     | 0.50              |
| 1:O:317:ARG:HB2  | 1:O:323:ILE:HG13 | 1.94                     | 0.50              |
| 1:O:408:VAL:O    | 1:O:409:ASP:HB3  | 2.11                     | 0.50              |
| 1:Y:111:ILE:O    | 1:Y:112:CYS:C    | 2.51                     | 0.50              |
| 1:Y:391:VAL:O    | 1:Y:392:LEU:C    | 2.55                     | 0.50              |
| 1:O:113:GLU:O    | 1:O:114:HIS:O    | 2.30                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:15:SER:CB    | 1:O:34:GLU:HA    | 2.41                     | 0.50              |
| 1:O:28:ILE:HG22  | 1:O:29:SER:N     | 2.27                     | 0.50              |
| 1:Y:94:GLY:CA    | 1:Y:171:TRP:HH2  | 2.25                     | 0.50              |
| 1:O:444:ALA:O    | 1:O:445:TYR:O    | 2.29                     | 0.50              |
| 1:O:90:GLU:CD    | 1:O:93:THR:HG21  | 2.37                     | 0.49              |
| 1:O:218:ARG:CG   | 1:O:218:ARG:HH11 | 2.25                     | 0.49              |
| 1:O:342:VAL:HA   | 1:O:365:PHE:O    | 2.12                     | 0.49              |
| 1:O:463:LYS:HZ3  | 1:O:465:VAL:HG23 | 1.77                     | 0.49              |
| 1:Y:197:LEU:N    | 1:Y:197:LEU:HD22 | 2.27                     | 0.49              |
| 1:O:216:GLU:OE2  | 1:O:218:ARG:HD3  | 2.11                     | 0.49              |
| 1:O:303:GLU:HG3  | 1:O:304:GLY:N    | 2.28                     | 0.49              |
| 1:Y:33:ARG:NH2   | 1:Y:58:TRP:HB3   | 2.27                     | 0.49              |
| 1:Y:273:MET:HB3  | 1:Y:395:MET:HE3  | 1.93                     | 0.49              |
| 1:Y:89:TRP:HD1   | 1:Y:90:GLU:O     | 1.95                     | 0.49              |
| 1:Y:242:ILE:HG22 | 1:Y:243:ALA:N    | 2.26                     | 0.49              |
| 1:O:168:TRP:O    | 1:O:169:LEU:C    | 2.54                     | 0.49              |
| 1:O:431:GLU:HB3  | 1:O:466:ILE:HG13 | 1.93                     | 0.49              |
| 1:O:438:VAL:HA   | 1:O:441:LEU:HD12 | 1.93                     | 0.49              |
| 1:O:44:TRP:N     | 1:O:44:TRP:CD1   | 2.80                     | 0.49              |
| 1:O:103:TRP:CD1  | 1:O:103:TRP:N    | 2.80                     | 0.49              |
| 1:O:108:THR:HG21 | 1:O:139:THR:C    | 2.37                     | 0.49              |
| 1:O:284:ASN:OD1  | 1:O:398:ASP:OD1  | 2.30                     | 0.49              |
| 1:Y:71:SER:HB3   | 1:Y:229:ILE:HG13 | 1.95                     | 0.49              |
| 1:Y:389:ARG:HB2  | 1:Y:426:LEU:CD1  | 2.42                     | 0.49              |
| 1:O:196:THR:HG22 | 1:O:198:ASP:N    | 2.28                     | 0.49              |
| 1:O:324:ASN:ND2  | 1:O:324:ASN:N    | 2.61                     | 0.49              |
| 1:O:478:GLU:O    | 1:O:482:ARG:HG2  | 2.12                     | 0.49              |
| 1:Y:80:THR:HG21  | 1:Y:248:ALA:HB2  | 1.94                     | 0.49              |
| 1:O:50:MET:O     | 1:O:53:TRP:HB3   | 2.12                     | 0.49              |
| 1:O:413:VAL:HA   | 1:O:419:MET:SD   | 2.53                     | 0.49              |
| 1:Y:237:ILE:CG2  | 1:Y:238:PRO:HD2  | 2.42                     | 0.49              |
| 1:O:80:THR:HG21  | 1:O:245:ASP:HA   | 1.94                     | 0.49              |
| 1:O:89:TRP:HB2   | 1:O:95:LYS:O     | 2.12                     | 0.49              |
| 1:O:115:LEU:O    | 1:O:116:LYS:C    | 2.56                     | 0.49              |
| 1:O:137:SER:HA   | 1:O:140:LYS:HB2  | 1.94                     | 0.49              |
| 1:O:389:ARG:O    | 1:O:393:GLU:HG2  | 2.11                     | 0.49              |
| 1:Y:142:LYS:O    | 1:Y:143:TRP:C    | 2.55                     | 0.49              |
| 1:Y:262:LYS:HZ1  | 1:Y:264:THR:HB   | 1.77                     | 0.49              |
| 1:O:182:ASP:OD2  | 1:O:184:THR:OG1  | 2.29                     | 0.49              |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:HA2  | 1.77                     | 0.49              |
| 1:O:415:ASN:ND2  | 1:O:418:LEU:HB2  | 2.28                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:221:SER:HB2  | 1:Y:450:ALA:HB2  | 1.93                     | 0.49              |
| 1:Y:249:ALA:HB2  | 1:Y:439:THR:OG1  | 2.13                     | 0.49              |
| 1:Y:339:THR:O    | 1:Y:339:THR:OG1  | 2.31                     | 0.49              |
| 1:Y:415:ASN:O    | 1:Y:419:MET:HG2  | 2.13                     | 0.49              |
| 1:O:143:TRP:HE3  | 1:O:144:ILE:HA   | 1.75                     | 0.49              |
| 1:O:448:GLY:O    | 1:O:451:VAL:HG12 | 2.13                     | 0.49              |
| 1:O:162:PHE:O    | 1:O:179:HIS:HE1  | 1.96                     | 0.48              |
| 1:O:272:LEU:HG   | 1:O:303:GLU:HB2  | 1.94                     | 0.48              |
| 1:O:348:PHE:CD1  | 1:O:348:PHE:N    | 2.78                     | 0.48              |
| 1:Y:143:TRP:CD2  | 1:Y:147:HIS:CD2  | 3.01                     | 0.48              |
| 1:Y:166:ASP:O    | 1:Y:167:THR:C    | 2.56                     | 0.48              |
| 1:Y:221:SER:HB2  | 1:Y:446:LEU:O    | 2.13                     | 0.48              |
| 1:Y:392:LEU:HD23 | 1:Y:393:GLU:HG2  | 1.94                     | 0.48              |
| 1:O:154:ARG:HA   | 1:O:159:GLU:HB3  | 1.95                     | 0.48              |
| 1:O:173:MET:HB3  | 1:O:227:THR:CG2  | 2.43                     | 0.48              |
| 1:O:132:ILE:O    | 1:O:133:ASP:HB2  | 2.13                     | 0.48              |
| 1:O:199:TRP:CZ2  | 1:O:215:PRO:HD2  | 2.48                     | 0.48              |
| 1:Y:18:ALA:HB2   | 1:Y:59:THR:HB    | 1.95                     | 0.48              |
| 1:Y:185:ASN:HD21 | 1:Y:244:GLY:CA   | 2.25                     | 0.48              |
| 1:Y:383:SER:O    | 1:Y:384:ILE:C    | 2.52                     | 0.48              |
| 1:O:137:SER:O    | 1:O:138:GLY:O    | 2.29                     | 0.48              |
| 1:O:144:ILE:HG22 | 1:O:148:VAL:CG2  | 2.43                     | 0.48              |
| 1:O:229:ILE:HG23 | 1:O:235:THR:O    | 2.13                     | 0.48              |
| 1:O:460:LEU:C    | 1:O:462:GLU:H    | 2.19                     | 0.48              |
| 1:Y:167:THR:HG21 | 1:Y:215:PRO:HG3  | 1.94                     | 0.48              |
| 1:Y:245:ASP:O    | 1:Y:249:ALA:N    | 2.41                     | 0.48              |
| 1:O:444:ALA:O    | 1:O:445:TYR:C    | 2.53                     | 0.48              |
| 1:Y:172:LYS:HD2  | 1:Y:172:LYS:HA   | 1.58                     | 0.48              |
| 1:Y:328:ASP:HB3  | 1:Y:332:PHE:HE2  | 1.79                     | 0.48              |
| 1:O:75:ALA:CB    | 1:O:453:PHE:HD2  | 2.26                     | 0.48              |
| 1:O:172:LYS:HD2  | 1:O:172:LYS:HA   | 1.45                     | 0.48              |
| 1:Y:184:THR:HA   | 1:Y:290:ILE:HG22 | 1.94                     | 0.48              |
| 1:O:441:LEU:HD23 | 1:O:445:TYR:CE1  | 2.48                     | 0.48              |
| 1:Y:170:ILE:O    | 1:Y:171:TRP:C    | 2.55                     | 0.48              |
| 1:Y:193:ASN:OD1  | 1:Y:195:HIS:N    | 2.44                     | 0.48              |
| 1:O:151:SER:O    | 1:O:154:ARG:HG3  | 2.13                     | 0.48              |
| 1:O:161:LEU:CD2  | 1:O:162:PHE:H    | 2.27                     | 0.48              |
| 1:O:184:THR:CA   | 1:O:290:ILE:HG22 | 2.43                     | 0.48              |
| 1:O:293:GLY:HA2  | 1:O:299:ASN:HD22 | 1.78                     | 0.48              |
| 1:Y:154:ARG:CA   | 1:Y:159:GLU:HB3  | 2.44                     | 0.48              |
| 1:Y:246:GLN:CG   | 1:Y:270:PHE:HB2  | 2.41                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:24:ASP:O     | 1:O:25:ALA:HB3   | 2.14                     | 0.48              |
| 1:O:193:ASN:HB3  | 1:O:196:THR:HB   | 1.95                     | 0.48              |
| 1:O:241:GLY:HA3  | 1:O:447:ALA:HB2  | 1.96                     | 0.48              |
| 1:O:406:LEU:HD23 | 1:O:407:ARG:H    | 1.79                     | 0.48              |
| 1:O:462:GLU:O    | 1:O:465:VAL:HG22 | 2.14                     | 0.48              |
| 1:Y:3:LYS:HA     | 1:Y:73:GLN:CA    | 2.43                     | 0.48              |
| 1:O:5:TYR:CB     | 1:O:74:ILE:HG22  | 2.35                     | 0.48              |
| 1:O:191:LEU:O    | 1:O:199:TRP:HE3  | 1.97                     | 0.48              |
| 1:O:419:MET:HA   | 1:O:419:MET:CE   | 2.35                     | 0.48              |
| 1:Y:326:ALA:O    | 1:Y:327:TYR:C    | 2.57                     | 0.47              |
| 1:O:408:VAL:HG23 | 1:O:413:VAL:HG11 | 1.95                     | 0.47              |
| 1:Y:33:ARG:CZ    | 1:Y:58:TRP:HB3   | 2.44                     | 0.47              |
| 1:Y:124:ILE:O    | 1:Y:128:THR:OG1  | 2.29                     | 0.47              |
| 1:O:437:GLU:N    | 1:O:437:GLU:OE1  | 2.48                     | 0.47              |
| 1:O:449:LEU:HD12 | 1:O:449:LEU:HA   | 1.72                     | 0.47              |
| 1:Y:169:LEU:O    | 1:Y:173:MET:HG2  | 2.14                     | 0.47              |
| 1:Y:425:ILE:HA   | 1:Y:479:ARG:HG2  | 1.96                     | 0.47              |
| 1:Y:468:ARG:HD2  | 1:Y:468:ARG:C    | 2.37                     | 0.47              |
| 1:Y:32:GLN:HA    | 1:Y:59:THR:CG2   | 2.45                     | 0.47              |
| 1:O:199:TRP:HZ2  | 1:O:215:PRO:HD2  | 1.79                     | 0.47              |
| 1:O:278:LYS:HD3  | 1:O:279:ALA:C    | 2.40                     | 0.47              |
| 1:O:466:ILE:O    | 1:O:466:ILE:HG22 | 2.08                     | 0.47              |
| 1:Y:207:LEU:CB   | 1:Y:209:ILE:HD12 | 2.44                     | 0.47              |
| 1:O:359:TYR:CD2  | 1:O:359:TYR:N    | 2.79                     | 0.47              |
| 1:O:405:ALA:HB2  | 1:O:429:ARG:HD2  | 1.96                     | 0.47              |
| 1:O:468:ARG:HG3  | 1:O:468:ARG:NH1  | 2.28                     | 0.47              |
| 1:Y:37:GLN:OE1   | 1:Y:47:HIS:HE1   | 1.97                     | 0.47              |
| 1:O:41:LYS:HG3   | 1:O:42:PRO:N     | 2.28                     | 0.47              |
| 1:O:102:VAL:O    | 1:O:103:TRP:C    | 2.57                     | 0.47              |
| 1:O:482:ARG:O    | 1:O:483:TYR:C    | 2.58                     | 0.47              |
| 1:Y:264:THR:HG23 | 1:Y:265:TYR:N    | 2.28                     | 0.47              |
| 1:Y:313:ILE:CD1  | 1:Y:380:THR:HG22 | 2.44                     | 0.47              |
| 1:Y:336:VAL:HG11 | 1:Y:375:HIS:CD2  | 2.49                     | 0.47              |
| 1:Y:429:ARG:HA   | 1:Y:470:PHE:O    | 2.15                     | 0.47              |
| 1:O:5:TYR:O      | 1:O:74:ILE:HA    | 2.14                     | 0.47              |
| 1:O:137:SER:CA   | 1:O:140:LYS:HD2  | 2.32                     | 0.47              |
| 1:O:240:SER:C    | 1:O:447:ALA:HA   | 2.40                     | 0.47              |
| 1:O:250:LEU:HD11 | 1:O:255:CYS:CB   | 2.42                     | 0.47              |
| 1:O:287:LEU:HD23 | 1:O:287:LEU:N    | 2.28                     | 0.47              |
| 1:O:354:PRO:O    | 1:O:356:TRP:HD1  | 1.97                     | 0.47              |
| 1:O:381:LEU:O    | 1:O:382:GLU:C    | 2.55                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:382:GLU:O    | 1:O:383:SER:C    | 2.55                     | 0.47              |
| 1:Y:222:GLU:HG2  | 1:Y:224:TYR:CE1  | 2.49                     | 0.47              |
| 1:O:94:GLY:HA2   | 1:O:171:TRP:CH2  | 2.49                     | 0.47              |
| 1:O:281:LYS:O    | 1:O:281:LYS:HG3  | 2.15                     | 0.47              |
| 1:Y:21:MET:HB3   | 1:Y:26:ASN:O     | 2.14                     | 0.47              |
| 1:Y:104:GLN:NE2  | 1:Y:308:MET:HE1  | 2.30                     | 0.47              |
| 1:Y:254:LEU:C    | 1:Y:256:VAL:H    | 2.23                     | 0.47              |
| 1:Y:375:HIS:O    | 1:Y:376:ILE:C    | 2.56                     | 0.47              |
| 1:O:105:CYS:SG   | 1:O:107:ARG:NH1  | 2.87                     | 0.47              |
| 1:O:123:TYR:CD2  | 1:O:203:MET:CE   | 2.98                     | 0.47              |
| 1:O:482:ARG:HH11 | 1:O:482:ARG:CG   | 2.27                     | 0.47              |
| 1:Y:13:THR:N     | 3:Y:601:ATF:O2G  | 2.39                     | 0.47              |
| 1:Y:48:ASP:O     | 1:Y:52:ILE:N     | 2.44                     | 0.47              |
| 3:Y:601:ATF:O3G  | 3:Y:601:ATF:O2B  | 2.33                     | 0.47              |
| 1:O:20:VAL:HG21  | 1:O:63:VAL:HG11  | 1.96                     | 0.47              |
| 1:O:340:ASN:ND2  | 1:O:371:VAL:CG2  | 2.77                     | 0.47              |
| 1:Y:151:SER:O    | 1:Y:152:ARG:C    | 2.55                     | 0.46              |
| 1:Y:253:GLN:HE22 | 1:Y:409:ASP:HB3  | 1.80                     | 0.46              |
| 1:Y:454:TRP:CD1  | 1:Y:460:LEU:HD11 | 2.50                     | 0.46              |
| 1:O:272:LEU:HD12 | 1:O:272:LEU:N    | 2.30                     | 0.46              |
| 1:O:386:TYR:HB3  | 1:O:486:TRP:CD2  | 2.49                     | 0.46              |
| 1:O:156:ARG:NH1  | 1:O:156:ARG:CB   | 2.79                     | 0.46              |
| 1:O:197:LEU:N    | 1:O:197:LEU:HD13 | 2.30                     | 0.46              |
| 1:O:197:LEU:HD13 | 1:O:197:LEU:H    | 1.80                     | 0.46              |
| 1:O:218:ARG:HG3  | 1:O:218:ARG:HH11 | 1.81                     | 0.46              |
| 1:Y:41:LYS:HG3   | 1:Y:42:PRO:HD2   | 1.97                     | 0.46              |
| 1:Y:44:TRP:CD1   | 1:Y:44:TRP:N     | 2.80                     | 0.46              |
| 1:Y:434:GLU:CB   | 1:Y:465:VAL:HB   | 2.41                     | 0.46              |
| 1:O:124:ILE:HG12 | 1:O:124:ILE:H    | 1.37                     | 0.46              |
| 1:O:161:LEU:HD23 | 1:O:162:PHE:H    | 1.80                     | 0.46              |
| 1:O:263:ASN:HB2  | 1:O:271:MET:HG3  | 1.96                     | 0.46              |
| 1:Y:16:SER:HB3   | 1:Y:56:GLN:HA    | 1.98                     | 0.46              |
| 1:Y:47:HIS:CB    | 1:Y:52:ILE:HD11  | 2.45                     | 0.46              |
| 1:Y:74:ILE:HD11  | 1:Y:237:ILE:CG1  | 2.15                     | 0.46              |
| 1:Y:115:LEU:HD21 | 1:Y:207:LEU:HD21 | 1.97                     | 0.46              |
| 1:O:21:MET:HE1   | 1:O:444:ALA:CB   | 2.45                     | 0.46              |
| 1:O:183:TYR:CD2  | 1:O:298:VAL:CG2  | 2.98                     | 0.46              |
| 1:O:416:ASN:O    | 1:O:417:PHE:C    | 2.59                     | 0.46              |
| 1:Y:87:ILE:HD13  | 1:Y:168:TRP:HB2  | 1.98                     | 0.46              |
| 1:Y:293:GLY:N    | 1:Y:297:GLU:O    | 2.36                     | 0.46              |
| 1:O:403:LEU:N    | 1:O:403:LEU:CD1  | 2.79                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:151:SER:O    | 1:Y:155:ALA:N    | 2.37                     | 0.46              |
| 1:Y:458:ASP:HA   | 1:Y:461:GLN:CB   | 2.44                     | 0.46              |
| 1:O:144:ILE:HD12 | 1:O:144:ILE:N    | 2.27                     | 0.46              |
| 1:Y:104:GLN:NE2  | 1:Y:308:MET:CE   | 2.79                     | 0.46              |
| 1:Y:120:LEU:O    | 1:Y:121:GLU:C    | 2.54                     | 0.46              |
| 1:Y:244:GLY:O    | 1:Y:245:ASP:C    | 2.59                     | 0.46              |
| 1:Y:284:ASN:OD1  | 1:Y:398:ASP:OD1  | 2.33                     | 0.46              |
| 1:O:113:GLU:O    | 1:O:117:ARG:HD3  | 2.15                     | 0.46              |
| 1:O:214:LEU:N    | 1:O:214:LEU:CD1  | 2.78                     | 0.46              |
| 1:Y:11:GLN:HE22  | 1:Y:82:GLN:HE21  | 1.62                     | 0.46              |
| 1:Y:185:ASN:HD21 | 1:Y:243:ALA:C    | 2.24                     | 0.46              |
| 1:Y:313:ILE:HD11 | 1:Y:381:LEU:HD23 | 1.98                     | 0.46              |
| 1:O:4:LYS:HB3    | 1:O:4:LYS:HE2    | 1.68                     | 0.46              |
| 1:O:161:LEU:CD2  | 1:O:162:PHE:N    | 2.79                     | 0.46              |
| 1:Y:142:LYS:O    | 1:Y:145:LEU:HB2  | 2.16                     | 0.46              |
| 1:Y:201:ASP:O    | 1:Y:204:LEU:HB2  | 2.16                     | 0.46              |
| 1:Y:401:ILE:CG2  | 1:Y:402:ARG:N    | 2.79                     | 0.46              |
| 1:O:6:ILE:HG13   | 1:O:7:VAL:N      | 2.30                     | 0.46              |
| 1:O:53:TRP:CZ3   | 1:O:173:MET:HE3  | 2.47                     | 0.46              |
| 1:O:81:ASN:OD1   | 1:O:165:VAL:HB   | 2.15                     | 0.46              |
| 1:O:293:GLY:CA   | 1:O:299:ASN:ND2  | 2.78                     | 0.46              |
| 1:Y:111:ILE:HG22 | 1:Y:115:LEU:HD11 | 1.96                     | 0.46              |
| 1:O:145:LEU:HD12 | 1:O:145:LEU:HA   | 1.78                     | 0.46              |
| 1:O:161:LEU:CD2  | 1:O:179:HIS:CE1  | 2.99                     | 0.46              |
| 1:O:194:ILE:HB   | 1:O:290:ILE:HD11 | 1.98                     | 0.46              |
| 1:O:457:LEU:HD12 | 1:O:457:LEU:HA   | 1.82                     | 0.46              |
| 1:O:487:LYS:O    | 1:O:488:LYS:C    | 2.56                     | 0.46              |
| 1:Y:41:LYS:O     | 1:Y:44:TRP:HB2   | 2.16                     | 0.45              |
| 1:Y:156:ARG:NH1  | 1:Y:156:ARG:CB   | 2.79                     | 0.45              |
| 1:O:53:TRP:CE3   | 1:O:169:LEU:CD1  | 3.00                     | 0.45              |
| 1:O:401:ILE:CG2  | 1:O:402:ARG:N    | 2.79                     | 0.45              |
| 1:Y:94:GLY:CA    | 1:Y:171:TRP:CH2  | 2.99                     | 0.45              |
| 1:Y:110:GLU:O    | 1:Y:113:GLU:N    | 2.49                     | 0.45              |
| 1:O:6:ILE:HD12   | 1:O:76:ALA:HB3   | 1.97                     | 0.45              |
| 1:O:53:TRP:O     | 1:O:54:ALA:C     | 2.58                     | 0.45              |
| 1:Y:48:ASP:HB3   | 1:Y:51:GLU:HB3   | 1.98                     | 0.45              |
| 1:Y:237:ILE:CG2  | 1:Y:238:PRO:N    | 2.79                     | 0.45              |
| 1:Y:372:ASN:OD1  | 1:Y:374:ASN:HB2  | 2.16                     | 0.45              |
| 1:Y:422:GLN:NE2  | 1:Y:426:LEU:CD2  | 2.79                     | 0.45              |
| 1:O:64:LEU:O     | 1:O:65:ALA:C     | 2.57                     | 0.45              |
| 1:O:69:ILE:N     | 1:O:69:ILE:CD1   | 2.80                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:144:ILE:HG22 | 1:O:148:VAL:HG21 | 1.97                     | 0.45              |
| 1:Y:199:TRP:CD2  | 1:Y:214:LEU:HD23 | 2.52                     | 0.45              |
| 1:Y:214:LEU:N    | 1:Y:214:LEU:CD1  | 2.79                     | 0.45              |
| 1:Y:316:LEU:HD23 | 1:Y:316:LEU:HA   | 1.49                     | 0.45              |
| 1:Y:382:GLU:HG2  | 1:Y:421:PHE:CZ   | 2.51                     | 0.45              |
| 1:Y:433:PRO:HA   | 1:Y:466:ILE:CD1  | 2.44                     | 0.45              |
| 1:Y:449:LEU:HD13 | 1:Y:454:TRP:O    | 2.15                     | 0.45              |
| 1:Y:457:LEU:C    | 1:Y:459:GLU:H    | 2.24                     | 0.45              |
| 1:O:6:ILE:CD1    | 1:O:76:ALA:HB3   | 2.46                     | 0.45              |
| 1:O:40:PRO:HG2   | 1:O:44:TRP:HB2   | 1.95                     | 0.45              |
| 1:O:44:TRP:CZ2   | 1:O:107:ARG:HB2  | 2.49                     | 0.45              |
| 1:O:262:LYS:HD2  | 1:O:262:LYS:C    | 2.42                     | 0.45              |
| 1:O:325:ASP:HB3  | 1:O:327:TYR:CB   | 2.45                     | 0.45              |
| 1:Y:170:ILE:HG22 | 1:Y:171:TRP:N    | 2.27                     | 0.45              |
| 1:Y:226:GLN:HB3  | 1:Y:237:ILE:O    | 2.17                     | 0.45              |
| 1:O:122:ASP:O    | 1:O:126:SER:OG   | 2.30                     | 0.45              |
| 1:O:230:GLY:HA2  | 1:O:235:THR:HB   | 1.96                     | 0.45              |
| 1:O:480:ASN:O    | 1:O:481:TYR:C    | 2.58                     | 0.45              |
| 1:Y:161:LEU:CD2  | 1:Y:179:HIS:NE2  | 2.80                     | 0.45              |
| 1:O:125:ARG:NH2  | 1:O:285:GLY:H    | 2.15                     | 0.45              |
| 1:O:207:LEU:CD2  | 1:O:207:LEU:N    | 2.79                     | 0.45              |
| 1:O:226:GLN:HE21 | 1:O:236:ARG:HG2  | 1.80                     | 0.45              |
| 1:O:482:ARG:HG3  | 1:O:482:ARG:HH11 | 1.81                     | 0.45              |
| 1:Y:351:LEU:HD22 | 1:Y:360:ALA:CB   | 2.47                     | 0.45              |
| 1:O:20:VAL:O     | 1:O:28:ILE:HB    | 2.17                     | 0.45              |
| 1:O:58:TRP:CE3   | 1:O:58:TRP:CA    | 2.99                     | 0.45              |
| 1:O:218:ARG:NH1  | 1:O:218:ARG:CG   | 2.80                     | 0.45              |
| 1:O:428:THR:HG23 | 1:O:429:ARG:N    | 2.32                     | 0.45              |
| 1:Y:172:LYS:O    | 1:Y:173:MET:C    | 2.57                     | 0.45              |
| 1:O:53:TRP:CZ3   | 1:O:173:MET:CE   | 3.00                     | 0.45              |
| 1:O:188:ARG:HD3  | 1:O:188:ARG:HA   | 1.28                     | 0.45              |
| 1:O:204:LEU:HD23 | 1:O:204:LEU:HA   | 1.51                     | 0.45              |
| 1:O:326:ALA:O    | 1:O:327:TYR:C    | 2.57                     | 0.45              |
| 1:O:377:ILE:O    | 1:O:378:ARG:C    | 2.60                     | 0.45              |
| 1:O:422:GLN:NE2  | 1:O:426:LEU:CD2  | 2.80                     | 0.45              |
| 1:Y:108:THR:HB   | 1:Y:139:THR:HB   | 1.99                     | 0.45              |
| 1:Y:189:THR:OG1  | 1:Y:191:LEU:HD12 | 2.17                     | 0.45              |
| 1:O:170:ILE:CG2  | 1:O:171:TRP:N    | 2.80                     | 0.45              |
| 1:O:179:HIS:CD2  | 1:O:215:PRO:CA   | 3.00                     | 0.45              |
| 1:O:191:LEU:O    | 1:O:192:PHE:HB2  | 2.17                     | 0.45              |
| 1:O:430:VAL:HB   | 1:O:470:PHE:HB2  | 1.97                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:17:ARG:HH22  | 1:Y:437:GLU:HG2  | 1.81                     | 0.45              |
| 1:Y:211:ARG:NH1  | 1:Y:211:ARG:CG   | 2.80                     | 0.45              |
| 1:Y:251:PHE:CD2  | 1:Y:446:LEU:CD2  | 3.00                     | 0.45              |
| 1:Y:498:GLU:OE2  | 1:O:488:LYS:HE2  | 2.17                     | 0.45              |
| 1:O:58:TRP:CD2   | 1:O:58:TRP:N     | 2.80                     | 0.45              |
| 1:O:58:TRP:O     | 1:O:62:GLU:N     | 2.42                     | 0.45              |
| 1:O:170:ILE:HA   | 1:O:173:MET:CG   | 2.47                     | 0.45              |
| 1:Y:193:ASN:HB3  | 1:Y:196:THR:HB   | 1.99                     | 0.44              |
| 1:Y:256:VAL:HG12 | 1:Y:294:PRO:HG3  | 1.97                     | 0.44              |
| 1:Y:468:ARG:CG   | 1:Y:468:ARG:NH1  | 2.80                     | 0.44              |
| 1:O:13:THR:O     | 1:O:13:THR:HG22  | 2.15                     | 0.44              |
| 1:O:179:HIS:CD2  | 1:O:215:PRO:CB   | 2.99                     | 0.44              |
| 1:O:264:THR:HG23 | 1:O:265:TYR:N    | 2.32                     | 0.44              |
| 1:O:350:GLY:HA2  | 1:O:360:ALA:HB3  | 1.99                     | 0.44              |
| 1:O:372:ASN:OD1  | 1:O:374:ASN:N    | 2.50                     | 0.44              |
| 1:O:403:LEU:N    | 1:O:403:LEU:HD12 | 2.31                     | 0.44              |
| 1:Y:108:THR:CB   | 1:Y:139:THR:HB   | 2.47                     | 0.44              |
| 1:Y:195:HIS:N    | 1:Y:195:HIS:ND1  | 2.65                     | 0.44              |
| 1:Y:342:VAL:HA   | 1:Y:365:PHE:O    | 2.18                     | 0.44              |
| 1:Y:403:LEU:N    | 1:Y:403:LEU:CD1  | 2.80                     | 0.44              |
| 1:O:37:GLN:OE1   | 1:O:47:HIS:HE1   | 1.99                     | 0.44              |
| 1:O:41:LYS:HB3   | 1:O:41:LYS:HE2   | 1.78                     | 0.44              |
| 1:O:58:TRP:CE3   | 1:O:58:TRP:N     | 2.85                     | 0.44              |
| 1:O:70:SER:O     | 1:O:72:ASP:N     | 2.50                     | 0.44              |
| 1:O:199:TRP:CZ2  | 1:O:214:LEU:HB3  | 2.52                     | 0.44              |
| 3:O:601:ATF:O1G  | 3:O:601:ATF:O2B  | 2.35                     | 0.44              |
| 1:Y:193:ASN:CG   | 1:Y:196:THR:HB   | 2.43                     | 0.44              |
| 1:Y:361:ARG:HD3  | 1:Y:361:ARG:HA   | 1.74                     | 0.44              |
| 1:Y:480:ASN:ND2  | 1:Y:480:ASN:N    | 2.64                     | 0.44              |
| 1:O:409:ASP:CA   | 1:O:413:VAL:HG11 | 2.47                     | 0.44              |
| 1:Y:50:MET:O     | 1:Y:51:GLU:C     | 2.60                     | 0.44              |
| 1:Y:348:PHE:HD2  | 1:O:368:THR:C    | 2.26                     | 0.44              |
| 1:Y:24:ASP:CB    | 1:Y:26:ASN:HD21  | 2.14                     | 0.44              |
| 1:Y:185:ASN:O    | 1:Y:188:ARG:HB2  | 2.16                     | 0.44              |
| 1:Y:281:LYS:O    | 1:Y:281:LYS:HG3  | 2.16                     | 0.44              |
| 1:O:251:PHE:CE1  | 1:O:256:VAL:CG2  | 2.99                     | 0.44              |
| 1:O:394:ALA:O    | 1:O:397:ALA:HB3  | 2.16                     | 0.44              |
| 1:Y:117:ARG:H    | 1:Y:117:ARG:HG3  | 1.68                     | 0.44              |
| 1:Y:150:GLY:O    | 1:Y:153:GLU:HB2  | 2.18                     | 0.44              |
| 1:Y:191:LEU:O    | 1:Y:199:TRP:HE3  | 2.01                     | 0.44              |
| 1:Y:393:GLU:HG2  | 1:Y:393:GLU:H    | 1.21                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:199:TRP:HB3  | 1:O:204:LEU:HD11 | 2.00                     | 0.44              |
| 1:O:53:TRP:HZ3   | 1:O:173:MET:CE   | 2.29                     | 0.44              |
| 1:O:78:GLY:CA    | 1:O:447:ALA:HB2  | 2.48                     | 0.44              |
| 1:O:183:TYR:CD1  | 1:O:217:VAL:CG1  | 3.00                     | 0.44              |
| 1:O:237:ILE:HG22 | 1:O:238:PRO:N    | 2.33                     | 0.44              |
| 1:O:278:LYS:HZ3  | 1:O:280:VAL:HB   | 1.77                     | 0.44              |
| 1:O:415:ASN:CG   | 1:O:418:LEU:HB2  | 2.42                     | 0.44              |
| 1:Y:67:ALA:HB1   | 1:Y:69:ILE:HG12  | 1.99                     | 0.44              |
| 1:Y:142:LYS:O    | 1:Y:146:ASP:OD1  | 2.36                     | 0.44              |
| 1:Y:466:ILE:HD13 | 1:Y:466:ILE:HA   | 1.51                     | 0.44              |
| 1:O:179:HIS:NE2  | 1:O:215:PRO:CB   | 2.80                     | 0.44              |
| 1:O:192:PHE:HE2  | 1:O:217:VAL:HG11 | 1.83                     | 0.44              |
| 1:Y:9:LEU:HD12   | 1:Y:9:LEU:HA     | 1.87                     | 0.44              |
| 1:Y:27:ILE:HD11  | 1:Y:30:VAL:CG2   | 2.45                     | 0.44              |
| 1:O:166:ASP:O    | 1:O:169:LEU:N    | 2.51                     | 0.44              |
| 1:O:219:ARG:HG2  | 1:O:222:GLU:CB   | 2.44                     | 0.44              |
| 1:Y:40:PRO:HD2   | 1:Y:44:TRP:HB2   | 1.99                     | 0.43              |
| 1:Y:110:GLU:O    | 1:Y:111:ILE:C    | 2.60                     | 0.43              |
| 1:O:316:LEU:HD23 | 1:O:316:LEU:HA   | 1.43                     | 0.43              |
| 1:O:428:THR:CG2  | 1:O:429:ARG:N    | 2.80                     | 0.43              |
| 1:Y:44:TRP:CZ2   | 1:Y:107:ARG:HB2  | 2.52                     | 0.43              |
| 1:Y:221:SER:OG   | 1:Y:221:SER:O    | 2.34                     | 0.43              |
| 1:O:156:ARG:O    | 1:O:212:GLU:HG2  | 2.18                     | 0.43              |
| 1:Y:324:ASN:N    | 1:Y:324:ASN:HD22 | 2.14                     | 0.43              |
| 1:Y:325:ASP:HB2  | 1:Y:328:ASP:CG   | 2.44                     | 0.43              |
| 1:Y:328:ASP:HB3  | 1:Y:332:PHE:CE2  | 2.53                     | 0.43              |
| 1:Y:347:ALA:HB2  | 1:Y:351:LEU:HD13 | 2.01                     | 0.43              |
| 1:Y:482:ARG:NH1  | 1:Y:482:ARG:CG   | 2.79                     | 0.43              |
| 1:Y:32:GLN:N     | 1:Y:59:THR:HG22  | 2.34                     | 0.43              |
| 1:Y:166:ASP:CG   | 1:Y:167:THR:H    | 2.26                     | 0.43              |
| 1:Y:240:SER:HB2  | 1:Y:450:ALA:CB   | 2.47                     | 0.43              |
| 1:Y:309:ALA:O    | 1:Y:310:GLY:C    | 2.59                     | 0.43              |
| 1:O:148:VAL:HB   | 1:O:151:SER:HB3  | 1.99                     | 0.43              |
| 1:O:251:PHE:CD2  | 1:O:446:LEU:HD13 | 2.51                     | 0.43              |
| 1:Y:134:PRO:O    | 1:Y:135:TYR:C    | 2.60                     | 0.43              |
| 1:Y:286:LEU:HD11 | 1:Y:394:ALA:CB   | 2.48                     | 0.43              |
| 1:Y:435:VAL:HG21 | 1:Y:441:LEU:HD11 | 2.01                     | 0.43              |
| 1:Y:457:LEU:C    | 1:Y:459:GLU:N    | 2.77                     | 0.43              |
| 1:O:183:TYR:CD2  | 1:O:298:VAL:HG22 | 2.53                     | 0.43              |
| 1:O:339:THR:O    | 1:O:339:THR:OG1  | 2.34                     | 0.43              |
| 1:Y:276:GLY:O    | 1:Y:300:TYR:N    | 2.51                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:386:TYR:HB3  | 1:Y:486:TRP:CE2  | 2.53                     | 0.43              |
| 1:O:11:GLN:NE2   | 1:O:82:GLN:HE21  | 2.17                     | 0.43              |
| 1:O:33:ARG:NH2   | 1:O:58:TRP:HB3   | 2.31                     | 0.43              |
| 1:O:84:GLU:OE1   | 1:O:103:TRP:HB3  | 2.19                     | 0.43              |
| 1:O:88:VAL:HG12  | 1:O:97:ILE:HG12  | 2.01                     | 0.43              |
| 1:O:130:LEU:HD13 | 1:O:136:PHE:CD1  | 2.54                     | 0.43              |
| 1:O:137:SER:O    | 1:O:140:LYS:N    | 2.52                     | 0.43              |
| 1:O:389:ARG:O    | 1:O:390:ASP:C    | 2.62                     | 0.43              |
| 1:Y:156:ARG:HH11 | 1:Y:156:ARG:CG   | 2.31                     | 0.43              |
| 1:Y:169:LEU:O    | 1:Y:172:LYS:HB2  | 2.18                     | 0.43              |
| 1:Y:408:VAL:HG23 | 1:Y:409:ASP:N    | 2.33                     | 0.43              |
| 1:Y:432:ARG:CG   | 1:Y:436:ARG:NH1  | 2.81                     | 0.43              |
| 1:O:108:THR:CB   | 1:O:139:THR:HB   | 2.48                     | 0.43              |
| 1:O:142:LYS:O    | 1:O:145:LEU:N    | 2.52                     | 0.43              |
| 1:O:271:MET:O    | 1:O:272:LEU:HD12 | 2.19                     | 0.43              |
| 1:Y:91:LYS:HE3   | 1:Y:91:LYS:HB3   | 1.80                     | 0.43              |
| 1:Y:228:ASN:HD21 | 1:Y:235:THR:N    | 2.16                     | 0.43              |
| 1:Y:250:LEU:HD12 | 1:Y:255:CYS:HB2  | 1.97                     | 0.43              |
| 1:Y:355:TYR:O    | 1:Y:356:TRP:C    | 2.59                     | 0.43              |
| 1:O:49:PRO:HA    | 1:O:52:ILE:HD12  | 2.00                     | 0.43              |
| 1:O:83:ARG:CZ    | 1:O:246:GLN:HG2  | 2.49                     | 0.43              |
| 1:O:180:VAL:HG21 | 1:O:218:ARG:HH11 | 1.84                     | 0.43              |
| 1:O:386:TYR:CB   | 1:O:486:TRP:CD2  | 3.01                     | 0.43              |
| 1:O:406:LEU:CD2  | 1:O:407:ARG:N    | 2.82                     | 0.43              |
| 1:O:87:ILE:O     | 1:O:88:VAL:HG23  | 2.19                     | 0.43              |
| 1:O:170:ILE:HA   | 1:O:173:MET:HG2  | 2.01                     | 0.43              |
| 1:O:185:ASN:HD21 | 1:O:244:GLY:N    | 2.17                     | 0.43              |
| 1:O:78:GLY:HA2   | 1:O:241:GLY:HA3  | 2.00                     | 0.43              |
| 1:O:263:ASN:HB2  | 1:O:271:MET:CG   | 2.48                     | 0.43              |
| 1:O:475:GLU:O    | 1:O:478:GLU:CB   | 2.67                     | 0.43              |
| 1:Y:170:ILE:HA   | 1:Y:173:MET:HG2  | 2.01                     | 0.42              |
| 1:Y:262:LYS:HZ2  | 1:Y:264:THR:HB   | 1.84                     | 0.42              |
| 1:Y:302:LEU:HA   | 1:Y:302:LEU:HD23 | 1.10                     | 0.42              |
| 1:O:136:PHE:HB3  | 1:O:188:ARG:O    | 2.19                     | 0.42              |
| 1:O:186:ALA:C    | 1:O:188:ARG:N    | 2.77                     | 0.42              |
| 1:O:250:LEU:HD12 | 1:O:255:CYS:HB2  | 2.01                     | 0.42              |
| 1:O:466:ILE:HD13 | 1:O:466:ILE:HA   | 1.61                     | 0.42              |
| 1:O:491:LYS:O    | 1:O:494:MET:HG3  | 2.19                     | 0.42              |
| 1:Y:81:ASN:ND2   | 1:Y:81:ASN:H     | 2.16                     | 0.42              |
| 1:Y:144:ILE:O    | 1:Y:147:HIS:N    | 2.33                     | 0.42              |
| 1:Y:357:ASP:OD2  | 1:Y:494:MET:HB3  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:415:ASN:ND2  | 1:Y:418:LEU:HB2  | 2.34                     | 0.42              |
| 1:O:40:PRO:CG    | 1:O:44:TRP:HB3   | 2.49                     | 0.42              |
| 1:O:161:LEU:HD23 | 1:O:161:LEU:HA   | 1.67                     | 0.42              |
| 1:O:413:VAL:HG23 | 1:O:432:ARG:HD2  | 2.01                     | 0.42              |
| 1:Y:23:HIS:ND1   | 1:Y:453:PHE:CE1  | 2.88                     | 0.42              |
| 1:Y:185:ASN:O    | 1:Y:186:ALA:C    | 2.61                     | 0.42              |
| 1:Y:484:ALA:O    | 1:Y:485:GLY:C    | 2.62                     | 0.42              |
| 1:O:48:ASP:O     | 1:O:51:GLU:HB3   | 2.19                     | 0.42              |
| 1:O:53:TRP:CH2   | 1:O:172:LYS:HB3  | 2.54                     | 0.42              |
| 1:O:359:TYR:HD1  | 1:O:497:GLU:HB3  | 1.85                     | 0.42              |
| 1:O:383:SER:O    | 1:O:387:GLN:HB2  | 2.19                     | 0.42              |
| 1:Y:144:ILE:HG23 | 1:Y:148:VAL:CG2  | 2.49                     | 0.42              |
| 1:Y:184:THR:HG22 | 1:Y:290:ILE:HG22 | 2.00                     | 0.42              |
| 1:Y:415:ASN:HD22 | 1:Y:415:ASN:C    | 2.26                     | 0.42              |
| 1:Y:467:GLU:OE2  | 1:Y:468:ARG:HB2  | 2.20                     | 0.42              |
| 1:Y:487:LYS:O    | 1:Y:488:LYS:C    | 2.59                     | 0.42              |
| 1:O:48:ASP:C     | 1:O:52:ILE:HD12  | 2.44                     | 0.42              |
| 1:O:90:GLU:HB3   | 1:O:93:THR:OG1   | 2.19                     | 0.42              |
| 1:O:278:LYS:O    | 1:O:278:LYS:HD2  | 2.18                     | 0.42              |
| 1:Y:40:PRO:HD2   | 1:Y:44:TRP:CB    | 2.49                     | 0.42              |
| 1:Y:50:MET:O     | 1:Y:53:TRP:HB3   | 2.19                     | 0.42              |
| 1:Y:124:ILE:HG12 | 1:Y:124:ILE:H    | 1.68                     | 0.42              |
| 1:Y:359:TYR:CD1  | 1:Y:359:TYR:N    | 2.87                     | 0.42              |
| 1:O:108:THR:CG2  | 1:O:139:THR:HB   | 2.50                     | 0.42              |
| 1:O:144:ILE:CG2  | 1:O:148:VAL:CG2  | 2.97                     | 0.42              |
| 1:O:389:ARG:HD2  | 1:O:393:GLU:OE2  | 2.20                     | 0.42              |
| 1:O:398:ASP:O    | 1:O:400:GLY:N    | 2.52                     | 0.42              |
| 1:Y:122:ASP:O    | 1:Y:126:SER:N    | 2.47                     | 0.42              |
| 1:Y:435:VAL:CG2  | 1:Y:436:ARG:N    | 2.80                     | 0.42              |
| 1:Y:441:LEU:HD23 | 1:Y:441:LEU:HA   | 1.89                     | 0.42              |
| 1:O:5:TYR:N      | 1:O:73:GLN:O     | 2.35                     | 0.42              |
| 1:O:130:LEU:HD23 | 1:O:130:LEU:N    | 2.33                     | 0.42              |
| 1:O:157:ARG:HG2  | 1:O:157:ARG:H    | 1.61                     | 0.42              |
| 1:O:264:THR:CG2  | 1:O:265:TYR:N    | 2.78                     | 0.42              |
| 1:Y:325:ASP:CB   | 1:Y:327:TYR:HB3  | 2.33                     | 0.42              |
| 1:Y:352:GLY:C    | 1:Y:356:TRP:H    | 2.24                     | 0.42              |
| 1:O:5:TYR:HE2    | 1:O:69:ILE:HG23  | 1.84                     | 0.42              |
| 1:O:11:GLN:HE22  | 1:O:82:GLN:HE21  | 1.66                     | 0.42              |
| 1:O:83:ARG:HE    | 4:O:600:GOL:H2   | 1.85                     | 0.42              |
| 1:O:193:ASN:CB   | 1:O:196:THR:HB   | 2.50                     | 0.42              |
| 1:O:262:LYS:HA   | 1:O:407:ARG:O    | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:47:HIS:HD2   | 1:Y:82:GLN:HE22  | 1.68                     | 0.42              |
| 1:Y:111:ILE:CG2  | 1:Y:115:LEU:HD11 | 2.50                     | 0.42              |
| 1:Y:111:ILE:CG2  | 1:Y:139:THR:HG22 | 2.46                     | 0.42              |
| 1:O:5:TYR:HB3    | 1:O:21:MET:O     | 2.20                     | 0.42              |
| 1:O:77:ILE:HB    | 1:O:238:PRO:O    | 2.20                     | 0.42              |
| 1:O:161:LEU:HD22 | 1:O:162:PHE:N    | 2.35                     | 0.42              |
| 1:O:161:LEU:HD22 | 1:O:179:HIS:CE1  | 2.55                     | 0.42              |
| 1:O:188:ARG:HH11 | 1:O:188:ARG:HD2  | 1.60                     | 0.42              |
| 1:Y:253:GLN:OE1  | 1:Y:407:ARG:HD2  | 2.20                     | 0.42              |
| 1:Y:408:VAL:O    | 1:Y:409:ASP:HB3  | 2.20                     | 0.42              |
| 1:O:64:LEU:HD12  | 1:O:64:LEU:N     | 2.35                     | 0.42              |
| 1:O:137:SER:O    | 1:O:140:LYS:HB2  | 2.20                     | 0.42              |
| 1:O:229:ILE:HG21 | 1:O:237:ILE:CG1  | 2.31                     | 0.42              |
| 1:O:351:LEU:HD13 | 1:O:351:LEU:HA   | 1.74                     | 0.42              |
| 1:Y:17:ARG:HH22  | 1:Y:437:GLU:CG   | 2.32                     | 0.42              |
| 1:Y:60:LEU:HD12  | 1:Y:60:LEU:HA    | 1.80                     | 0.42              |
| 1:Y:117:ARG:HH11 | 1:Y:117:ARG:HG3  | 1.85                     | 0.42              |
| 1:Y:127:ASN:CB   | 1:Y:193:ASN:ND2  | 2.80                     | 0.42              |
| 1:O:187:SER:CB   | 1:O:290:ILE:HB   | 2.50                     | 0.42              |
| 1:Y:103:TRP:HA   | 1:Y:140:LYS:HE3  | 2.02                     | 0.41              |
| 1:Y:320:MET:HE1  | 1:O:376:ILE:HG13 | 2.01                     | 0.41              |
| 1:Y:360:ALA:HA   | 1:Y:493:ALA:O    | 2.19                     | 0.41              |
| 1:O:32:GLN:HA    | 1:O:59:THR:CG2   | 2.50                     | 0.41              |
| 1:O:40:PRO:HD2   | 1:O:44:TRP:C     | 2.45                     | 0.41              |
| 1:O:46:GLU:HB3   | 1:O:100:ALA:O    | 2.20                     | 0.41              |
| 1:O:60:LEU:O     | 1:O:63:VAL:HB    | 2.20                     | 0.41              |
| 1:O:393:GLU:HG2  | 1:O:393:GLU:H    | 1.63                     | 0.41              |
| 1:Y:87:ILE:HD13  | 1:Y:168:TRP:CB   | 2.50                     | 0.41              |
| 1:Y:132:ILE:HD13 | 1:Y:132:ILE:HG21 | 1.86                     | 0.41              |
| 1:Y:251:PHE:CD2  | 1:Y:446:LEU:HD22 | 2.55                     | 0.41              |
| 1:Y:458:ASP:HA   | 1:Y:461:GLN:HB2  | 2.01                     | 0.41              |
| 1:O:20:VAL:CG1   | 1:O:21:MET:N     | 2.80                     | 0.41              |
| 1:O:133:ASP:HA   | 1:O:134:PRO:HD3  | 1.92                     | 0.41              |
| 1:O:278:LYS:HD2  | 1:O:278:LYS:C    | 2.46                     | 0.41              |
| 1:O:441:LEU:CD2  | 1:O:445:TYR:CE1  | 3.03                     | 0.41              |
| 1:O:457:LEU:C    | 1:O:459:GLU:N    | 2.78                     | 0.41              |
| 1:Y:97:ILE:O     | 1:Y:98:TYR:HB2   | 2.21                     | 0.41              |
| 1:Y:103:TRP:CD1  | 1:Y:103:TRP:N    | 2.88                     | 0.41              |
| 1:Y:130:LEU:HB3  | 1:Y:131:VAL:H    | 1.51                     | 0.41              |
| 1:Y:164:THR:O    | 1:Y:165:VAL:C    | 2.60                     | 0.41              |
| 1:Y:490:VAL:H    | 1:Y:490:VAL:HG23 | 1.60                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:444:ALA:O    | 1:Y:445:TYR:C    | 2.62                     | 0.41              |
| 1:Y:490:VAL:O    | 1:Y:491:LYS:C    | 2.62                     | 0.41              |
| 1:O:38:ILE:O     | 1:O:45:VAL:HA    | 2.20                     | 0.41              |
| 1:O:128:THR:HG21 | 1:O:190:MET:HA   | 2.02                     | 0.41              |
| 1:O:143:TRP:CE3  | 1:O:143:TRP:C    | 2.98                     | 0.41              |
| 1:O:263:ASN:ND2  | 1:O:265:TYR:CZ   | 2.88                     | 0.41              |
| 1:Y:70:SER:C     | 1:Y:72:ASP:N     | 2.77                     | 0.41              |
| 1:Y:114:HIS:CD2  | 1:Y:114:HIS:H    | 2.38                     | 0.41              |
| 1:Y:145:LEU:HD12 | 1:Y:145:LEU:HA   | 1.59                     | 0.41              |
| 1:O:28:ILE:HA    | 1:O:28:ILE:HD12  | 1.85                     | 0.41              |
| 1:O:113:GLU:OE1  | 1:O:113:GLU:HA   | 2.20                     | 0.41              |
| 1:Y:16:SER:HB3   | 1:Y:56:GLN:OE1   | 2.21                     | 0.41              |
| 1:Y:23:HIS:HA    | 1:Y:453:PHE:HE1  | 1.86                     | 0.41              |
| 1:Y:189:THR:O    | 1:Y:190:MET:HB3  | 2.21                     | 0.41              |
| 1:Y:256:VAL:HG11 | 1:Y:294:PRO:HB3  | 2.02                     | 0.41              |
| 1:Y:428:THR:HG23 | 1:Y:429:ARG:N    | 2.36                     | 0.41              |
| 1:O:55:THR:O     | 1:O:58:TRP:HB2   | 2.21                     | 0.41              |
| 1:O:89:TRP:CZ2   | 1:O:161:LEU:HD13 | 2.56                     | 0.41              |
| 1:O:174:THR:HG21 | 1:O:178:VAL:HG23 | 2.02                     | 0.41              |
| 1:O:392:LEU:O    | 1:O:392:LEU:HG   | 2.15                     | 0.41              |
| 1:O:458:ASP:HA   | 1:O:461:GLN:HB2  | 2.01                     | 0.41              |
| 1:O:484:ALA:O    | 1:O:487:LYS:N    | 2.54                     | 0.41              |
| 1:Y:70:SER:H     | 1:Y:73:GLN:CD    | 2.29                     | 0.41              |
| 1:Y:445:TYR:O    | 1:Y:449:LEU:N    | 2.39                     | 0.41              |
| 1:O:54:ALA:C     | 1:O:58:TRP:NE1   | 2.79                     | 0.41              |
| 1:O:441:LEU:HD22 | 1:O:445:TYR:CZ   | 2.55                     | 0.41              |
| 1:Y:257:LYS:HG3  | 1:Y:260:MET:SD   | 2.61                     | 0.41              |
| 1:Y:258:GLU:N    | 1:Y:274:ASN:OD1  | 2.54                     | 0.41              |
| 1:O:70:SER:C     | 1:O:72:ASP:N     | 2.78                     | 0.41              |
| 1:O:156:ARG:CG   | 1:O:156:ARG:HH11 | 2.34                     | 0.41              |
| 1:O:325:ASP:HB2  | 1:O:328:ASP:CG   | 2.46                     | 0.41              |
| 1:Y:3:LYS:HG2    | 1:Y:72:ASP:O     | 2.21                     | 0.41              |
| 1:Y:23:HIS:HE1   | 1:Y:453:PHE:O    | 2.04                     | 0.41              |
| 1:Y:117:ARG:CG   | 1:Y:117:ARG:NH1  | 2.80                     | 0.41              |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CG   | 2.56                     | 0.41              |
| 1:Y:169:LEU:N    | 1:Y:169:LEU:HD22 | 2.36                     | 0.41              |
| 1:Y:205:GLU:C    | 1:Y:208:ASP:H    | 2.28                     | 0.41              |
| 1:Y:222:GLU:HG2  | 1:Y:224:TYR:CD1  | 2.56                     | 0.41              |
| 1:Y:250:LEU:HD13 | 1:Y:262:LYS:HG2  | 2.03                     | 0.41              |
| 1:Y:251:PHE:O    | 1:Y:254:LEU:HD12 | 2.21                     | 0.41              |
| 1:Y:377:ILE:O    | 1:Y:378:ARG:C    | 2.58                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:70:SER:O     | 1:O:71:SER:C     | 2.63                     | 0.41              |
| 1:O:192:PHE:CE1  | 1:O:197:LEU:HA   | 2.56                     | 0.41              |
| 1:O:226:GLN:NE2  | 1:O:236:ARG:CB   | 2.79                     | 0.41              |
| 1:O:412:ALA:C    | 1:O:414:ALA:N    | 2.78                     | 0.41              |
| 1:O:487:LYS:O    | 1:O:490:VAL:HG23 | 2.21                     | 0.41              |
| 1:Y:183:TYR:CD1  | 1:Y:217:VAL:CG1  | 2.98                     | 0.41              |
| 1:Y:219:ARG:O    | 1:Y:224:TYR:OH   | 2.28                     | 0.41              |
| 1:Y:266:GLY:O    | 1:Y:267:THR:C    | 2.64                     | 0.41              |
| 1:Y:11:GLN:NE2   | 1:Y:82:GLN:HG2   | 2.36                     | 0.40              |
| 1:Y:84:GLU:HB2   | 1:Y:103:TRP:CB   | 2.42                     | 0.40              |
| 1:Y:237:ILE:CG2  | 1:Y:238:PRO:CD   | 2.99                     | 0.40              |
| 1:Y:269:CYS:C    | 1:Y:270:PHE:CG   | 2.99                     | 0.40              |
| 1:O:6:ILE:CG1    | 1:O:7:VAL:N      | 2.84                     | 0.40              |
| 1:O:86:THR:HG1   | 1:O:137:SER:HB3  | 1.83                     | 0.40              |
| 1:Y:180:VAL:HG21 | 1:Y:218:ARG:HG3  | 2.03                     | 0.40              |
| 1:O:155:ALA:O    | 1:O:212:GLU:HB2  | 2.20                     | 0.40              |
| 1:O:162:PHE:CD1  | 1:O:162:PHE:C    | 2.98                     | 0.40              |
| 1:O:166:ASP:CG   | 1:O:167:THR:N    | 2.78                     | 0.40              |
| 1:O:180:VAL:CG2  | 1:O:218:ARG:CG   | 2.99                     | 0.40              |
| 1:O:402:ARG:NH1  | 1:O:402:ARG:C    | 2.80                     | 0.40              |
| 1:Y:226:GLN:HE21 | 1:Y:236:ARG:HB3  | 1.85                     | 0.40              |
| 1:Y:256:VAL:CG1  | 1:Y:294:PRO:CB   | 3.00                     | 0.40              |
| 1:Y:295:THR:N    | 1:Y:297:GLU:OE1  | 2.50                     | 0.40              |
| 1:Y:481:TYR:HD2  | 1:Y:482:ARG:HD2  | 1.86                     | 0.40              |
| 1:O:41:LYS:CB    | 1:O:42:PRO:CD    | 2.99                     | 0.40              |
| 1:O:251:PHE:CD1  | 1:O:256:VAL:CG2  | 3.04                     | 0.40              |
| 1:O:457:LEU:O    | 1:O:459:GLU:N    | 2.54                     | 0.40              |
| 1:O:474:ILE:HA   | 1:O:474:ILE:HD12 | 1.60                     | 0.40              |
| 1:Y:41:LYS:CB    | 1:Y:42:PRO:CD    | 3.00                     | 0.40              |
| 1:Y:74:ILE:HD13  | 1:Y:237:ILE:HG21 | 2.02                     | 0.40              |
| 1:Y:169:LEU:HA   | 1:Y:169:LEU:HD13 | 1.50                     | 0.40              |
| 1:Y:256:VAL:CG1  | 1:Y:294:PRO:CG   | 2.99                     | 0.40              |
| 1:O:45:VAL:HG12  | 1:O:46:GLU:N     | 2.36                     | 0.40              |
| 1:O:152:ARG:C    | 1:O:155:ALA:HB3  | 2.46                     | 0.40              |
| 1:O:437:GLU:O    | 1:O:438:VAL:C    | 2.62                     | 0.40              |
| 1:O:477:THR:O    | 1:O:479:ARG:N    | 2.55                     | 0.40              |
| 1:Y:87:ILE:CG2   | 1:Y:88:VAL:N     | 2.83                     | 0.40              |
| 1:Y:133:ASP:HA   | 1:Y:134:PRO:HD3  | 1.91                     | 0.40              |
| 1:Y:156:ARG:C    | 1:Y:158:GLY:N    | 2.79                     | 0.40              |
| 1:Y:201:ASP:O    | 1:Y:205:GLU:HG2  | 2.21                     | 0.40              |
| 1:Y:229:ILE:HG13 | 1:Y:230:GLY:N    | 2.37                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:Y:402:ARG:NH1 | 1:Y:402:ARG:C    | 2.80                     | 0.40              |
| 1:Y:432:ARG:CD  | 1:Y:436:ARG:NH2  | 2.82                     | 0.40              |
| 1:O:160:LEU:O   | 1:O:213:MET:HB3  | 2.22                     | 0.40              |
| 1:O:409:ASP:HB2 | 1:O:438:VAL:HG21 | 2.04                     | 0.40              |
| 1:O:484:ALA:O   | 1:O:485:GLY:C    | 2.65                     | 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:Y:58:TRP:CZ2 | 1:Y:58:TRP:CZ2[3_655] | 2.10                     | 0.10              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers | Percentiles |           |
|-----|-------|----------------|-----------|-----------|----------|-------------|-----------|
| 1   | O     | 490/501 (98%)  | 375 (76%) | 87 (18%)  | 28 (6%)  | <b>1</b>    | <b>8</b>  |
| 1   | Y     | 490/501 (98%)  | 404 (82%) | 68 (14%)  | 18 (4%)  | <b>2</b>    | <b>15</b> |
| All | All   | 980/1002 (98%) | 779 (80%) | 155 (16%) | 46 (5%)  | <b>2</b>    | <b>11</b> |

All (46) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 71  | SER  |
| 1   | Y     | 151 | SER  |
| 1   | Y     | 153 | GLU  |
| 1   | Y     | 175 | GLN  |
| 1   | O     | 60  | LEU  |
| 1   | O     | 445 | TYR  |
| 1   | O     | 446 | LEU  |
| 1   | O     | 456 | ASN  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 61  | VAL  |
| 1   | Y     | 196 | THR  |
| 1   | O     | 63  | VAL  |
| 1   | O     | 75  | ALA  |
| 1   | O     | 111 | ILE  |
| 1   | O     | 118 | ASP  |
| 1   | O     | 151 | SER  |
| 1   | O     | 199 | TRP  |
| 1   | O     | 477 | THR  |
| 1   | O     | 478 | GLU  |
| 1   | Y     | 111 | ILE  |
| 1   | Y     | 456 | ASN  |
| 1   | O     | 71  | SER  |
| 1   | O     | 98  | TYR  |
| 1   | Y     | 60  | LEU  |
| 1   | Y     | 62  | GLU  |
| 1   | Y     | 64  | LEU  |
| 1   | Y     | 98  | TYR  |
| 1   | O     | 110 | GLU  |
| 1   | O     | 114 | HIS  |
| 1   | O     | 138 | GLY  |
| 1   | O     | 176 | GLY  |
| 1   | O     | 202 | LYS  |
| 1   | O     | 441 | LEU  |
| 1   | Y     | 202 | LYS  |
| 1   | Y     | 258 | GLU  |
| 1   | O     | 99  | ASN  |
| 1   | O     | 149 | GLU  |
| 1   | O     | 196 | THR  |
| 1   | O     | 479 | ARG  |
| 1   | Y     | 138 | GLY  |
| 1   | Y     | 411 | GLY  |
| 1   | O     | 187 | SER  |
| 1   | O     | 242 | ILE  |
| 1   | O     | 258 | GLU  |
| 1   | O     | 458 | ASP  |
| 1   | Y     | 176 | GLY  |
| 1   | Y     | 442 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | O     | 408/412 (99%) | 251 (62%) | 157 (38%) | 0           | 1 |
| 1   | Y     | 408/412 (99%) | 258 (63%) | 150 (37%) | 0           | 1 |
| All | All   | 816/824 (99%) | 509 (62%) | 307 (38%) | 0           | 1 |

All (307) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 2   | GLU  |
| 1   | Y     | 3   | LYS  |
| 1   | Y     | 6   | ILE  |
| 1   | Y     | 9   | LEU  |
| 1   | Y     | 11  | GLN  |
| 1   | Y     | 21  | MET  |
| 1   | Y     | 27  | ILE  |
| 1   | Y     | 28  | ILE  |
| 1   | Y     | 33  | ARG  |
| 1   | Y     | 34  | GLU  |
| 1   | Y     | 41  | LYS  |
| 1   | Y     | 52  | ILE  |
| 1   | Y     | 62  | GLU  |
| 1   | Y     | 63  | VAL  |
| 1   | Y     | 66  | LYS  |
| 1   | Y     | 69  | ILE  |
| 1   | Y     | 70  | SER  |
| 1   | Y     | 71  | SER  |
| 1   | Y     | 73  | GLN  |
| 1   | Y     | 79  | ILE  |
| 1   | Y     | 80  | THR  |
| 1   | Y     | 81  | ASN  |
| 1   | Y     | 83  | ARG  |
| 1   | Y     | 91  | LYS  |
| 1   | Y     | 92  | GLU  |
| 1   | Y     | 93  | THR  |
| 1   | Y     | 95  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 102 | VAL  |
| 1   | Y     | 107 | ARG  |
| 1   | Y     | 110 | GLU  |
| 1   | Y     | 111 | ILE  |
| 1   | Y     | 116 | LYS  |
| 1   | Y     | 117 | ARG  |
| 1   | Y     | 118 | ASP  |
| 1   | Y     | 121 | GLU  |
| 1   | Y     | 124 | ILE  |
| 1   | Y     | 131 | VAL  |
| 1   | Y     | 136 | PHE  |
| 1   | Y     | 137 | SER  |
| 1   | Y     | 139 | THR  |
| 1   | Y     | 141 | VAL  |
| 1   | Y     | 145 | LEU  |
| 1   | Y     | 146 | ASP  |
| 1   | Y     | 148 | VAL  |
| 1   | Y     | 151 | SER  |
| 1   | Y     | 153 | GLU  |
| 1   | Y     | 154 | ARG  |
| 1   | Y     | 156 | ARG  |
| 1   | Y     | 157 | ARG  |
| 1   | Y     | 169 | LEU  |
| 1   | Y     | 170 | ILE  |
| 1   | Y     | 172 | LYS  |
| 1   | Y     | 173 | MET  |
| 1   | Y     | 175 | GLN  |
| 1   | Y     | 178 | VAL  |
| 1   | Y     | 181 | THR  |
| 1   | Y     | 185 | ASN  |
| 1   | Y     | 187 | SER  |
| 1   | Y     | 191 | LEU  |
| 1   | Y     | 195 | HIS  |
| 1   | Y     | 196 | THR  |
| 1   | Y     | 197 | LEU  |
| 1   | Y     | 198 | ASP  |
| 1   | Y     | 201 | ASP  |
| 1   | Y     | 202 | LYS  |
| 1   | Y     | 205 | GLU  |
| 1   | Y     | 206 | VAL  |
| 1   | Y     | 209 | ILE  |
| 1   | Y     | 211 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 212 | GLU  |
| 1   | Y     | 214 | LEU  |
| 1   | Y     | 219 | ARG  |
| 1   | Y     | 221 | SER  |
| 1   | Y     | 222 | GLU  |
| 1   | Y     | 226 | GLN  |
| 1   | Y     | 227 | THR  |
| 1   | Y     | 229 | ILE  |
| 1   | Y     | 235 | THR  |
| 1   | Y     | 236 | ARG  |
| 1   | Y     | 237 | ILE  |
| 1   | Y     | 242 | ILE  |
| 1   | Y     | 245 | ASP  |
| 1   | Y     | 246 | GLN  |
| 1   | Y     | 250 | LEU  |
| 1   | Y     | 254 | LEU  |
| 1   | Y     | 257 | LYS  |
| 1   | Y     | 258 | GLU  |
| 1   | Y     | 262 | LYS  |
| 1   | Y     | 264 | THR  |
| 1   | Y     | 281 | LYS  |
| 1   | Y     | 288 | THR  |
| 1   | Y     | 290 | ILE  |
| 1   | Y     | 295 | THR  |
| 1   | Y     | 302 | LEU  |
| 1   | Y     | 312 | SER  |
| 1   | Y     | 313 | ILE  |
| 1   | Y     | 317 | ARG  |
| 1   | Y     | 318 | ASP  |
| 1   | Y     | 319 | GLU  |
| 1   | Y     | 323 | ILE  |
| 1   | Y     | 324 | ASN  |
| 1   | Y     | 335 | LYS  |
| 1   | Y     | 337 | GLN  |
| 1   | Y     | 339 | THR  |
| 1   | Y     | 351 | LEU  |
| 1   | Y     | 368 | THR  |
| 1   | Y     | 384 | ILE  |
| 1   | Y     | 389 | ARG  |
| 1   | Y     | 391 | VAL  |
| 1   | Y     | 392 | LEU  |
| 1   | Y     | 393 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 395 | MET  |
| 1   | Y     | 402 | ARG  |
| 1   | Y     | 406 | LEU  |
| 1   | Y     | 407 | ARG  |
| 1   | Y     | 408 | VAL  |
| 1   | Y     | 415 | ASN  |
| 1   | Y     | 418 | LEU  |
| 1   | Y     | 423 | SER  |
| 1   | Y     | 426 | LEU  |
| 1   | Y     | 428 | THR  |
| 1   | Y     | 429 | ARG  |
| 1   | Y     | 434 | GLU  |
| 1   | Y     | 438 | VAL  |
| 1   | Y     | 439 | THR  |
| 1   | Y     | 445 | TYR  |
| 1   | Y     | 446 | LEU  |
| 1   | Y     | 449 | LEU  |
| 1   | Y     | 451 | VAL  |
| 1   | Y     | 455 | GLN  |
| 1   | Y     | 456 | ASN  |
| 1   | Y     | 457 | LEU  |
| 1   | Y     | 461 | GLN  |
| 1   | Y     | 462 | GLU  |
| 1   | Y     | 463 | LYS  |
| 1   | Y     | 465 | VAL  |
| 1   | Y     | 466 | ILE  |
| 1   | Y     | 467 | GLU  |
| 1   | Y     | 468 | ARG  |
| 1   | Y     | 469 | GLU  |
| 1   | Y     | 474 | ILE  |
| 1   | Y     | 475 | GLU  |
| 1   | Y     | 476 | THR  |
| 1   | Y     | 478 | GLU  |
| 1   | Y     | 482 | ARG  |
| 1   | Y     | 490 | VAL  |
| 1   | Y     | 492 | ARG  |
| 1   | Y     | 494 | MET  |
| 1   | Y     | 498 | GLU  |
| 1   | Y     | 499 | HIS  |
| 1   | O     | 2   | GLU  |
| 1   | O     | 3   | LYS  |
| 1   | O     | 5   | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 9   | LEU  |
| 1   | O     | 11  | GLN  |
| 1   | O     | 21  | MET  |
| 1   | O     | 27  | ILE  |
| 1   | O     | 28  | ILE  |
| 1   | O     | 33  | ARG  |
| 1   | O     | 34  | GLU  |
| 1   | O     | 41  | LYS  |
| 1   | O     | 45  | VAL  |
| 1   | O     | 46  | GLU  |
| 1   | O     | 50  | MET  |
| 1   | O     | 51  | GLU  |
| 1   | O     | 57  | SER  |
| 1   | O     | 59  | THR  |
| 1   | O     | 60  | LEU  |
| 1   | O     | 64  | LEU  |
| 1   | O     | 69  | ILE  |
| 1   | O     | 70  | SER  |
| 1   | O     | 71  | SER  |
| 1   | O     | 80  | THR  |
| 1   | O     | 81  | ASN  |
| 1   | O     | 83  | ARG  |
| 1   | O     | 87  | ILE  |
| 1   | O     | 91  | LYS  |
| 1   | O     | 92  | GLU  |
| 1   | O     | 93  | THR  |
| 1   | O     | 102 | VAL  |
| 1   | O     | 106 | ARG  |
| 1   | O     | 107 | ARG  |
| 1   | O     | 110 | GLU  |
| 1   | O     | 115 | LEU  |
| 1   | O     | 117 | ARG  |
| 1   | O     | 118 | ASP  |
| 1   | O     | 124 | ILE  |
| 1   | O     | 125 | ARG  |
| 1   | O     | 131 | VAL  |
| 1   | O     | 136 | PHE  |
| 1   | O     | 137 | SER  |
| 1   | O     | 140 | LYS  |
| 1   | O     | 141 | VAL  |
| 1   | O     | 145 | LEU  |
| 1   | O     | 146 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 148 | VAL  |
| 1   | O     | 152 | ARG  |
| 1   | O     | 154 | ARG  |
| 1   | O     | 156 | ARG  |
| 1   | O     | 157 | ARG  |
| 1   | O     | 161 | LEU  |
| 1   | O     | 162 | PHE  |
| 1   | O     | 164 | THR  |
| 1   | O     | 169 | LEU  |
| 1   | O     | 170 | ILE  |
| 1   | O     | 172 | LYS  |
| 1   | O     | 173 | MET  |
| 1   | O     | 175 | GLN  |
| 1   | O     | 178 | VAL  |
| 1   | O     | 180 | VAL  |
| 1   | O     | 181 | THR  |
| 1   | O     | 187 | SER  |
| 1   | O     | 188 | ARG  |
| 1   | O     | 190 | MET  |
| 1   | O     | 191 | LEU  |
| 1   | O     | 194 | ILE  |
| 1   | O     | 195 | HIS  |
| 1   | O     | 196 | THR  |
| 1   | O     | 197 | LEU  |
| 1   | O     | 198 | ASP  |
| 1   | O     | 201 | ASP  |
| 1   | O     | 202 | LYS  |
| 1   | O     | 206 | VAL  |
| 1   | O     | 207 | LEU  |
| 1   | O     | 211 | ARG  |
| 1   | O     | 213 | MET  |
| 1   | O     | 214 | LEU  |
| 1   | O     | 218 | ARG  |
| 1   | O     | 219 | ARG  |
| 1   | O     | 221 | SER  |
| 1   | O     | 222 | GLU  |
| 1   | O     | 226 | GLN  |
| 1   | O     | 227 | THR  |
| 1   | O     | 229 | ILE  |
| 1   | O     | 235 | THR  |
| 1   | O     | 236 | ARG  |
| 1   | O     | 253 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 254 | LEU  |
| 1   | O     | 256 | VAL  |
| 1   | O     | 257 | LYS  |
| 1   | O     | 258 | GLU  |
| 1   | O     | 264 | THR  |
| 1   | O     | 267 | THR  |
| 1   | O     | 269 | CYS  |
| 1   | O     | 271 | MET  |
| 1   | O     | 278 | LYS  |
| 1   | O     | 280 | VAL  |
| 1   | O     | 281 | LYS  |
| 1   | O     | 287 | LEU  |
| 1   | O     | 288 | THR  |
| 1   | O     | 290 | ILE  |
| 1   | O     | 313 | ILE  |
| 1   | O     | 317 | ARG  |
| 1   | O     | 322 | LEU  |
| 1   | O     | 324 | ASN  |
| 1   | O     | 339 | THR  |
| 1   | O     | 351 | LEU  |
| 1   | O     | 368 | THR  |
| 1   | O     | 387 | GLN  |
| 1   | O     | 389 | ARG  |
| 1   | O     | 391 | VAL  |
| 1   | O     | 392 | LEU  |
| 1   | O     | 393 | GLU  |
| 1   | O     | 395 | MET  |
| 1   | O     | 399 | SER  |
| 1   | O     | 402 | ARG  |
| 1   | O     | 406 | LEU  |
| 1   | O     | 407 | ARG  |
| 1   | O     | 408 | VAL  |
| 1   | O     | 413 | VAL  |
| 1   | O     | 415 | ASN  |
| 1   | O     | 418 | LEU  |
| 1   | O     | 423 | SER  |
| 1   | O     | 425 | ILE  |
| 1   | O     | 426 | LEU  |
| 1   | O     | 428 | THR  |
| 1   | O     | 429 | ARG  |
| 1   | O     | 434 | GLU  |
| 1   | O     | 438 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 439 | THR  |
| 1   | O     | 441 | LEU  |
| 1   | O     | 445 | TYR  |
| 1   | O     | 446 | LEU  |
| 1   | O     | 451 | VAL  |
| 1   | O     | 453 | PHE  |
| 1   | O     | 455 | GLN  |
| 1   | O     | 457 | LEU  |
| 1   | O     | 459 | GLU  |
| 1   | O     | 460 | LEU  |
| 1   | O     | 461 | GLN  |
| 1   | O     | 462 | GLU  |
| 1   | O     | 463 | LYS  |
| 1   | O     | 465 | VAL  |
| 1   | O     | 466 | ILE  |
| 1   | O     | 467 | GLU  |
| 1   | O     | 468 | ARG  |
| 1   | O     | 474 | ILE  |
| 1   | O     | 475 | GLU  |
| 1   | O     | 476 | THR  |
| 1   | O     | 477 | THR  |
| 1   | O     | 478 | GLU  |
| 1   | O     | 482 | ARG  |
| 1   | O     | 487 | LYS  |
| 1   | O     | 488 | LYS  |
| 1   | O     | 490 | VAL  |
| 1   | O     | 494 | MET  |
| 1   | O     | 498 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 11  | GLN  |
| 1   | Y     | 26  | ASN  |
| 1   | Y     | 47  | HIS  |
| 1   | Y     | 56  | GLN  |
| 1   | Y     | 73  | GLN  |
| 1   | Y     | 81  | ASN  |
| 1   | Y     | 104 | GLN  |
| 1   | Y     | 114 | HIS  |
| 1   | Y     | 127 | ASN  |
| 1   | Y     | 147 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 185 | ASN  |
| 1   | Y     | 226 | GLN  |
| 1   | Y     | 246 | GLN  |
| 1   | Y     | 253 | GLN  |
| 1   | Y     | 324 | ASN  |
| 1   | Y     | 340 | ASN  |
| 1   | Y     | 396 | GLN  |
| 1   | Y     | 404 | HIS  |
| 1   | Y     | 415 | ASN  |
| 1   | Y     | 461 | GLN  |
| 1   | Y     | 480 | ASN  |
| 1   | Y     | 499 | HIS  |
| 1   | O     | 11  | GLN  |
| 1   | O     | 26  | ASN  |
| 1   | O     | 47  | HIS  |
| 1   | O     | 81  | ASN  |
| 1   | O     | 179 | HIS  |
| 1   | O     | 185 | ASN  |
| 1   | O     | 226 | GLN  |
| 1   | O     | 263 | ASN  |
| 1   | O     | 324 | ASN  |
| 1   | O     | 340 | ASN  |
| 1   | O     | 404 | HIS  |
| 1   | O     | 415 | ASN  |
| 1   | O     | 420 | GLN  |
| 1   | O     | 461 | GLN  |
| 1   | O     | 480 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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   | GOL  | Y     | 600 | -    | 5,5,5        | 0.65 | 0           | 5,5,5       | 0.95 | 0           |
| 3   | ATF  | O     | 601 | 2    | 31,35,35     | 2.04 | 7 (22%)     | 43,57,57    | 1.42 | 5 (11%)     |
| 3   | ATF  | Y     | 601 | 2    | 31,35,35     | 2.19 | 6 (19%)     | 43,57,57    | 1.80 | 7 (16%)     |
| 4   | GOL  | O     | 600 | -    | 5,5,5        | 0.63 | 0           | 5,5,5       | 0.59 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | GOL  | Y     | 600 | -    | -       | 2/4/4/4    | -       |
| 3   | ATF  | O     | 601 | 2    | -       | 5/19/50/50 | 0/3/3/3 |
| 3   | ATF  | Y     | 601 | 2    | -       | 7/19/50/50 | 0/3/3/3 |
| 4   | GOL  | O     | 600 | -    | -       | 4/4/4/4    | -       |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | Y     | 601 | ATF  | PB-O2B  | 6.64  | 1.69        | 1.56     |
| 3   | O     | 601 | ATF  | PB-O2B  | 5.63  | 1.67        | 1.56     |
| 3   | Y     | 601 | ATF  | PG-O3G  | 5.59  | 1.69        | 1.54     |
| 3   | O     | 601 | ATF  | PG-O2G  | 5.32  | 1.68        | 1.54     |
| 3   | Y     | 601 | ATF  | PG-O2G  | 5.05  | 1.68        | 1.54     |
| 3   | O     | 601 | ATF  | PG-O3G  | 3.96  | 1.65        | 1.54     |
| 3   | O     | 601 | ATF  | PB-O1B  | -3.79 | 1.44        | 1.51     |
| 3   | Y     | 601 | ATF  | PA-O3A  | 3.52  | 1.63        | 1.59     |
| 3   | Y     | 601 | ATF  | PB-O3A  | 2.90  | 1.61        | 1.58     |
| 3   | O     | 601 | ATF  | O2'-C2' | 2.40  | 1.48        | 1.43     |
| 3   | O     | 601 | ATF  | PA-O2A  | 2.23  | 1.65        | 1.55     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | O     | 601 | ATF  | C4-N3  | -2.10 | 1.30        | 1.34     |
| 3   | Y     | 601 | ATF  | PA-O1A | -2.06 | 1.43        | 1.50     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | Y     | 601 | ATF  | PB-O3A-PA   | -5.91 | 113.82      | 132.22   |
| 3   | Y     | 601 | ATF  | O2'-C2'-C1' | -5.50 | 91.17       | 110.10   |
| 3   | O     | 601 | ATF  | PB-O3A-PA   | -3.77 | 120.49      | 132.22   |
| 3   | O     | 601 | ATF  | O2'-C2'-C1' | -3.55 | 97.89       | 110.10   |
| 3   | Y     | 601 | ATF  | O4'-C1'-N9  | 3.52  | 114.84      | 108.09   |
| 3   | O     | 601 | ATF  | C1'-N9-C8   | -3.37 | 119.62      | 127.09   |
| 3   | Y     | 601 | ATF  | O5'-C5'-C4' | 3.21  | 119.91      | 108.99   |
| 3   | Y     | 601 | ATF  | C5'-C4'-C3' | -2.74 | 105.36      | 115.21   |
| 3   | O     | 601 | ATF  | C4-N9-C1'   | 2.58  | 132.67      | 126.63   |
| 3   | O     | 601 | ATF  | O3'-C3'-C2' | 2.30  | 119.20      | 111.82   |
| 3   | Y     | 601 | ATF  | O3G-PG-O2G  | 2.22  | 114.51      | 108.24   |
| 3   | Y     | 601 | ATF  | O2A-PA-O3A  | 2.20  | 113.23      | 107.27   |

There are no chirality outliers.

All (18) torsion outliers are listed below:

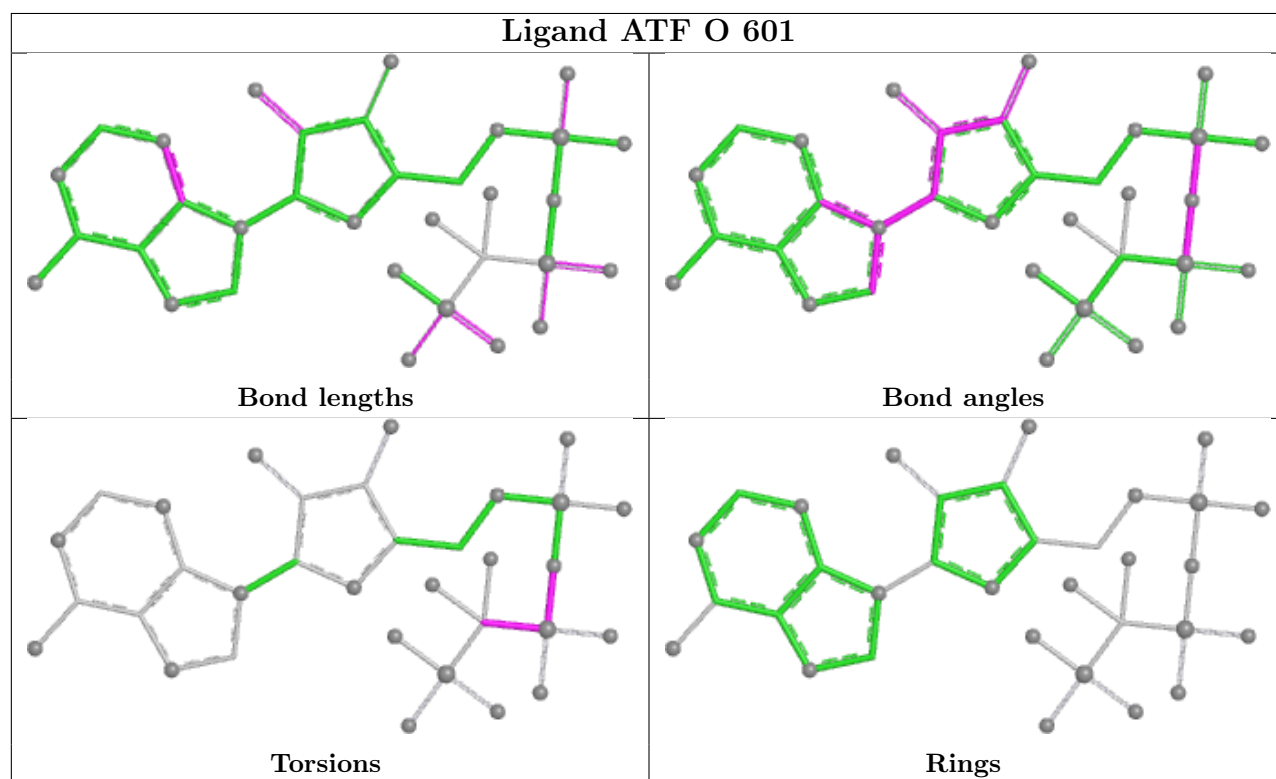
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | Y     | 601 | ATF  | F1B-C3B-PB-O1B |
| 3   | Y     | 601 | ATF  | F2B-C3B-PB-O1B |
| 3   | Y     | 601 | ATF  | F1B-C3B-PB-O3A |
| 3   | Y     | 601 | ATF  | F2B-C3B-PB-O3A |
| 3   | Y     | 601 | ATF  | C5'-O5'-PA-O2A |
| 3   | Y     | 601 | ATF  | C5'-O5'-PA-O3A |
| 3   | Y     | 601 | ATF  | C4'-C5'-O5'-PA |
| 3   | O     | 601 | ATF  | F1B-C3B-PB-O1B |
| 3   | O     | 601 | ATF  | F2B-C3B-PB-O1B |
| 3   | O     | 601 | ATF  | F1B-C3B-PB-O3A |
| 3   | O     | 601 | ATF  | F2B-C3B-PB-O3A |
| 4   | Y     | 600 | GOL  | C1-C2-C3-O3    |
| 4   | O     | 600 | GOL  | O1-C1-C2-C3    |
| 4   | O     | 600 | GOL  | C1-C2-C3-O3    |
| 4   | O     | 600 | GOL  | O2-C2-C3-O3    |
| 4   | Y     | 600 | GOL  | O2-C2-C3-O3    |
| 4   | O     | 600 | GOL  | O1-C1-C2-O2    |
| 3   | O     | 601 | ATF  | PA-O3A-PB-O2B  |

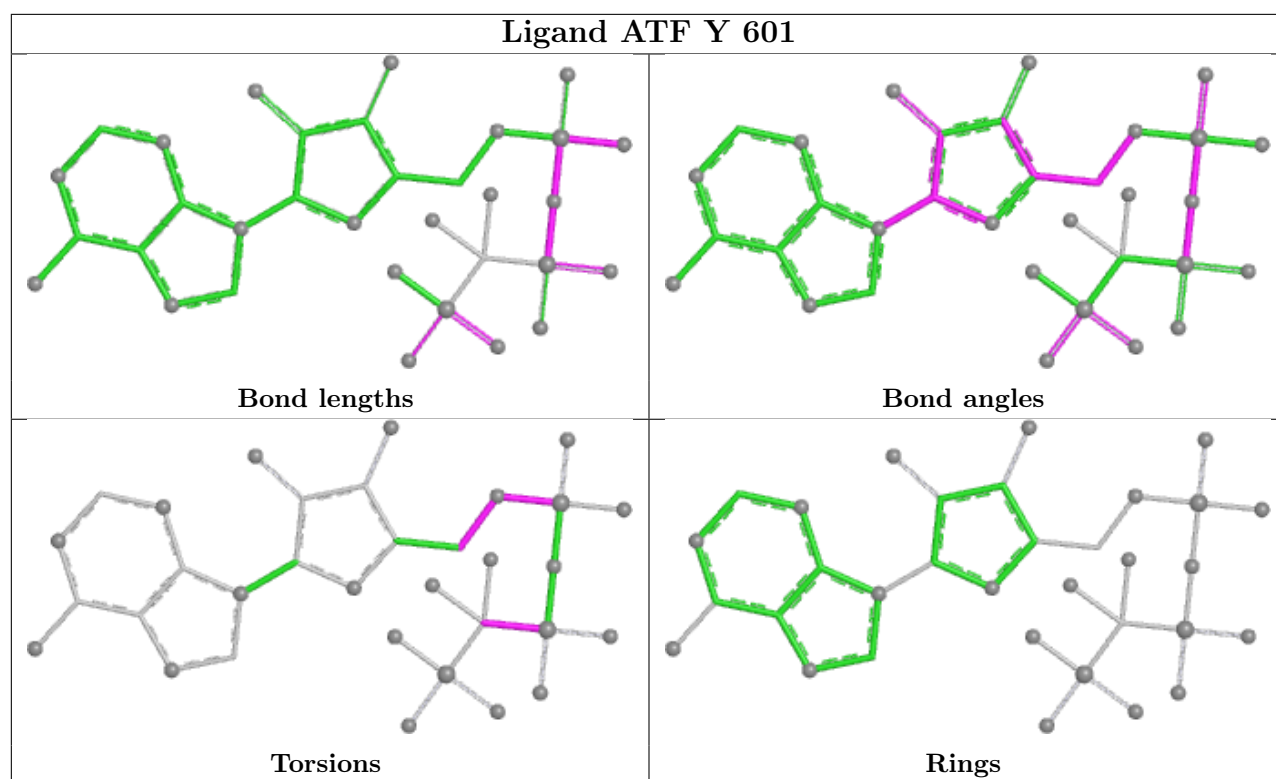
There are no ring outliers.

4 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | Y     | 600 | GOL  | 1       | 0            |
| 3   | O     | 601 | ATF  | 2       | 0            |
| 3   | Y     | 601 | ATF  | 3       | 0            |
| 4   | O     | 600 | GOL  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 [i](#)

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

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | O     | 494/501 (98%)  | -0.58  | 1 (0%) 91 83 | 9, 52, 92, 100        | 0     |
| 1   | Y     | 494/501 (98%)  | -0.79  | 0 100 100    | 7, 41, 80, 100        | 0     |
| All | All   | 988/1002 (98%) | -0.69  | 1 (0%) 92 86 | 7, 47, 88, 100        | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 296 | GLY  | 2.6  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | MG   | Y     | 602 | 1/1   | 0.80 | 0.16 | 43,43,43,43                | 0     |
| 2   | MG   | O     | 602 | 1/1   | 0.87 | 0.18 | 56,56,56,56                | 0     |
| 3   | ATF  | Y     | 601 | 33/33 | 0.92 | 0.10 | 42,42,42,42                | 0     |
| 3   | ATF  | O     | 601 | 33/33 | 0.95 | 0.08 | 56,56,56,56                | 0     |

*Continued on next page...*

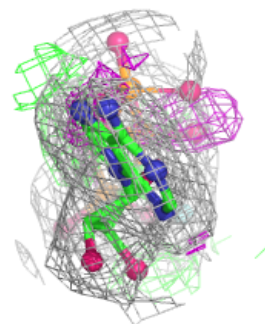
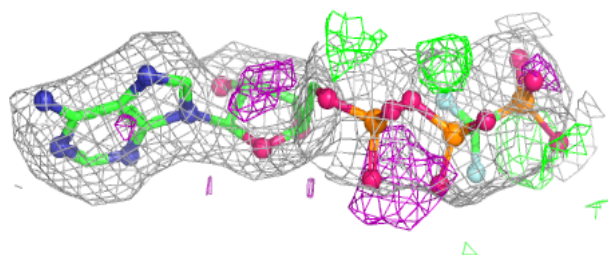
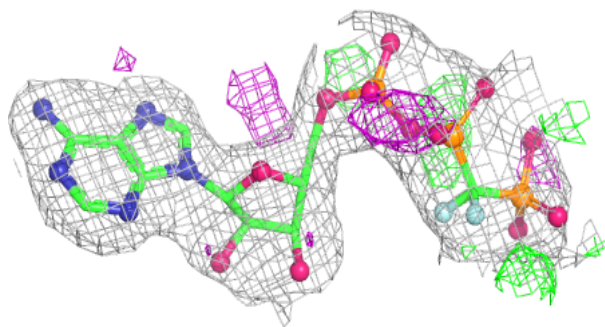
*Continued from previous page...*

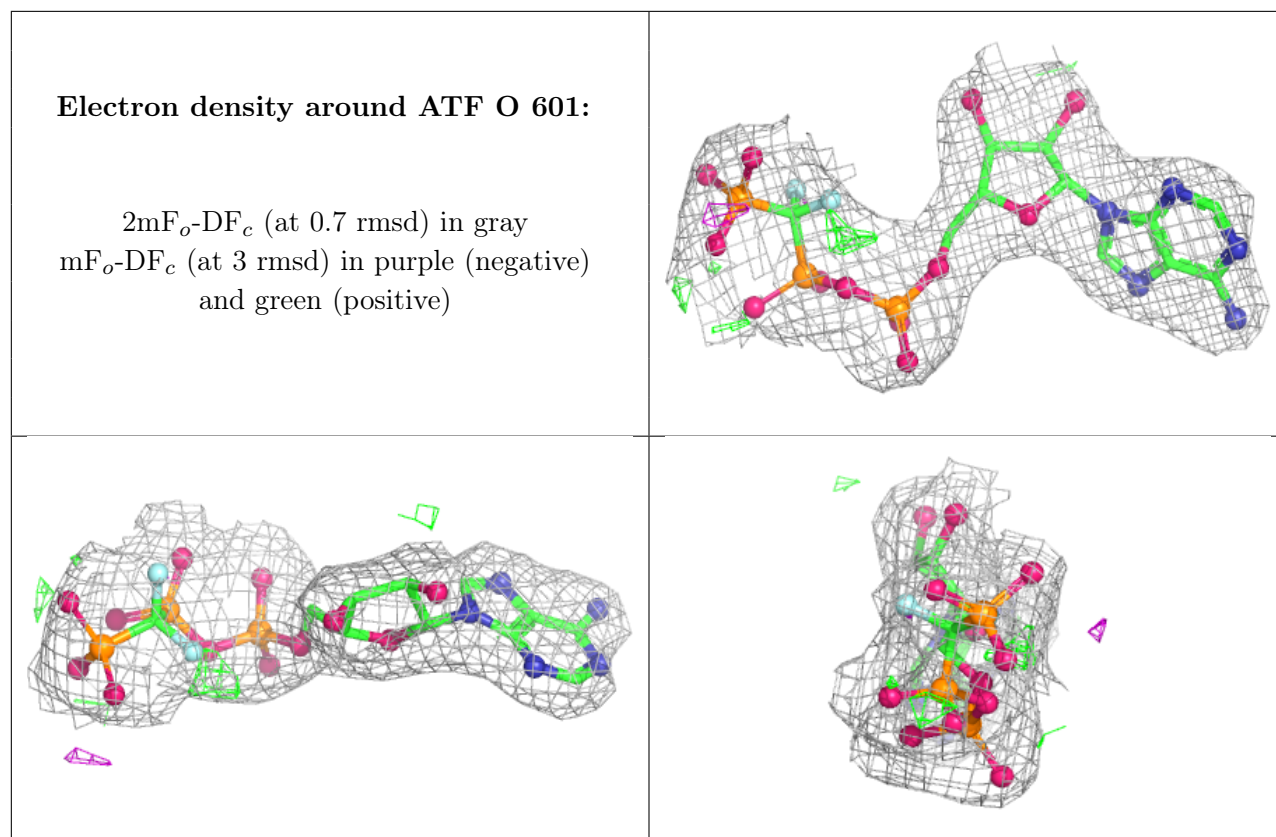
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | GOL  | O     | 600 | 6/6   | 0.96 | 0.07 | 31,31,31,31                 | 0     |
| 4   | GOL  | Y     | 600 | 6/6   | 0.98 | 0.05 | 14,14,14,14                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ATF Y 601:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.