



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:36 AM UTC

PDB ID : 4V7G / pdb\_00004v7g  
Title : Crystal Structure of Lumazine Synthase from Bacillus Anthracis  
Authors : Morgunova, E.; Illarionov, B.; Saller, S.; Popov, A.; Sambaiah, T.; Bacher, A.;  
Cushman, M.; Fischer, M.; Ladenstein, R.  
Deposited on : 2009-09-16  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

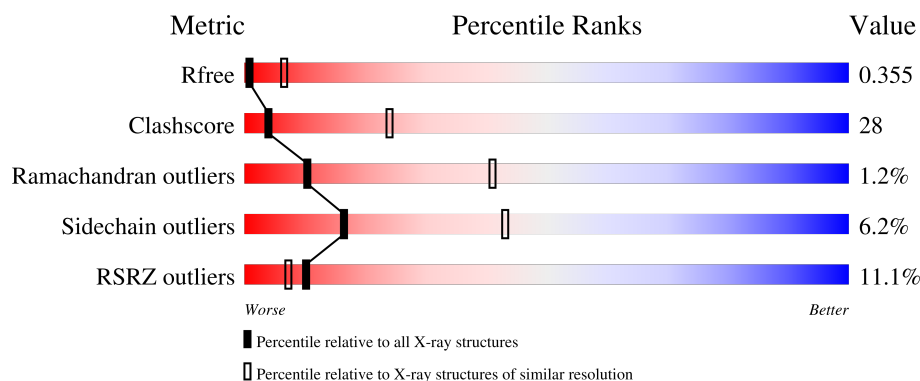
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |

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   | A1    | 153    |                  |
| 1   | A2    | 153    |                  |
| 1   | A3    | 153    |                  |
| 1   | A4    | 153    |                  |
| 1   | AA    | 153    |                  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AB    | 153    |                  |
| 1   | AC    | 153    |                  |
| 1   | AD    | 153    |                  |
| 1   | AE    | 153    |                  |
| 1   | AF    | 153    |                  |
| 1   | AG    | 153    |                  |
| 1   | AH    | 153    |                  |
| 1   | AI    | 153    |                  |
| 1   | AJ    | 153    |                  |
| 1   | AK    | 153    |                  |
| 1   | AL    | 153    |                  |
| 1   | AM    | 153    |                  |
| 1   | AN    | 153    |                  |
| 1   | AO    | 153    |                  |
| 1   | AP    | 153    |                  |
| 1   | AQ    | 153    |                  |
| 1   | AR    | 153    |                  |
| 1   | AS    | 153    |                  |
| 1   | AT    | 153    |                  |
| 1   | AU    | 153    |                  |
| 1   | AV    | 153    |                  |
| 1   | AW    | 153    |                  |
| 1   | AX    | 153    |                  |
| 1   | AY    | 153    |                  |
| 1   | AZ    | 153    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | B1    | 153    |                  |
| 1   | B2    | 153    |                  |
| 1   | B3    | 153    |                  |
| 1   | B4    | 153    |                  |
| 1   | BA    | 153    |                  |
| 1   | BB    | 153    |                  |
| 1   | BC    | 153    |                  |
| 1   | BD    | 153    |                  |
| 1   | BE    | 153    |                  |
| 1   | BF    | 153    |                  |
| 1   | BG    | 153    |                  |
| 1   | BH    | 153    |                  |
| 1   | BI    | 153    |                  |
| 1   | BJ    | 153    |                  |
| 1   | BK    | 153    |                  |
| 1   | BL    | 153    |                  |
| 1   | BM    | 153    |                  |
| 1   | BN    | 153    |                  |
| 1   | BO    | 153    |                  |
| 1   | BP    | 153    |                  |
| 1   | BQ    | 153    |                  |
| 1   | BR    | 153    |                  |
| 1   | BS    | 153    |                  |
| 1   | BT    | 153    |                  |
| 1   | BU    | 153    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | BV    | 153    |                  |
| 1   | BW    | 153    |                  |
| 1   | BX    | 153    |                  |
| 1   | BY    | 153    |                  |
| 1   | BZ    | 153    |                  |
| 1   | C1    | 153    |                  |
| 1   | C2    | 153    |                  |
| 1   | C3    | 153    |                  |
| 1   | C4    | 153    |                  |
| 1   | CA    | 153    |                  |
| 1   | CB    | 153    |                  |
| 1   | CC    | 153    |                  |
| 1   | CD    | 153    |                  |
| 1   | CE    | 153    |                  |
| 1   | CF    | 153    |                  |
| 1   | CG    | 153    |                  |
| 1   | CH    | 153    |                  |
| 1   | CI    | 153    |                  |
| 1   | CJ    | 153    |                  |
| 1   | CK    | 153    |                  |
| 1   | CL    | 153    |                  |
| 1   | CM    | 153    |                  |
| 1   | CN    | 153    |                  |
| 1   | CO    | 153    |                  |
| 1   | CP    | 153    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | CQ    | 153    |                  |
| 1   | CR    | 153    |                  |
| 1   | CS    | 153    |                  |
| 1   | CT    | 153    |                  |
| 1   | CU    | 153    |                  |
| 1   | CV    | 153    |                  |
| 1   | CW    | 153    |                  |
| 1   | CX    | 153    |                  |
| 1   | CY    | 153    |                  |
| 1   | CZ    | 153    |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | PO4  | A2    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | A4    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AC    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AE    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AH    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AJ    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AM    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AO    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AR    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AT    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | AW    | 201  | -         | -        | X       | -                |
| 2   | PO4  | AY    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | B2    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | B4    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BC    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BE    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BH    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BJ    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BM    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BO    | 1001 | -         | -        | X       | -                |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | PO4  | BR    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BT    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BW    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | BY    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | C2    | 2201 | -         | -        | X       | -                |
| 2   | PO4  | C4    | 4201 | -         | -        | X       | -                |
| 2   | PO4  | CC    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | CE    | 1001 | -         | -        | X       | -                |
| 2   | PO4  | CH    | 2201 | -         | -        | X       | -                |
| 2   | PO4  | CJ    | 4201 | -         | -        | X       | -                |
| 2   | PO4  | CM    | 2201 | -         | -        | X       | -                |
| 2   | PO4  | CO    | 4201 | -         | -        | X       | -                |
| 2   | PO4  | CR    | 2201 | -         | -        | X       | -                |
| 2   | PO4  | CT    | 4201 | -         | -        | X       | -                |
| 2   | PO4  | CW    | 2201 | -         | -        | X       | -                |
| 2   | PO4  | CY    | 4201 | -         | -        | X       | -                |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 102534 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 6,7-dimethyl-8-ribityllumazine synthase.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AA    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AB    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AC    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AD    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AE    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AF    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AG    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AH    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AI    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AJ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AK    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AL    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AM    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AN    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AO    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AP    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AQ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AR    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AS    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AT    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AU    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AV    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | AW    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AX    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AY    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | AZ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | A1    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 723 | 193 | 210 | 3 |         |         |       |
| 1   | A2    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | A3    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | A4    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1132  | 724 | 193 | 212 | 3 |         |         |       |
| 1   | BA    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BB    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BC    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BD    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BE    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BF    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BG    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | BH    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BI    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BJ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BK    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BL    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BM    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BN    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BO    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BP    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BQ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BR    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BS    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BT    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BU    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BV    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BW    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BX    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BY    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | BZ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | B1    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | B2    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

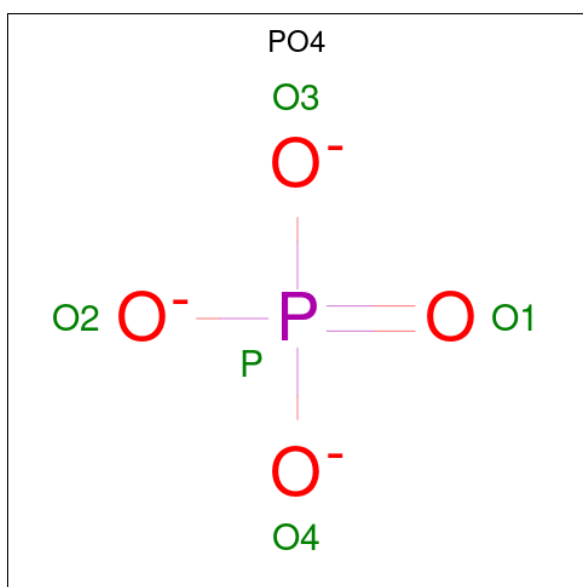
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | B3    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | B4    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CA    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CB    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CC    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CD    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CE    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CF    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CG    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CH    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CI    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CJ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CK    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CL    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CM    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CN    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CO    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CP    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CQ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CR    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CS    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | CT    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CU    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CV    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CW    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CX    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CY    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | CZ    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | C1    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | C2    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | C3    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |
| 1   | C4    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 193 | 214 | 3 |         |         |       |

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | AA    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AB    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AC    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AD    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AE    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AF    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AG    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AH    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AI    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AJ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AK    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AL    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AM    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AN    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AO    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AP    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AQ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AR    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AS    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AT    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AU    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AV    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | AW    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AX    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AY    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | AZ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A1    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A2    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A3    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A4    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BA    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BB    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BC    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BD    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BE    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BF    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BG    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BH    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BI    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BJ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BK    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BL    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BM    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | BN    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BO    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BP    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BQ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BR    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BS    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BT    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BU    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BV    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BW    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BX    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BY    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | BZ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B1    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B2    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B3    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B4    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CA    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CB    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CC    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CD    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | CE    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CF    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CG    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CH    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CI    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CJ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CK    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CL    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CM    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CN    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CO    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CP    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CQ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CR    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CS    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CT    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CU    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CV    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CW    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CX    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | CY    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

*Continued on next page...*

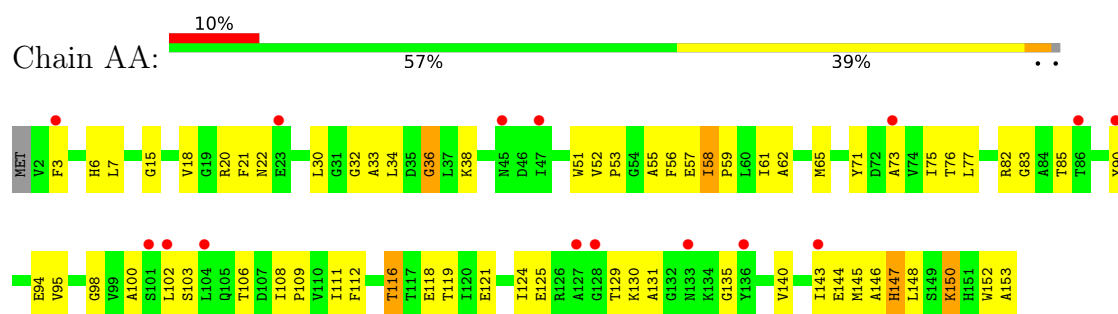
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | CZ    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C1    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C2    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C3    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C4    | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

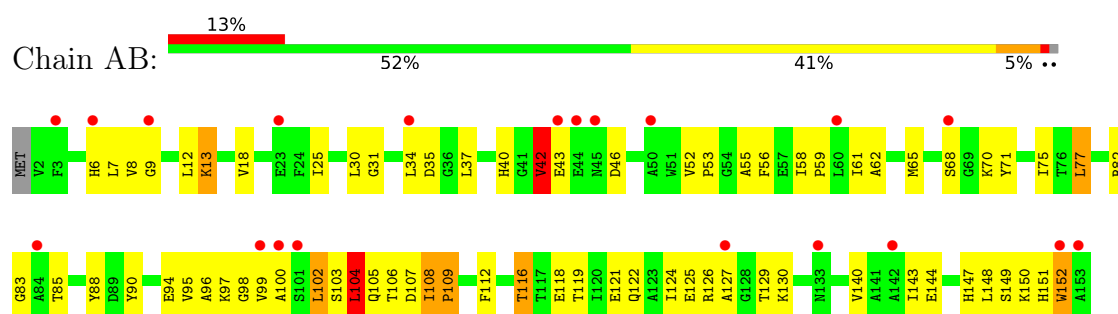
### 3 Residue-property plots [i](#)

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.

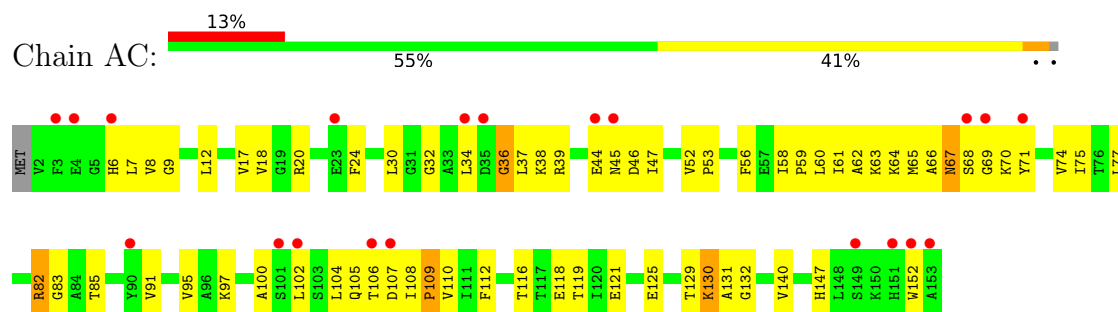
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

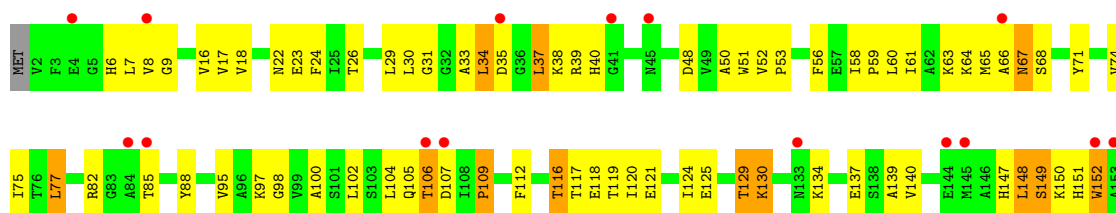


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

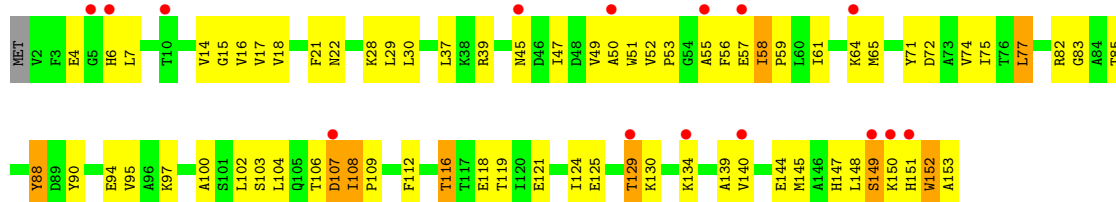


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

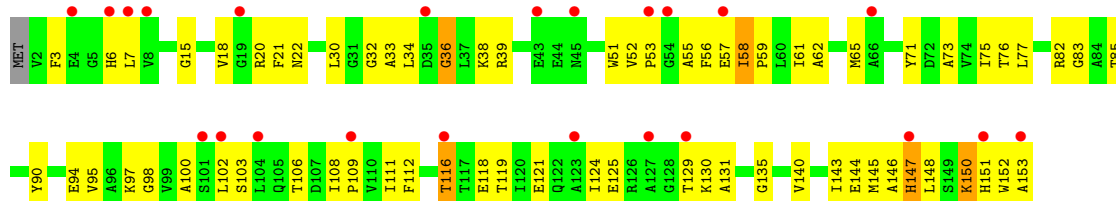




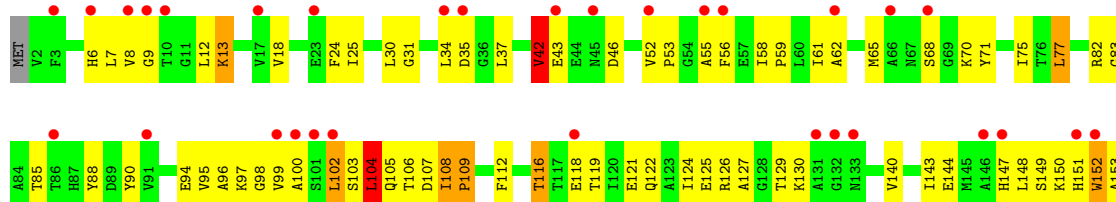
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



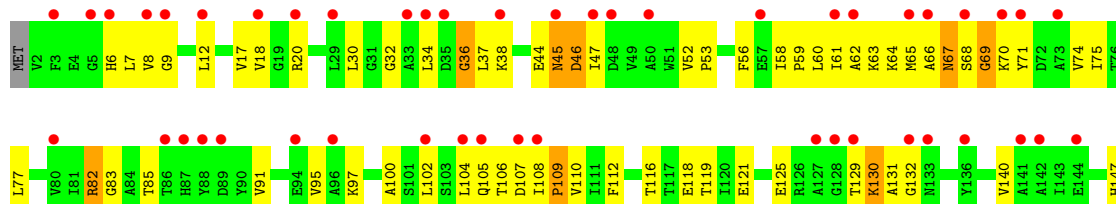
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

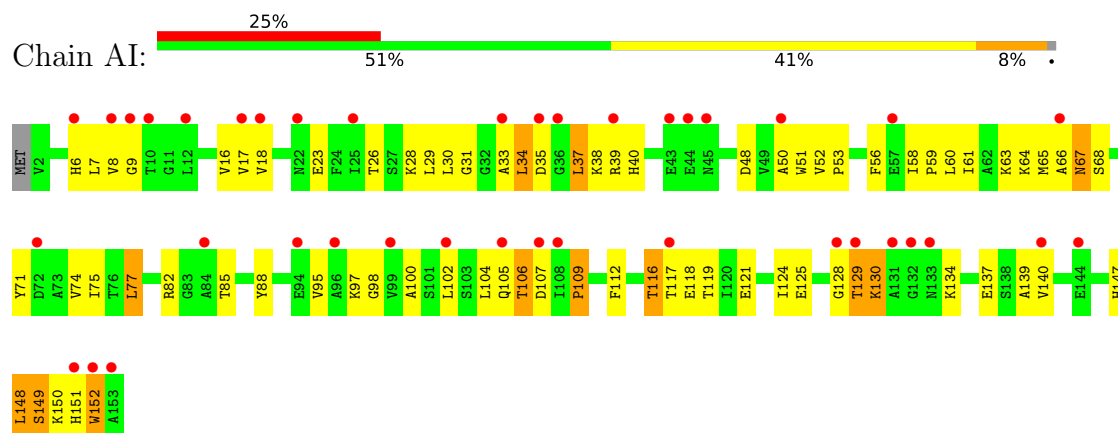


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

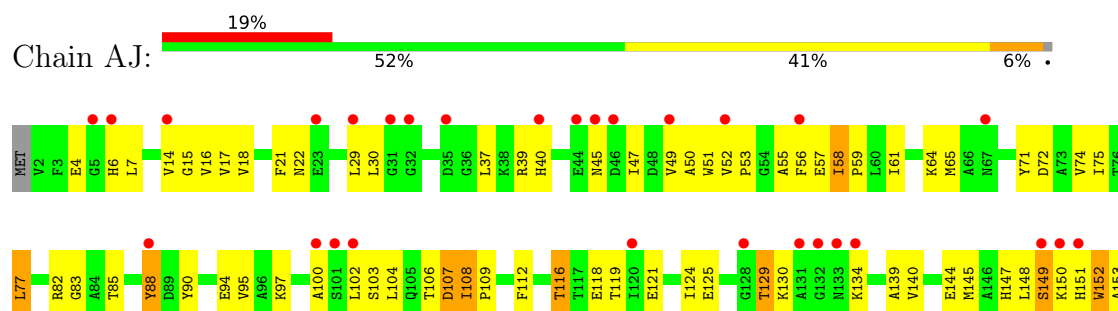




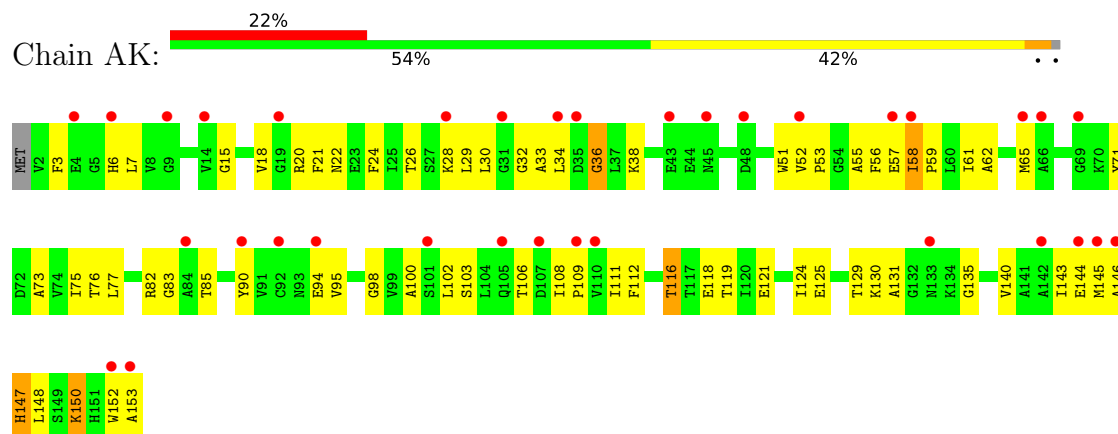
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



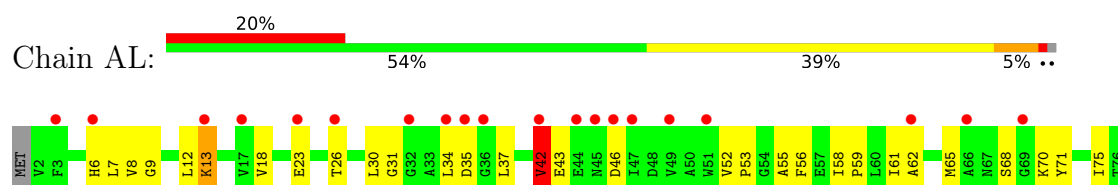
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

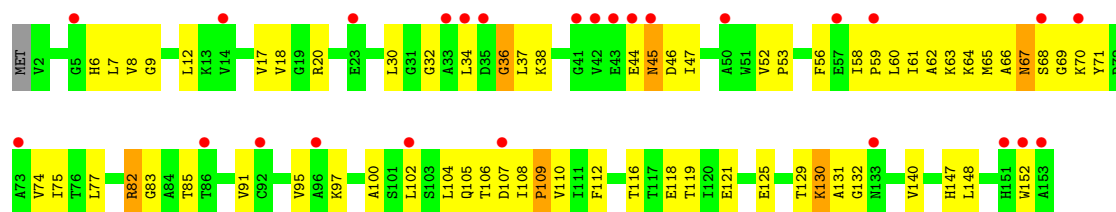


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase





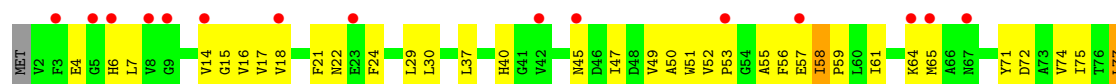
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



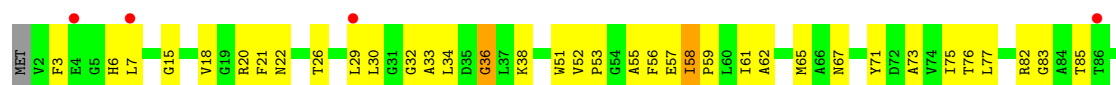
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

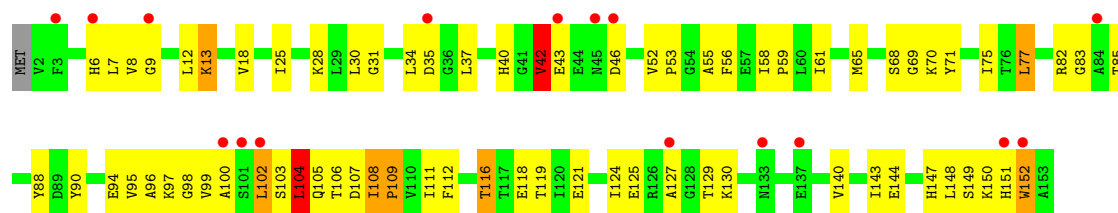


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

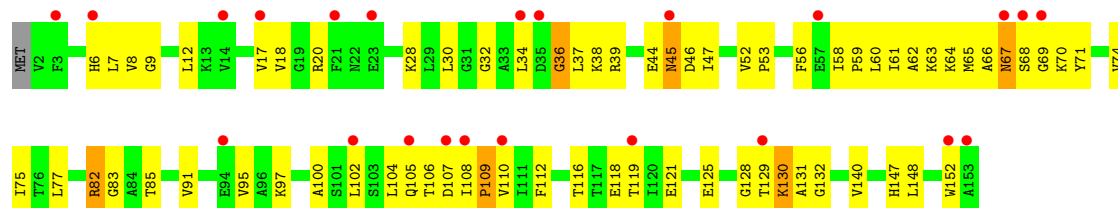


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

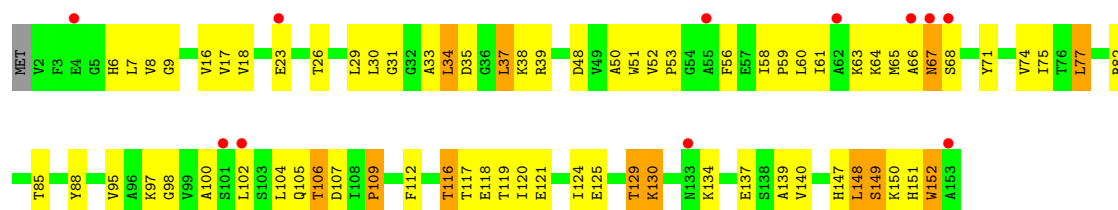




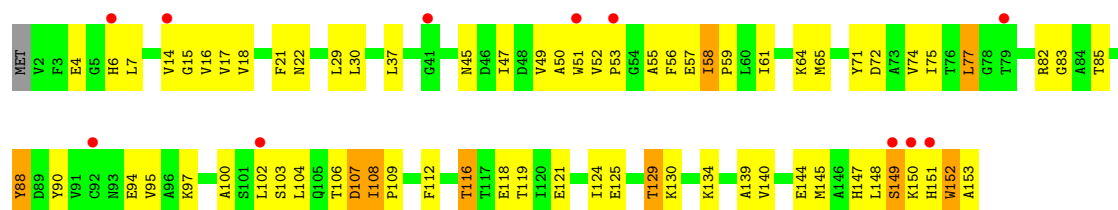
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



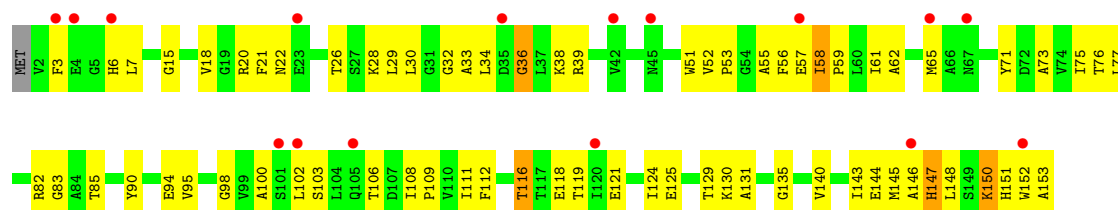
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



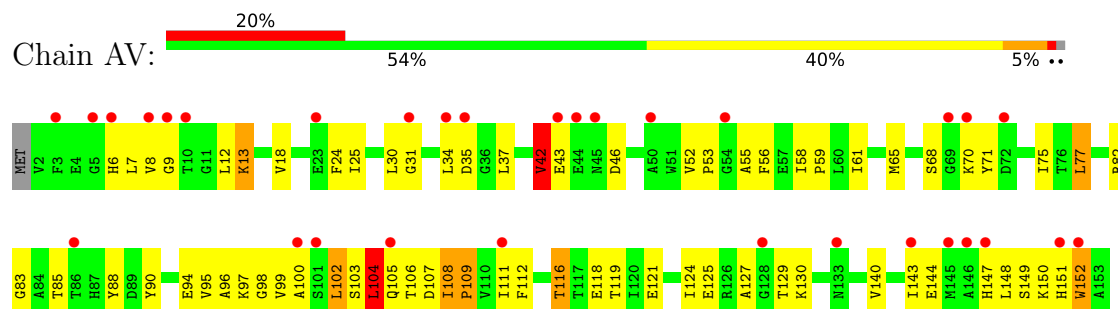
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



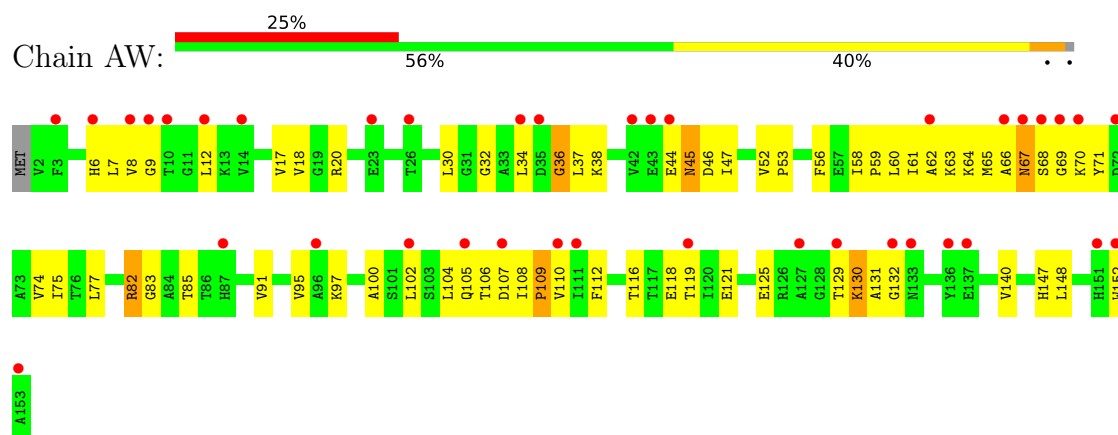
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



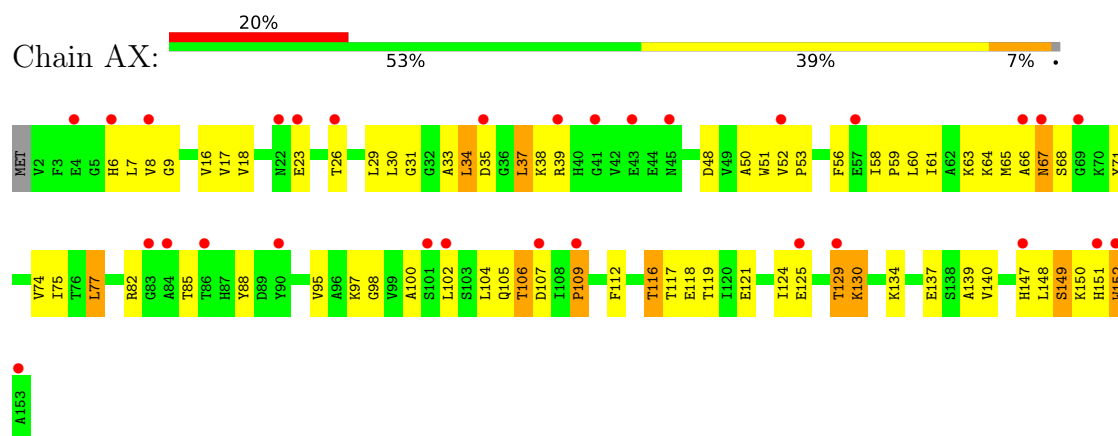
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



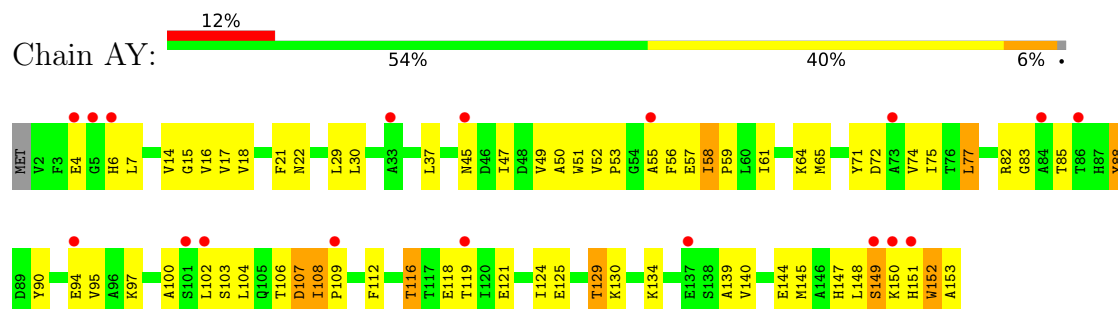
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



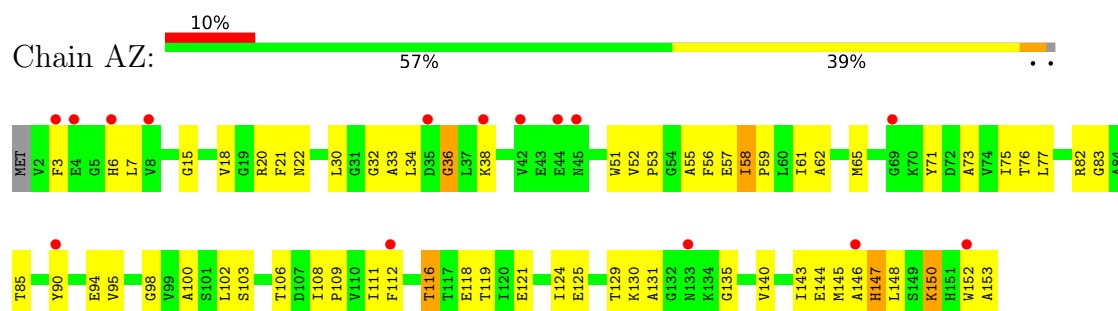
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



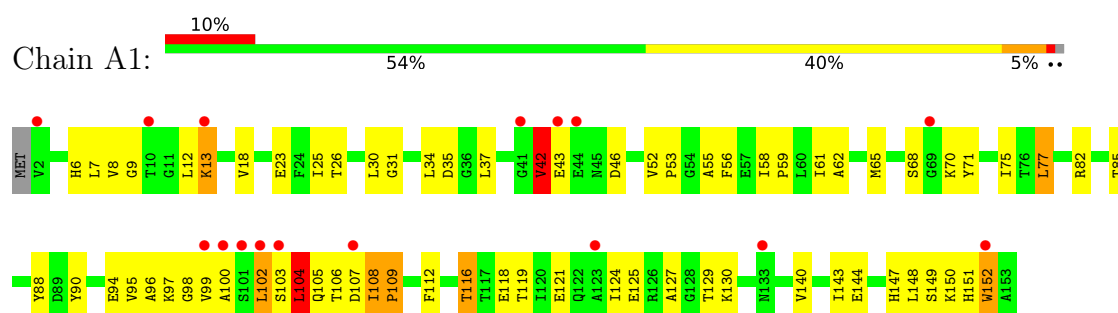
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



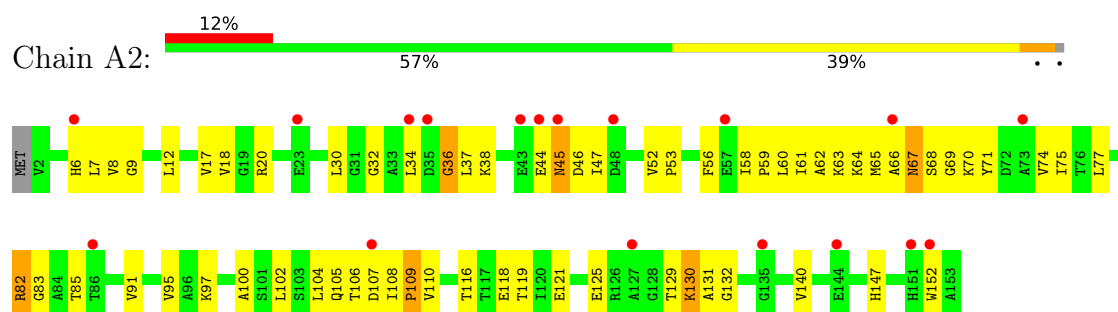
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



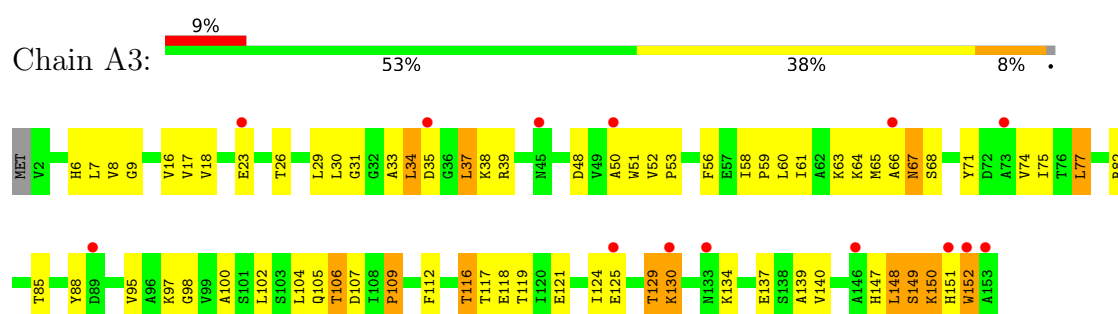
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



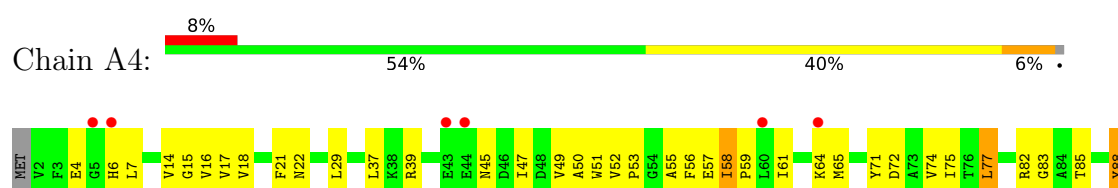
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase





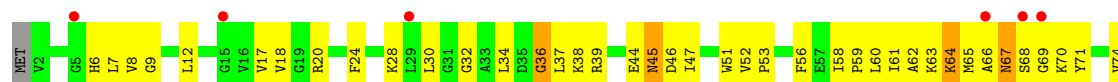
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



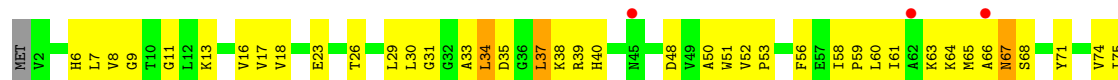
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

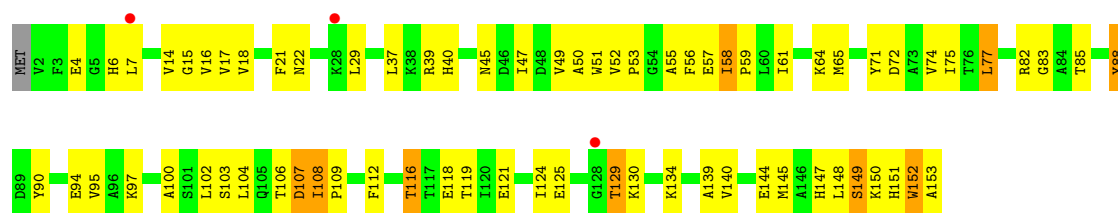


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

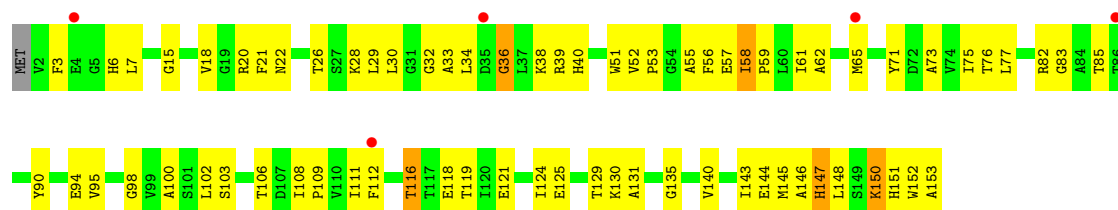


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

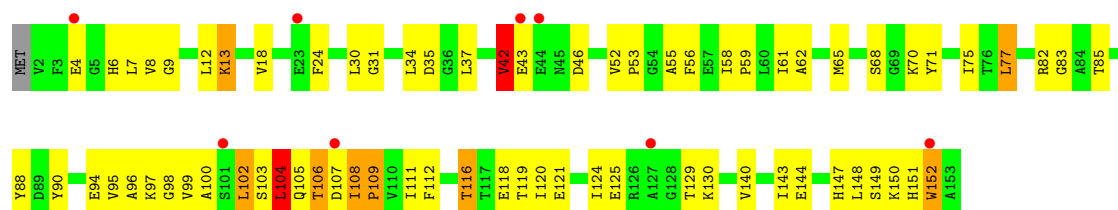




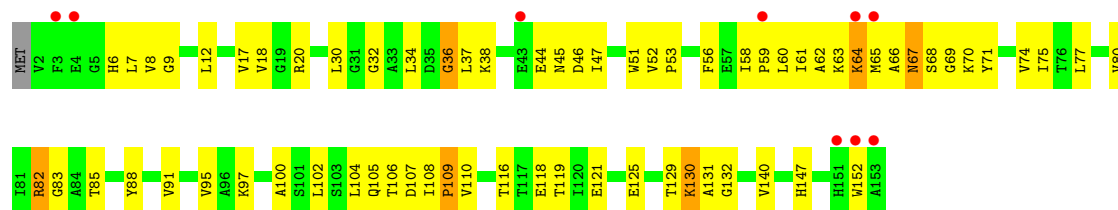
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



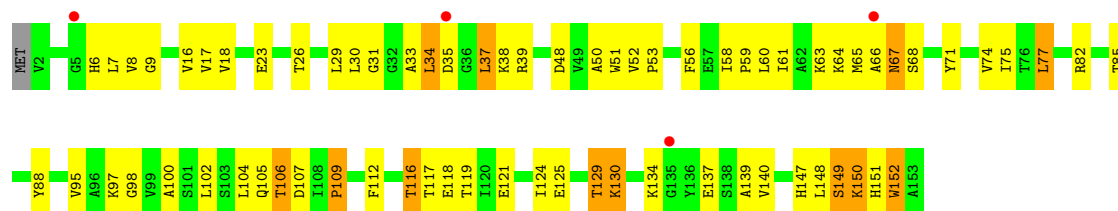
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

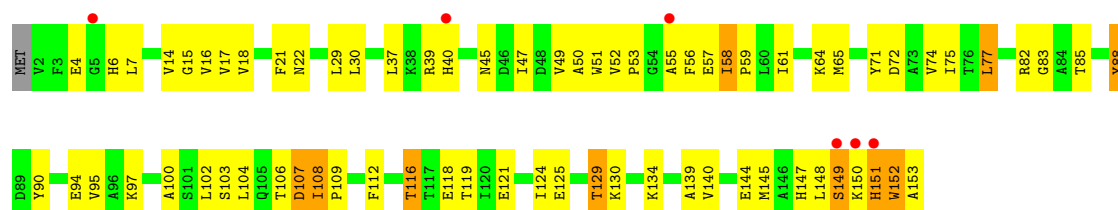


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



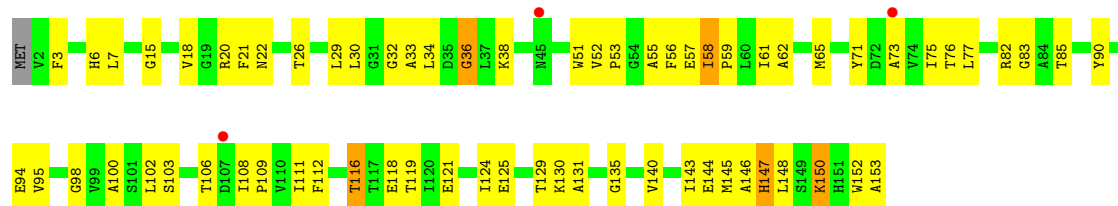
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BJ: 



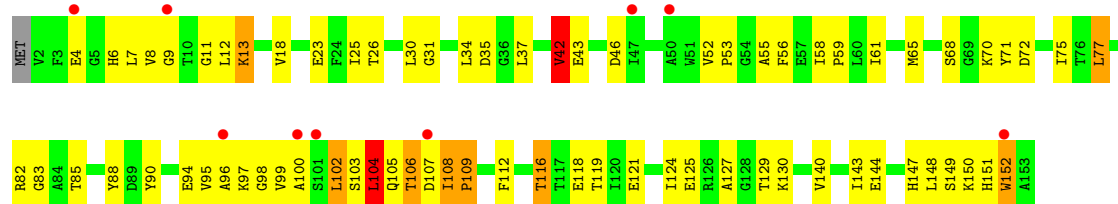
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BK: 



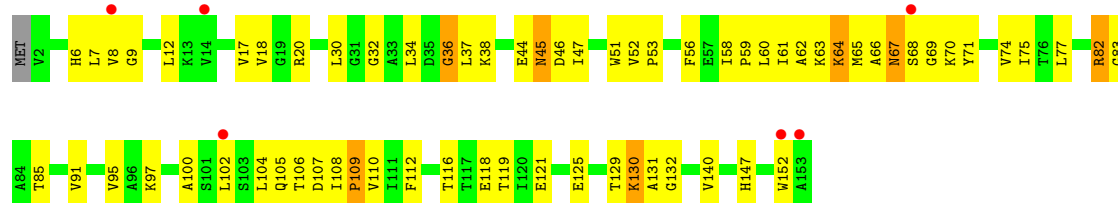
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BL: 



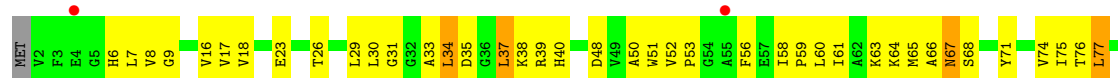
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

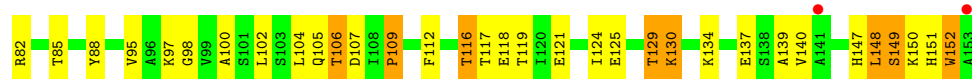
Chain BM: 



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BN: 





- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



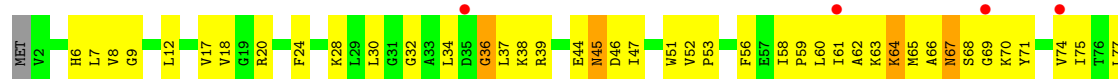
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

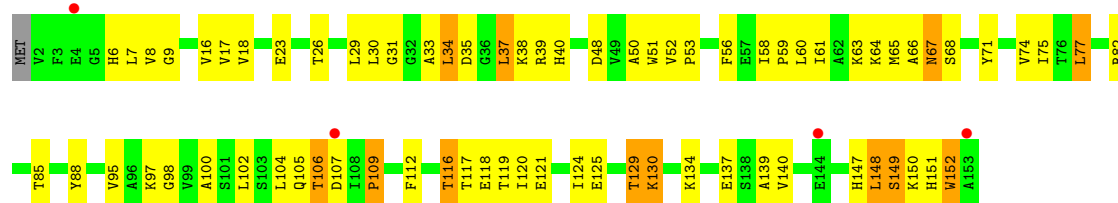


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

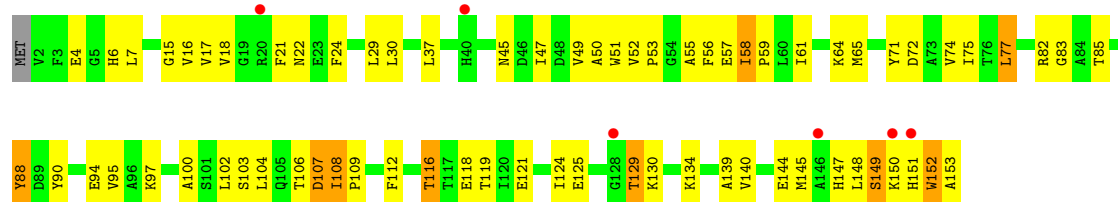


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

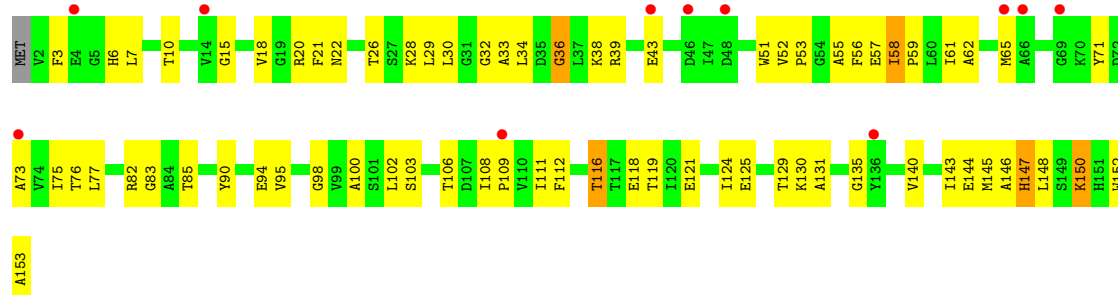




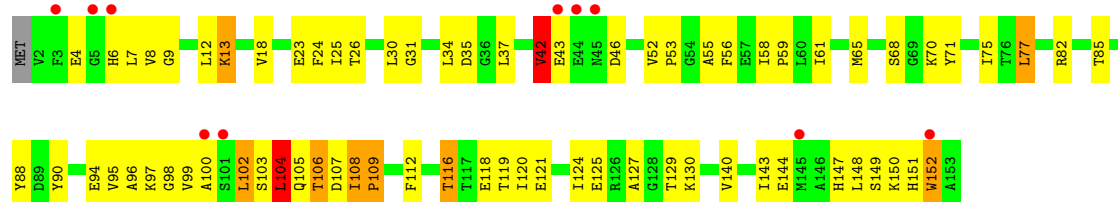
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

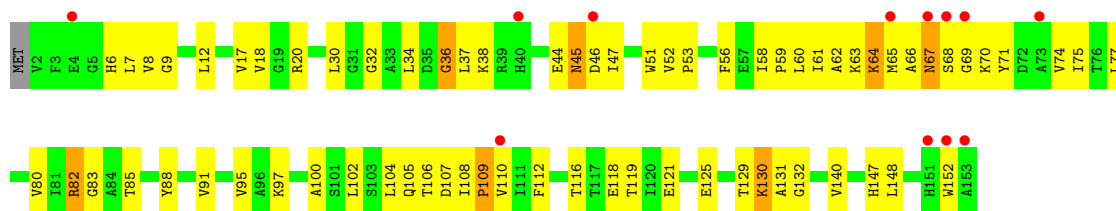


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

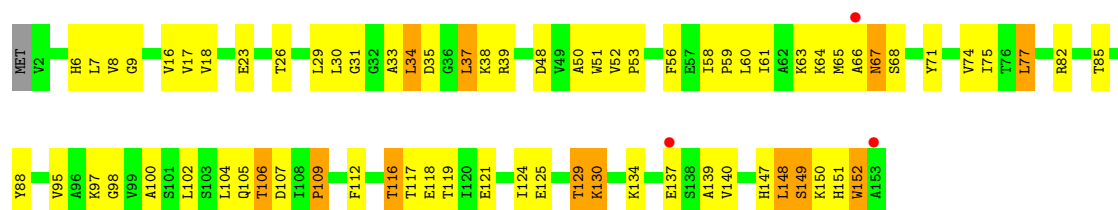


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

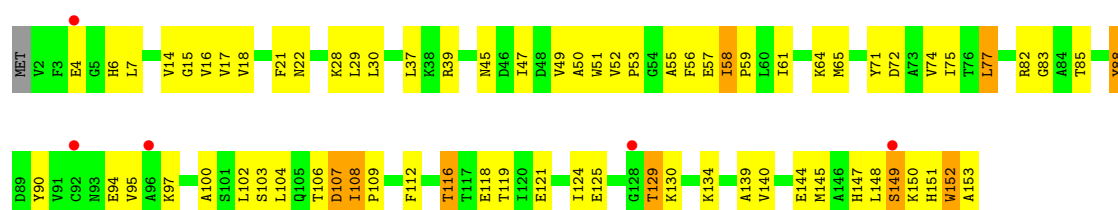




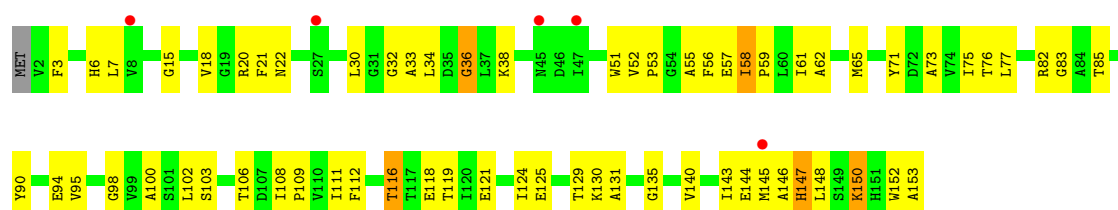
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



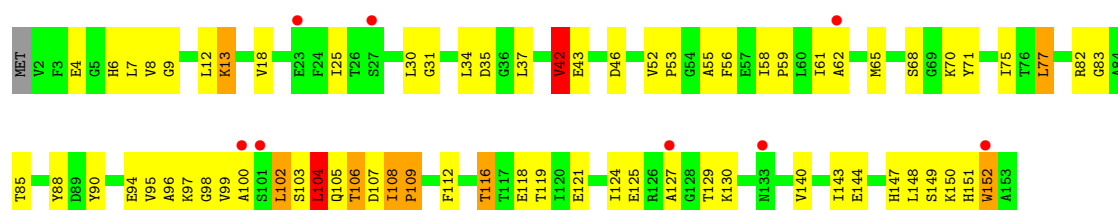
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

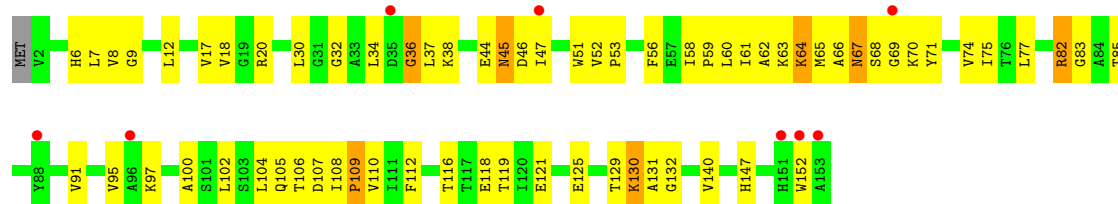


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



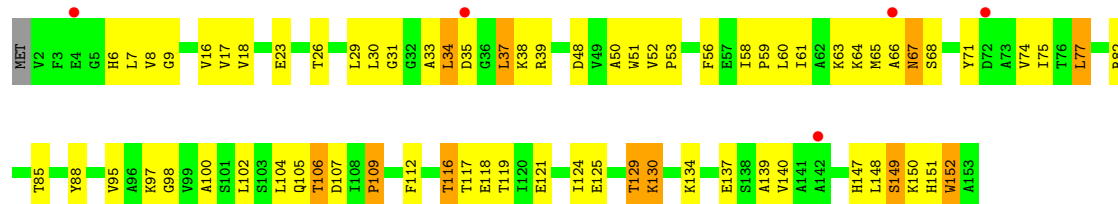
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B2: 



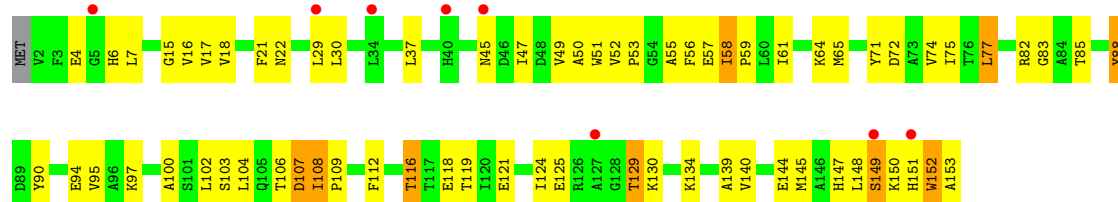
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B3: 



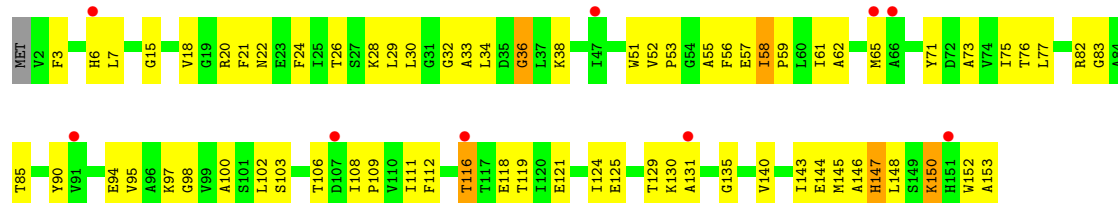
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B4: 



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CA: 



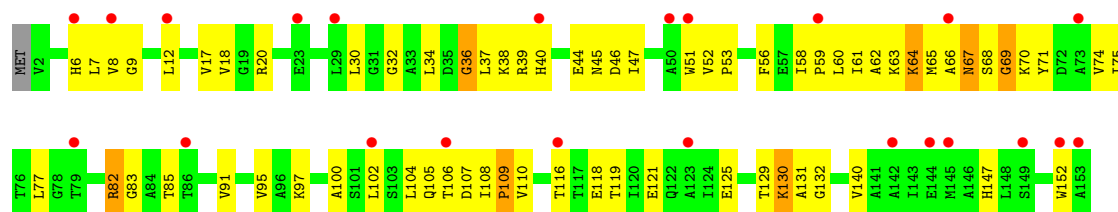
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CB: 

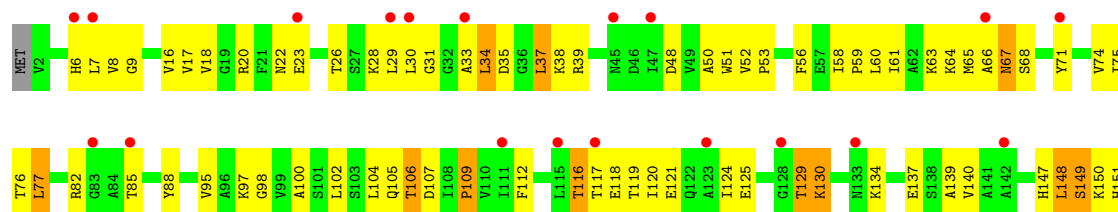




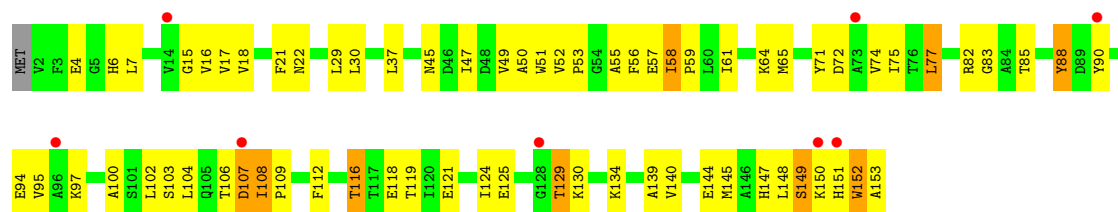
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



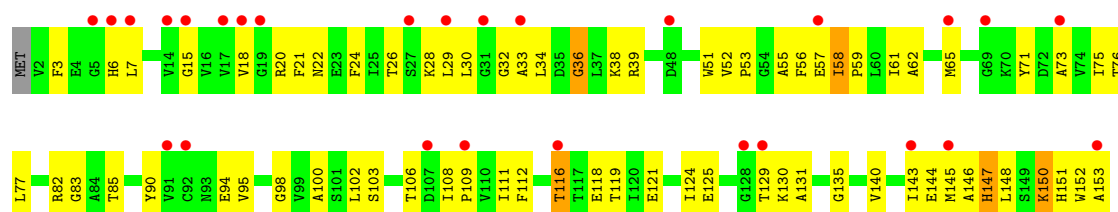
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



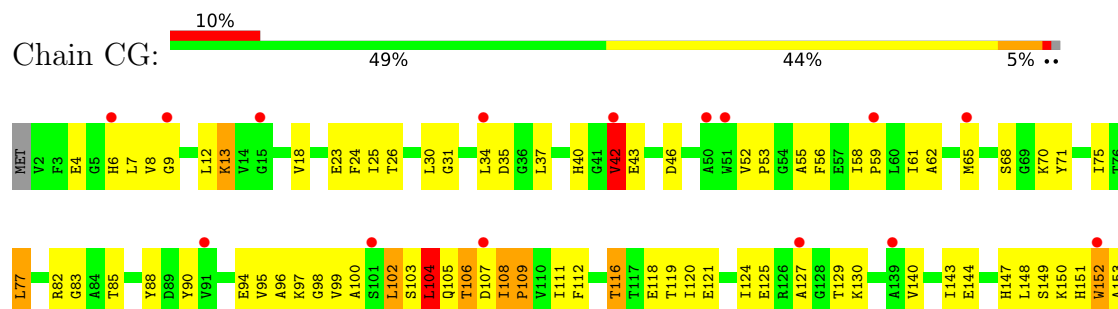
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



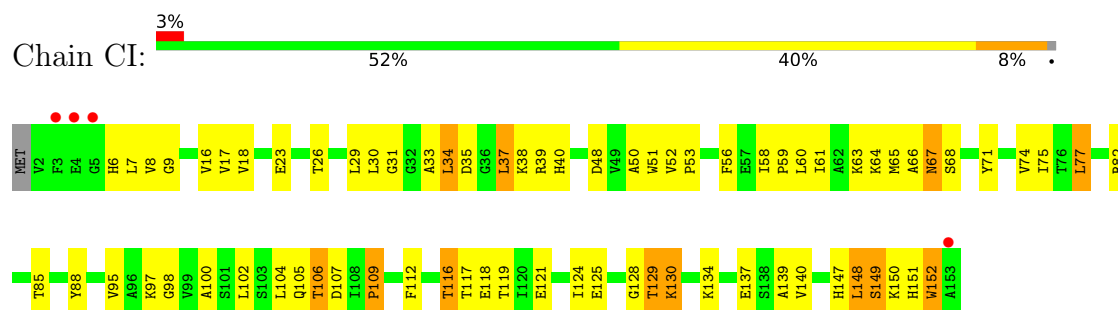
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



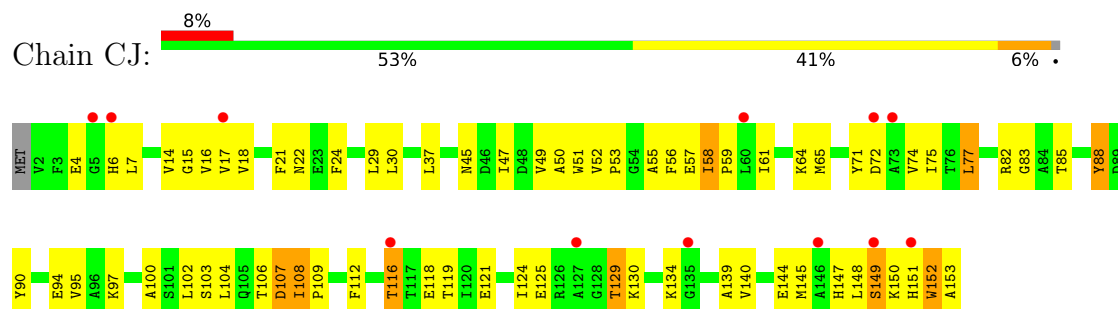
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



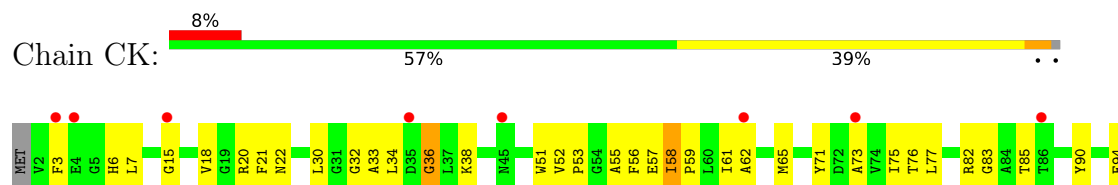
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

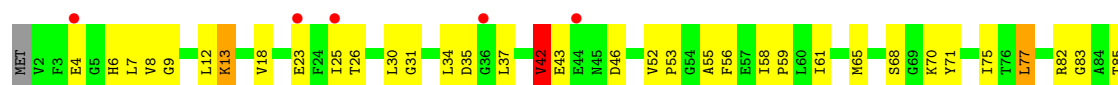


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

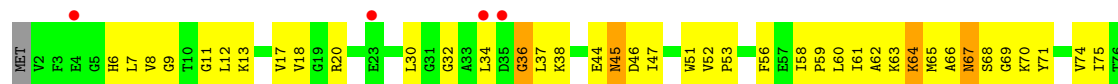




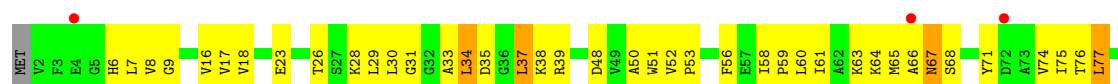
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



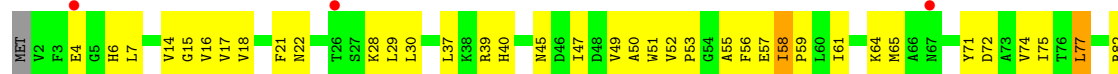
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

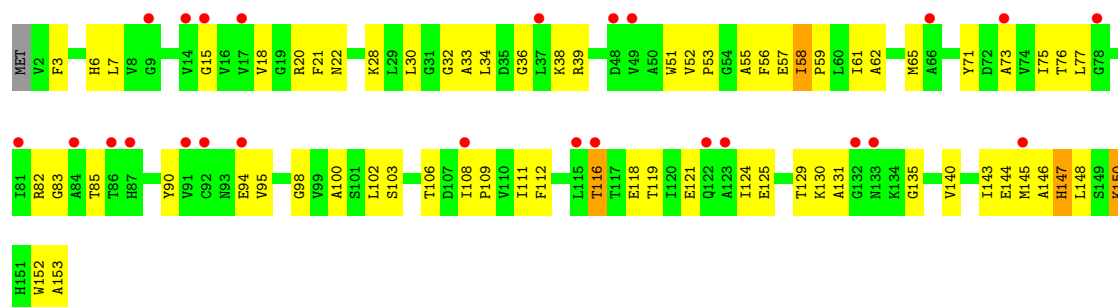


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

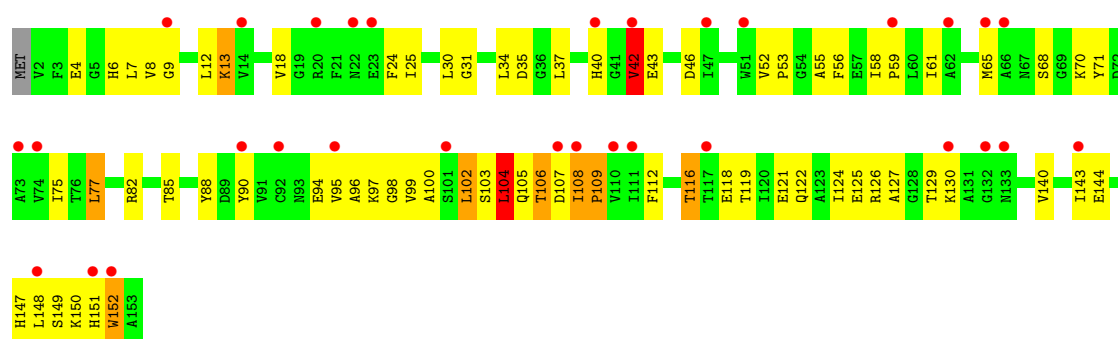


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

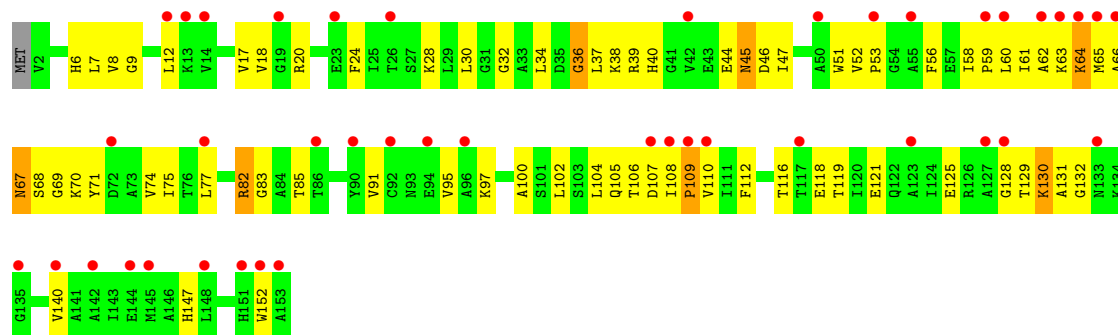




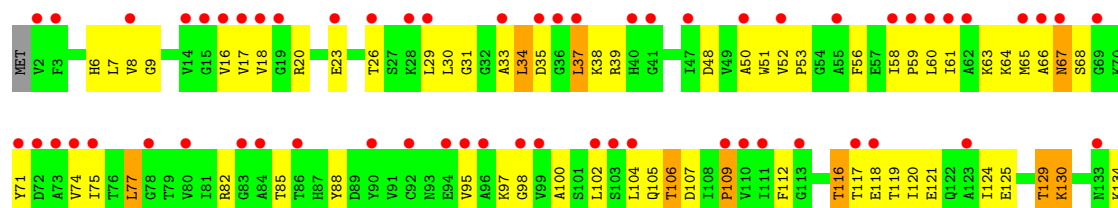
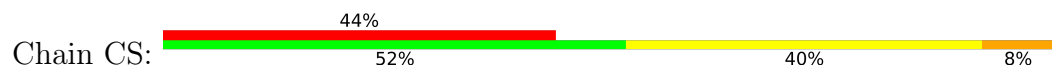
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

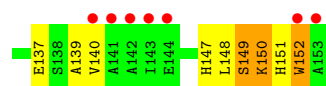


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

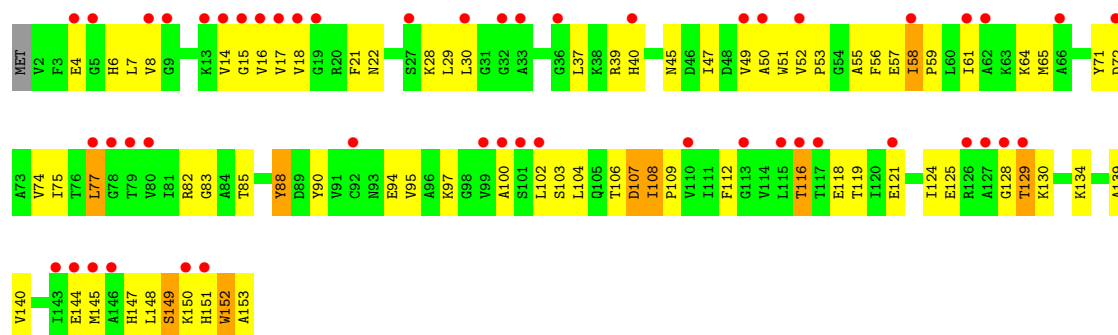


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

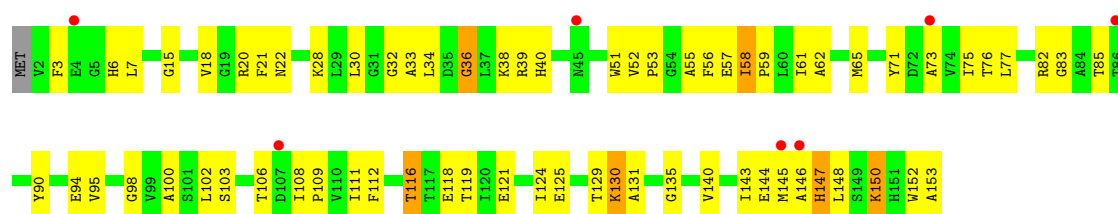




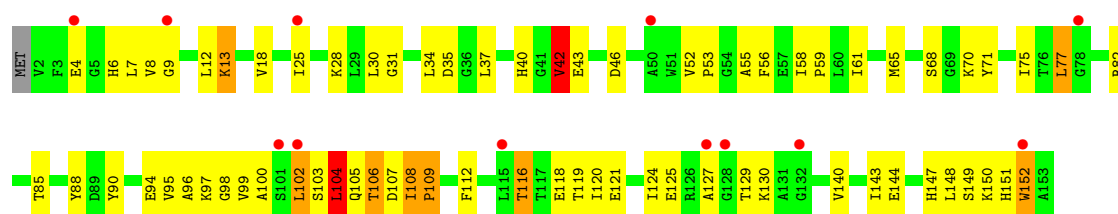
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



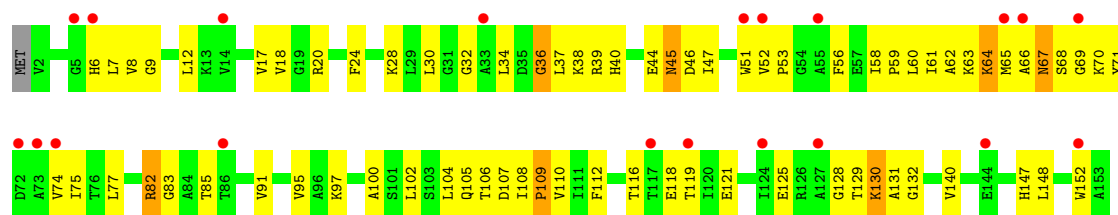
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



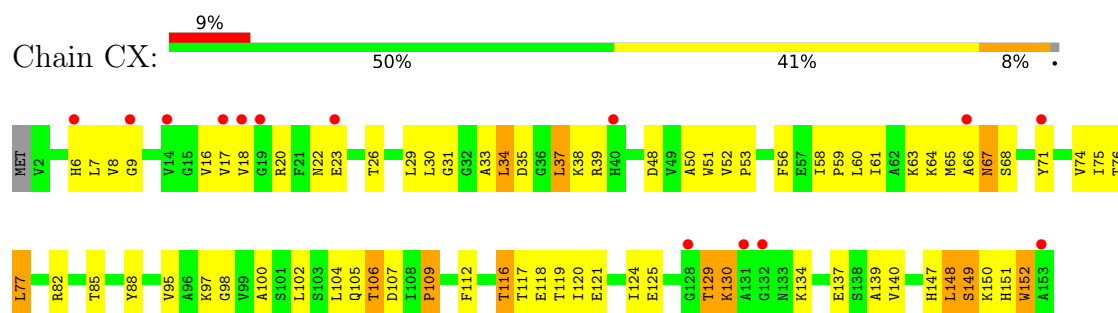
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



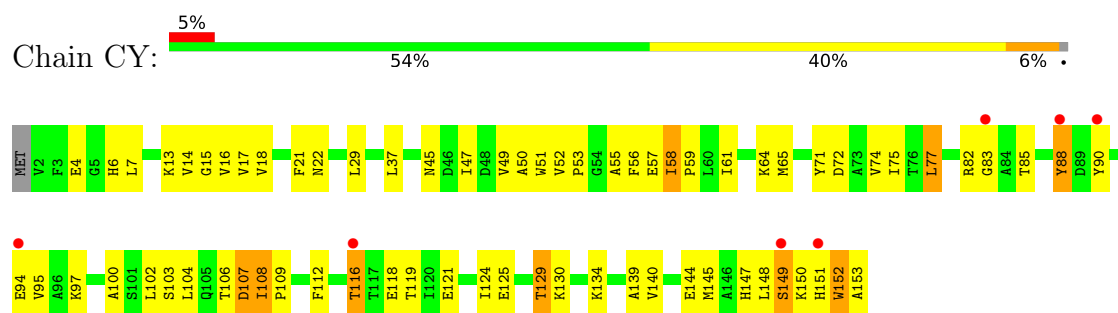
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



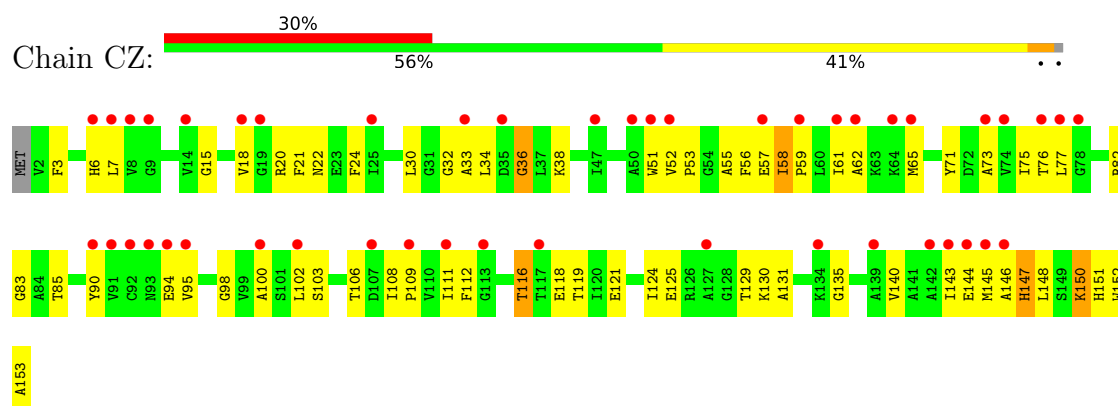
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



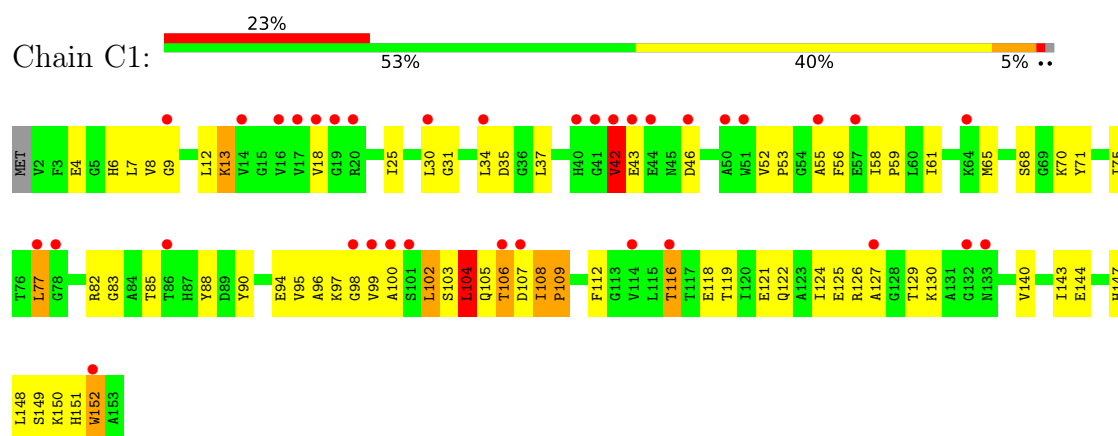
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

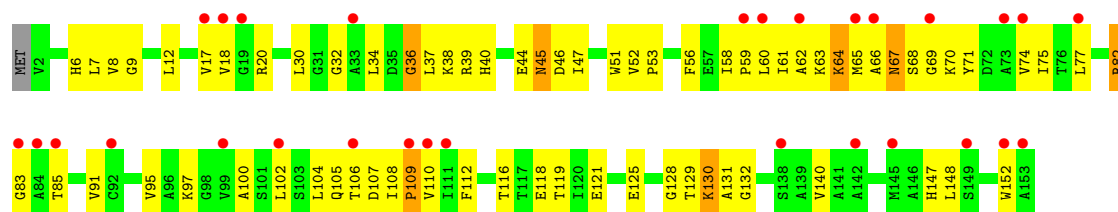


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



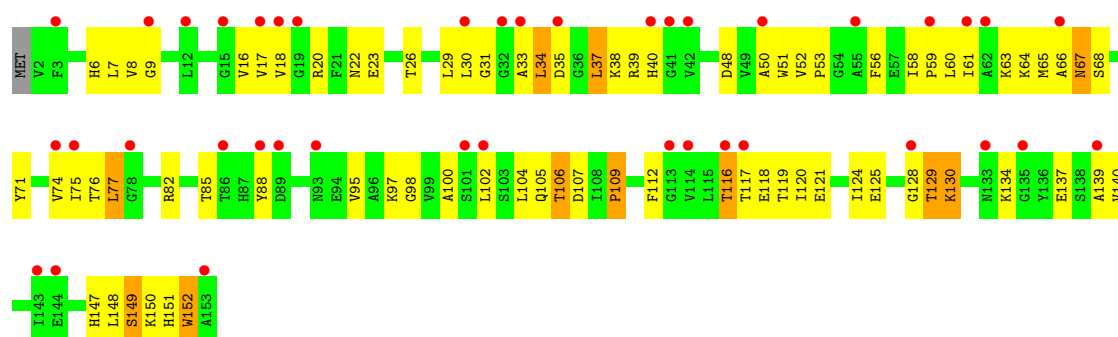
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C2: 



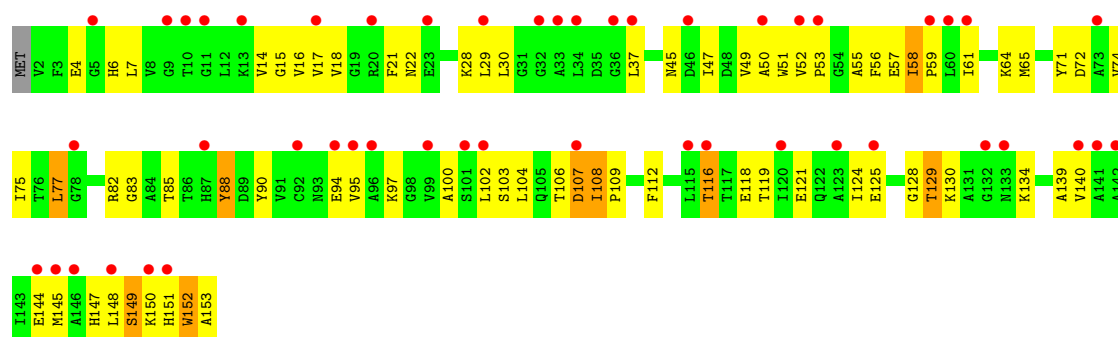
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C3: 



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C4: 



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 157.20Å 222.24Å 473.49Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 15.00 – 3.50<br>15.00 – 3.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.8 (15.00-3.50)<br>91.7 (15.00-3.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.29                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.93 (at 3.48Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.235 , 0.286<br>0.351 , 0.355                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3896 reflections (1.86%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.104                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.21 , 36.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.74                                                        | EDS              |
| Total number of atoms                                                   | 102534                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 104.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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   | A1    | 0.59         | 0/1149      | 1.06        | 9/1558 (0.6%)  |
| 1   | A2    | 0.43         | 0/1152      | 1.03        | 4/1562 (0.3%)  |
| 1   | A3    | 0.43         | 0/1152      | 1.26        | 11/1562 (0.7%) |
| 1   | A4    | 0.47         | 0/1152      | 0.89        | 5/1562 (0.3%)  |
| 1   | AA    | 0.43         | 0/1149      | 0.82        | 2/1558 (0.1%)  |
| 1   | AB    | 0.59         | 0/1149      | 1.06        | 9/1558 (0.6%)  |
| 1   | AC    | 0.43         | 0/1152      | 1.03        | 4/1562 (0.3%)  |
| 1   | AD    | 0.43         | 0/1152      | 1.26        | 11/1562 (0.7%) |
| 1   | AE    | 0.47         | 0/1152      | 0.89        | 5/1562 (0.3%)  |
| 1   | AF    | 0.43         | 0/1149      | 0.82        | 2/1558 (0.1%)  |
| 1   | AG    | 0.59         | 0/1149      | 1.06        | 9/1558 (0.6%)  |
| 1   | AH    | 0.43         | 0/1152      | 1.03        | 4/1562 (0.3%)  |
| 1   | AI    | 0.43         | 0/1152      | 1.26        | 11/1562 (0.7%) |
| 1   | AJ    | 0.47         | 0/1152      | 0.89        | 5/1562 (0.3%)  |
| 1   | AK    | 0.43         | 0/1149      | 0.82        | 2/1558 (0.1%)  |
| 1   | AL    | 0.59         | 0/1149      | 1.06        | 9/1558 (0.6%)  |
| 1   | AM    | 0.43         | 0/1152      | 1.03        | 4/1562 (0.3%)  |
| 1   | AN    | 0.43         | 0/1152      | 1.26        | 11/1562 (0.7%) |
| 1   | AO    | 0.47         | 0/1152      | 0.89        | 5/1562 (0.3%)  |
| 1   | AP    | 0.43         | 0/1149      | 0.82        | 2/1558 (0.1%)  |
| 1   | AQ    | 0.59         | 0/1149      | 1.06        | 9/1558 (0.6%)  |
| 1   | AR    | 0.43         | 0/1152      | 1.02        | 4/1562 (0.3%)  |
| 1   | AS    | 0.43         | 0/1152      | 1.26        | 11/1562 (0.7%) |
| 1   | AT    | 0.47         | 0/1152      | 0.89        | 5/1562 (0.3%)  |
| 1   | AU    | 0.43         | 0/1149      | 0.82        | 2/1558 (0.1%)  |
| 1   | AV    | 0.59         | 0/1149      | 1.06        | 9/1558 (0.6%)  |
| 1   | AW    | 0.43         | 0/1152      | 1.03        | 4/1562 (0.3%)  |
| 1   | AX    | 0.43         | 0/1152      | 1.26        | 11/1562 (0.7%) |
| 1   | AY    | 0.47         | 0/1152      | 0.89        | 5/1562 (0.3%)  |
| 1   | AZ    | 0.43         | 0/1149      | 0.82        | 2/1558 (0.1%)  |
| 1   | B1    | 0.59         | 0/1156      | 1.06        | 9/1567 (0.6%)  |
| 1   | B2    | 0.43         | 0/1156      | 1.02        | 4/1567 (0.3%)  |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | B3    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | B4    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | BA    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | BB    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | BC    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | BD    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | BE    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | BF    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | BG    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | BH    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | BI    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | BJ    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | BK    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | BL    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | BM    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | BN    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | BO    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | BP    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | BQ    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | BR    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | BS    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | BT    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | BU    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | BV    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | BW    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | BX    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | BY    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | BZ    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | C1    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | C2    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | C3    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | C4    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | CA    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | CB    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | CC    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | CD    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | CE    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | CF    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |
| 1   | CG    | 0.59         | 0/1156  | 1.06        | 9/1567 (0.6%)  |
| 1   | CH    | 0.43         | 0/1156  | 1.02        | 4/1567 (0.3%)  |
| 1   | CI    | 0.43         | 0/1156  | 1.25        | 11/1567 (0.7%) |
| 1   | CJ    | 0.47         | 0/1156  | 0.89        | 5/1567 (0.3%)  |
| 1   | CK    | 0.43         | 0/1156  | 0.82        | 2/1567 (0.1%)  |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 1   | CL    | 0.59         | 0/1156   | 1.06        | 9/1567 (0.6%)     |
| 1   | CM    | 0.43         | 0/1156   | 1.02        | 4/1567 (0.3%)     |
| 1   | CN    | 0.43         | 0/1156   | 1.25        | 11/1567 (0.7%)    |
| 1   | CO    | 0.47         | 0/1156   | 0.89        | 5/1567 (0.3%)     |
| 1   | CP    | 0.43         | 0/1156   | 0.82        | 2/1567 (0.1%)     |
| 1   | CQ    | 0.59         | 0/1156   | 1.06        | 9/1567 (0.6%)     |
| 1   | CR    | 0.43         | 0/1156   | 1.02        | 4/1567 (0.3%)     |
| 1   | CS    | 0.43         | 0/1156   | 1.25        | 11/1567 (0.7%)    |
| 1   | CT    | 0.47         | 0/1156   | 0.89        | 5/1567 (0.3%)     |
| 1   | CU    | 0.43         | 0/1156   | 0.82        | 2/1567 (0.1%)     |
| 1   | CV    | 0.59         | 0/1156   | 1.06        | 9/1567 (0.6%)     |
| 1   | CW    | 0.43         | 0/1156   | 1.02        | 4/1567 (0.3%)     |
| 1   | CX    | 0.43         | 0/1156   | 1.25        | 11/1567 (0.7%)    |
| 1   | CY    | 0.47         | 0/1156   | 0.89        | 5/1567 (0.3%)     |
| 1   | CZ    | 0.43         | 0/1156   | 0.82        | 2/1567 (0.1%)     |
| All | All   | 0.47         | 0/103884 | 1.02        | 558/140832 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A1    | 0                   | 1                   |
| 1   | AB    | 0                   | 1                   |
| 1   | AG    | 0                   | 1                   |
| 1   | AL    | 0                   | 1                   |
| 1   | AQ    | 0                   | 1                   |
| 1   | AV    | 0                   | 1                   |
| 1   | B1    | 0                   | 1                   |
| 1   | BB    | 0                   | 1                   |
| 1   | BG    | 0                   | 1                   |
| 1   | BL    | 0                   | 1                   |
| 1   | BQ    | 0                   | 1                   |
| 1   | BV    | 0                   | 1                   |
| 1   | C1    | 0                   | 1                   |
| 1   | CB    | 0                   | 1                   |
| 1   | CG    | 0                   | 1                   |
| 1   | CL    | 0                   | 1                   |
| 1   | CQ    | 0                   | 1                   |
| 1   | CV    | 0                   | 1                   |
| All | All   | 0                   | 18                  |

There are no bond length outliers.

All (558) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | CX    | 150 | LYS  | N-CA-CB | -16.32 | 86.14       | 110.12   |
| 1   | C3    | 150 | LYS  | N-CA-CB | -16.31 | 86.14       | 110.12   |
| 1   | BN    | 150 | LYS  | N-CA-CB | -16.31 | 86.14       | 110.12   |
| 1   | BD    | 150 | LYS  | N-CA-CB | -16.31 | 86.15       | 110.12   |
| 1   | AN    | 150 | LYS  | N-CA-CB | -16.30 | 86.16       | 110.12   |
| 1   | CS    | 150 | LYS  | N-CA-CB | -16.30 | 86.16       | 110.12   |
| 1   | BI    | 150 | LYS  | N-CA-CB | -16.30 | 86.16       | 110.12   |
| 1   | CD    | 150 | LYS  | N-CA-CB | -16.29 | 86.17       | 110.12   |
| 1   | AI    | 150 | LYS  | N-CA-CB | -16.29 | 86.18       | 110.12   |
| 1   | AD    | 150 | LYS  | N-CA-CB | -16.28 | 86.19       | 110.12   |
| 1   | AS    | 150 | LYS  | N-CA-CB | -16.28 | 86.19       | 110.12   |
| 1   | A3    | 150 | LYS  | N-CA-CB | -16.27 | 86.20       | 110.12   |
| 1   | BS    | 150 | LYS  | N-CA-CB | -16.27 | 86.20       | 110.12   |
| 1   | B3    | 150 | LYS  | N-CA-CB | -16.27 | 86.21       | 110.12   |
| 1   | CN    | 150 | LYS  | N-CA-CB | -16.27 | 86.21       | 110.12   |
| 1   | AX    | 150 | LYS  | N-CA-CB | -16.26 | 86.22       | 110.12   |
| 1   | CI    | 150 | LYS  | N-CA-CB | -16.26 | 86.22       | 110.12   |
| 1   | BX    | 150 | LYS  | N-CA-CB | -16.24 | 86.24       | 110.12   |
| 1   | BD    | 149 | SER  | CB-CA-C | -16.22 | 81.78       | 109.99   |
| 1   | CD    | 149 | SER  | CB-CA-C | -16.21 | 81.79       | 109.99   |
| 1   | C3    | 149 | SER  | CB-CA-C | -16.20 | 81.80       | 109.99   |
| 1   | CX    | 149 | SER  | CB-CA-C | -16.20 | 81.81       | 109.99   |
| 1   | BI    | 149 | SER  | CB-CA-C | -16.19 | 81.81       | 109.99   |
| 1   | AS    | 149 | SER  | CB-CA-C | -16.19 | 81.82       | 109.99   |
| 1   | CS    | 149 | SER  | CB-CA-C | -16.19 | 81.83       | 109.99   |
| 1   | AD    | 149 | SER  | CB-CA-C | -16.18 | 81.83       | 109.99   |
| 1   | AX    | 149 | SER  | CB-CA-C | -16.18 | 81.83       | 109.99   |
| 1   | B3    | 149 | SER  | CB-CA-C | -16.18 | 81.83       | 109.99   |
| 1   | AI    | 149 | SER  | CB-CA-C | -16.18 | 81.83       | 109.99   |
| 1   | BX    | 149 | SER  | CB-CA-C | -16.18 | 81.84       | 109.99   |
| 1   | CI    | 149 | SER  | CB-CA-C | -16.18 | 81.84       | 109.99   |
| 1   | BN    | 149 | SER  | CB-CA-C | -16.17 | 81.85       | 109.99   |
| 1   | BS    | 149 | SER  | CB-CA-C | -16.17 | 81.85       | 109.99   |
| 1   | AN    | 149 | SER  | CB-CA-C | -16.16 | 81.86       | 109.99   |
| 1   | A3    | 149 | SER  | CB-CA-C | -16.16 | 81.88       | 109.99   |
| 1   | CN    | 149 | SER  | CB-CA-C | -16.16 | 81.88       | 109.99   |
| 1   | AN    | 149 | SER  | N-CA-C  | 16.14  | 137.81      | 113.61   |
| 1   | A3    | 149 | SER  | N-CA-C  | 16.10  | 137.76      | 113.61   |
| 1   | CS    | 149 | SER  | N-CA-C  | 16.10  | 137.76      | 113.61   |
| 1   | AS    | 149 | SER  | N-CA-C  | 16.10  | 137.76      | 113.61   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | BS    | 149 | SER  | N-CA-C  | 16.10  | 137.76      | 113.61   |
| 1   | BN    | 149 | SER  | N-CA-C  | 16.10  | 137.75      | 113.61   |
| 1   | AD    | 149 | SER  | N-CA-C  | 16.09  | 137.75      | 113.61   |
| 1   | CI    | 149 | SER  | N-CA-C  | 16.09  | 137.75      | 113.61   |
| 1   | BD    | 149 | SER  | N-CA-C  | 16.09  | 137.75      | 113.61   |
| 1   | B3    | 149 | SER  | N-CA-C  | 16.09  | 137.75      | 113.61   |
| 1   | AI    | 149 | SER  | N-CA-C  | 16.09  | 137.74      | 113.61   |
| 1   | BI    | 149 | SER  | N-CA-C  | 16.08  | 137.72      | 113.61   |
| 1   | CD    | 149 | SER  | N-CA-C  | 16.08  | 137.72      | 113.61   |
| 1   | AX    | 149 | SER  | N-CA-C  | 16.08  | 137.72      | 113.61   |
| 1   | C3    | 149 | SER  | N-CA-C  | 16.07  | 137.72      | 113.61   |
| 1   | CN    | 149 | SER  | N-CA-C  | 16.07  | 137.71      | 113.61   |
| 1   | BX    | 149 | SER  | N-CA-C  | 16.07  | 137.71      | 113.61   |
| 1   | CX    | 149 | SER  | N-CA-C  | 16.05  | 137.69      | 113.61   |
| 1   | CI    | 109 | PRO  | CA-N-CD | -12.83 | 94.04       | 112.00   |
| 1   | B3    | 109 | PRO  | CA-N-CD | -12.82 | 94.05       | 112.00   |
| 1   | BX    | 109 | PRO  | CA-N-CD | -12.81 | 94.06       | 112.00   |
| 1   | A3    | 109 | PRO  | CA-N-CD | -12.81 | 94.07       | 112.00   |
| 1   | CS    | 109 | PRO  | CA-N-CD | -12.81 | 94.07       | 112.00   |
| 1   | AD    | 109 | PRO  | CA-N-CD | -12.80 | 94.07       | 112.00   |
| 1   | BD    | 109 | PRO  | CA-N-CD | -12.80 | 94.07       | 112.00   |
| 1   | BS    | 109 | PRO  | CA-N-CD | -12.80 | 94.08       | 112.00   |
| 1   | BN    | 109 | PRO  | CA-N-CD | -12.80 | 94.08       | 112.00   |
| 1   | CD    | 109 | PRO  | CA-N-CD | -12.80 | 94.08       | 112.00   |
| 1   | AN    | 109 | PRO  | CA-N-CD | -12.80 | 94.08       | 112.00   |
| 1   | BI    | 109 | PRO  | CA-N-CD | -12.80 | 94.08       | 112.00   |
| 1   | AI    | 109 | PRO  | CA-N-CD | -12.79 | 94.09       | 112.00   |
| 1   | AX    | 109 | PRO  | CA-N-CD | -12.78 | 94.10       | 112.00   |
| 1   | C3    | 109 | PRO  | CA-N-CD | -12.79 | 94.10       | 112.00   |
| 1   | CX    | 109 | PRO  | CA-N-CD | -12.78 | 94.11       | 112.00   |
| 1   | AS    | 109 | PRO  | CA-N-CD | -12.78 | 94.11       | 112.00   |
| 1   | CN    | 109 | PRO  | CA-N-CD | -12.77 | 94.12       | 112.00   |
| 1   | CG    | 109 | PRO  | CA-N-CD | -12.18 | 94.94       | 112.00   |
| 1   | CV    | 109 | PRO  | CA-N-CD | -12.17 | 94.96       | 112.00   |
| 1   | BL    | 109 | PRO  | CA-N-CD | -12.17 | 94.97       | 112.00   |
| 1   | B1    | 109 | PRO  | CA-N-CD | -12.17 | 94.97       | 112.00   |
| 1   | AG    | 109 | PRO  | CA-N-CD | -12.16 | 94.97       | 112.00   |
| 1   | BG    | 109 | PRO  | CA-N-CD | -12.16 | 94.97       | 112.00   |
| 1   | BB    | 109 | PRO  | CA-N-CD | -12.16 | 94.98       | 112.00   |
| 1   | BQ    | 109 | PRO  | CA-N-CD | -12.15 | 94.98       | 112.00   |
| 1   | AB    | 109 | PRO  | CA-N-CD | -12.15 | 94.99       | 112.00   |
| 1   | BV    | 109 | PRO  | CA-N-CD | -12.15 | 95.00       | 112.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | CQ    | 109 | PRO  | CA-N-CD    | -12.15 | 95.00       | 112.00   |
| 1   | AQ    | 109 | PRO  | CA-N-CD    | -12.14 | 95.00       | 112.00   |
| 1   | A1    | 109 | PRO  | CA-N-CD    | -12.14 | 95.00       | 112.00   |
| 1   | CB    | 109 | PRO  | CA-N-CD    | -12.14 | 95.00       | 112.00   |
| 1   | AV    | 109 | PRO  | CA-N-CD    | -12.13 | 95.02       | 112.00   |
| 1   | CL    | 109 | PRO  | CA-N-CD    | -12.13 | 95.02       | 112.00   |
| 1   | AL    | 109 | PRO  | CA-N-CD    | -12.12 | 95.03       | 112.00   |
| 1   | C1    | 109 | PRO  | CA-N-CD    | -12.12 | 95.03       | 112.00   |
| 1   | AN    | 105 | GLN  | OE1-CD-NE2 | -10.65 | 111.95      | 122.60   |
| 1   | BS    | 105 | GLN  | OE1-CD-NE2 | -10.63 | 111.97      | 122.60   |
| 1   | AI    | 105 | GLN  | OE1-CD-NE2 | -10.62 | 111.98      | 122.60   |
| 1   | CI    | 105 | GLN  | OE1-CD-NE2 | -10.62 | 111.98      | 122.60   |
| 1   | CX    | 105 | GLN  | OE1-CD-NE2 | -10.61 | 111.99      | 122.60   |
| 1   | CD    | 105 | GLN  | OE1-CD-NE2 | -10.61 | 112.00      | 122.60   |
| 1   | CS    | 105 | GLN  | OE1-CD-NE2 | -10.60 | 112.00      | 122.60   |
| 1   | AS    | 105 | GLN  | OE1-CD-NE2 | -10.60 | 112.00      | 122.60   |
| 1   | B3    | 105 | GLN  | OE1-CD-NE2 | -10.59 | 112.01      | 122.60   |
| 1   | A3    | 105 | GLN  | OE1-CD-NE2 | -10.59 | 112.01      | 122.60   |
| 1   | BD    | 105 | GLN  | OE1-CD-NE2 | -10.59 | 112.01      | 122.60   |
| 1   | BI    | 105 | GLN  | OE1-CD-NE2 | -10.59 | 112.01      | 122.60   |
| 1   | AD    | 105 | GLN  | OE1-CD-NE2 | -10.58 | 112.02      | 122.60   |
| 1   | C3    | 105 | GLN  | OE1-CD-NE2 | -10.58 | 112.02      | 122.60   |
| 1   | CN    | 105 | GLN  | OE1-CD-NE2 | -10.58 | 112.02      | 122.60   |
| 1   | BN    | 105 | GLN  | OE1-CD-NE2 | -10.55 | 112.05      | 122.60   |
| 1   | AX    | 105 | GLN  | OE1-CD-NE2 | -10.55 | 112.05      | 122.60   |
| 1   | BX    | 105 | GLN  | OE1-CD-NE2 | -10.50 | 112.10      | 122.60   |
| 1   | CH    | 105 | GLN  | OE1-CD-NE2 | -9.76  | 112.84      | 122.60   |
| 1   | CW    | 105 | GLN  | OE1-CD-NE2 | -9.75  | 112.85      | 122.60   |
| 1   | CR    | 105 | GLN  | OE1-CD-NE2 | -9.74  | 112.86      | 122.60   |
| 1   | BC    | 105 | GLN  | OE1-CD-NE2 | -9.74  | 112.86      | 122.60   |
| 1   | BH    | 105 | GLN  | OE1-CD-NE2 | -9.74  | 112.86      | 122.60   |
| 1   | A2    | 105 | GLN  | OE1-CD-NE2 | -9.73  | 112.87      | 122.60   |
| 1   | BW    | 105 | GLN  | OE1-CD-NE2 | -9.73  | 112.87      | 122.60   |
| 1   | AW    | 105 | GLN  | OE1-CD-NE2 | -9.73  | 112.87      | 122.60   |
| 1   | AH    | 105 | GLN  | OE1-CD-NE2 | -9.72  | 112.88      | 122.60   |
| 1   | AC    | 105 | GLN  | OE1-CD-NE2 | -9.72  | 112.88      | 122.60   |
| 1   | CC    | 105 | GLN  | OE1-CD-NE2 | -9.72  | 112.88      | 122.60   |
| 1   | AR    | 105 | GLN  | OE1-CD-NE2 | -9.71  | 112.89      | 122.60   |
| 1   | B2    | 105 | GLN  | OE1-CD-NE2 | -9.71  | 112.89      | 122.60   |
| 1   | AM    | 105 | GLN  | OE1-CD-NE2 | -9.71  | 112.89      | 122.60   |
| 1   | C2    | 105 | GLN  | OE1-CD-NE2 | -9.70  | 112.90      | 122.60   |
| 1   | BM    | 105 | GLN  | OE1-CD-NE2 | -9.70  | 112.90      | 122.60   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | CM    | 105 | GLN  | OE1-CD-NE2 | -9.70 | 112.90      | 122.60   |
| 1   | BR    | 105 | GLN  | OE1-CD-NE2 | -9.69 | 112.91      | 122.60   |
| 1   | CG    | 105 | GLN  | OE1-CD-NE2 | -9.25 | 113.35      | 122.60   |
| 1   | BV    | 105 | GLN  | OE1-CD-NE2 | -9.23 | 113.37      | 122.60   |
| 1   | AL    | 105 | GLN  | OE1-CD-NE2 | -9.23 | 113.37      | 122.60   |
| 1   | CQ    | 105 | GLN  | OE1-CD-NE2 | -9.22 | 113.38      | 122.60   |
| 1   | AV    | 105 | GLN  | OE1-CD-NE2 | -9.21 | 113.39      | 122.60   |
| 1   | BG    | 105 | GLN  | OE1-CD-NE2 | -9.21 | 113.39      | 122.60   |
| 1   | AG    | 105 | GLN  | OE1-CD-NE2 | -9.21 | 113.39      | 122.60   |
| 1   | BQ    | 105 | GLN  | OE1-CD-NE2 | -9.21 | 113.39      | 122.60   |
| 1   | BB    | 105 | GLN  | OE1-CD-NE2 | -9.19 | 113.41      | 122.60   |
| 1   | C1    | 105 | GLN  | OE1-CD-NE2 | -9.19 | 113.41      | 122.60   |
| 1   | BL    | 105 | GLN  | OE1-CD-NE2 | -9.19 | 113.42      | 122.60   |
| 1   | AB    | 105 | GLN  | OE1-CD-NE2 | -9.18 | 113.42      | 122.60   |
| 1   | CL    | 105 | GLN  | OE1-CD-NE2 | -9.18 | 113.42      | 122.60   |
| 1   | AQ    | 105 | GLN  | OE1-CD-NE2 | -9.17 | 113.43      | 122.60   |
| 1   | B1    | 105 | GLN  | OE1-CD-NE2 | -9.17 | 113.43      | 122.60   |
| 1   | A1    | 105 | GLN  | OE1-CD-NE2 | -9.15 | 113.45      | 122.60   |
| 1   | CV    | 105 | GLN  | OE1-CD-NE2 | -9.14 | 113.45      | 122.60   |
| 1   | CB    | 105 | GLN  | OE1-CD-NE2 | -9.12 | 113.48      | 122.60   |
| 1   | CW    | 46  | ASP  | N-CA-C     | -8.69 | 99.46       | 113.19   |
| 1   | C2    | 46  | ASP  | N-CA-C     | -8.69 | 99.46       | 113.19   |
| 1   | B2    | 46  | ASP  | N-CA-C     | -8.68 | 99.47       | 113.19   |
| 1   | AW    | 46  | ASP  | N-CA-C     | -8.68 | 99.48       | 113.19   |
| 1   | BM    | 46  | ASP  | N-CA-C     | -8.68 | 99.47       | 113.19   |
| 1   | AC    | 46  | ASP  | N-CA-C     | -8.67 | 99.49       | 113.19   |
| 1   | AM    | 46  | ASP  | N-CA-C     | -8.67 | 99.49       | 113.19   |
| 1   | BR    | 46  | ASP  | N-CA-C     | -8.67 | 99.49       | 113.19   |
| 1   | AR    | 46  | ASP  | N-CA-C     | -8.67 | 99.49       | 113.19   |
| 1   | CM    | 46  | ASP  | N-CA-C     | -8.67 | 99.49       | 113.19   |
| 1   | BW    | 46  | ASP  | N-CA-C     | -8.67 | 99.50       | 113.19   |
| 1   | CC    | 46  | ASP  | N-CA-C     | -8.67 | 99.50       | 113.19   |
| 1   | CH    | 46  | ASP  | N-CA-C     | -8.66 | 99.50       | 113.19   |
| 1   | A2    | 46  | ASP  | N-CA-C     | -8.65 | 99.52       | 113.19   |
| 1   | AH    | 46  | ASP  | N-CA-C     | -8.65 | 99.52       | 113.19   |
| 1   | CR    | 46  | ASP  | N-CA-C     | -8.65 | 99.52       | 113.19   |
| 1   | BC    | 46  | ASP  | N-CA-C     | -8.65 | 99.53       | 113.19   |
| 1   | BH    | 46  | ASP  | N-CA-C     | -8.64 | 99.53       | 113.19   |
| 1   | B2    | 109 | PRO  | CA-N-CD    | -8.37 | 100.28      | 112.00   |
| 1   | BR    | 109 | PRO  | CA-N-CD    | -8.37 | 100.28      | 112.00   |
| 1   | BM    | 109 | PRO  | CA-N-CD    | -8.36 | 100.30      | 112.00   |
| 1   | BW    | 109 | PRO  | CA-N-CD    | -8.36 | 100.30      | 112.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | CR    | 109 | PRO  | CA-N-CD | -8.35 | 100.30      | 112.00   |
| 1   | AH    | 109 | PRO  | CA-N-CD | -8.35 | 100.31      | 112.00   |
| 1   | BH    | 109 | PRO  | CA-N-CD | -8.34 | 100.32      | 112.00   |
| 1   | AC    | 109 | PRO  | CA-N-CD | -8.34 | 100.33      | 112.00   |
| 1   | CW    | 109 | PRO  | CA-N-CD | -8.34 | 100.33      | 112.00   |
| 1   | C2    | 109 | PRO  | CA-N-CD | -8.33 | 100.33      | 112.00   |
| 1   | AM    | 109 | PRO  | CA-N-CD | -8.33 | 100.34      | 112.00   |
| 1   | AW    | 109 | PRO  | CA-N-CD | -8.33 | 100.34      | 112.00   |
| 1   | A2    | 109 | PRO  | CA-N-CD | -8.32 | 100.35      | 112.00   |
| 1   | BC    | 109 | PRO  | CA-N-CD | -8.32 | 100.35      | 112.00   |
| 1   | AR    | 109 | PRO  | CA-N-CD | -8.32 | 100.35      | 112.00   |
| 1   | CH    | 109 | PRO  | CA-N-CD | -8.31 | 100.36      | 112.00   |
| 1   | CM    | 109 | PRO  | CA-N-CD | -8.30 | 100.37      | 112.00   |
| 1   | CC    | 109 | PRO  | CA-N-CD | -8.30 | 100.38      | 112.00   |
| 1   | B1    | 150 | LYS  | N-CA-C  | -8.16 | 95.61       | 109.24   |
| 1   | CB    | 150 | LYS  | N-CA-C  | -8.16 | 95.61       | 109.24   |
| 1   | CQ    | 150 | LYS  | N-CA-C  | -8.15 | 95.63       | 109.24   |
| 1   | BQ    | 150 | LYS  | N-CA-C  | -8.15 | 95.63       | 109.24   |
| 1   | CV    | 150 | LYS  | N-CA-C  | -8.15 | 95.63       | 109.24   |
| 1   | CG    | 150 | LYS  | N-CA-C  | -8.15 | 95.64       | 109.24   |
| 1   | AQ    | 150 | LYS  | N-CA-C  | -8.14 | 95.64       | 109.24   |
| 1   | BV    | 150 | LYS  | N-CA-C  | -8.14 | 95.64       | 109.24   |
| 1   | AB    | 150 | LYS  | N-CA-C  | -8.14 | 95.64       | 109.24   |
| 1   | AV    | 150 | LYS  | N-CA-C  | -8.14 | 95.65       | 109.24   |
| 1   | BL    | 150 | LYS  | N-CA-C  | -8.14 | 95.65       | 109.24   |
| 1   | CL    | 150 | LYS  | N-CA-C  | -8.14 | 95.65       | 109.24   |
| 1   | A1    | 150 | LYS  | N-CA-C  | -8.13 | 95.66       | 109.24   |
| 1   | BB    | 150 | LYS  | N-CA-C  | -8.13 | 95.66       | 109.24   |
| 1   | BG    | 150 | LYS  | N-CA-C  | -8.13 | 95.66       | 109.24   |
| 1   | AG    | 150 | LYS  | N-CA-C  | -8.13 | 95.67       | 109.24   |
| 1   | AL    | 150 | LYS  | N-CA-C  | -8.13 | 95.67       | 109.24   |
| 1   | C1    | 150 | LYS  | N-CA-C  | -8.12 | 95.67       | 109.24   |
| 1   | BS    | 34  | LEU  | N-CA-C  | 8.09  | 119.87      | 111.14   |
| 1   | CD    | 34  | LEU  | N-CA-C  | 8.08  | 119.87      | 111.14   |
| 1   | AN    | 34  | LEU  | N-CA-C  | 8.08  | 119.86      | 111.14   |
| 1   | BD    | 34  | LEU  | N-CA-C  | 8.08  | 119.86      | 111.14   |
| 1   | BN    | 34  | LEU  | N-CA-C  | 8.08  | 119.86      | 111.14   |
| 1   | B3    | 34  | LEU  | N-CA-C  | 8.08  | 119.86      | 111.14   |
| 1   | C3    | 34  | LEU  | N-CA-C  | 8.08  | 119.86      | 111.14   |
| 1   | AS    | 34  | LEU  | N-CA-C  | 8.07  | 119.85      | 111.14   |
| 1   | CX    | 34  | LEU  | N-CA-C  | 8.07  | 119.85      | 111.14   |
| 1   | AD    | 34  | LEU  | N-CA-C  | 8.06  | 119.85      | 111.14   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | CI    | 34  | LEU  | N-CA-C    | 8.06  | 119.85      | 111.14   |
| 1   | CS    | 34  | LEU  | N-CA-C    | 8.06  | 119.84      | 111.14   |
| 1   | CN    | 34  | LEU  | N-CA-C    | 8.06  | 119.84      | 111.14   |
| 1   | BX    | 34  | LEU  | N-CA-C    | 8.05  | 119.83      | 111.14   |
| 1   | AI    | 34  | LEU  | N-CA-C    | 8.04  | 119.83      | 111.14   |
| 1   | BI    | 34  | LEU  | N-CA-C    | 8.04  | 119.83      | 111.14   |
| 1   | AX    | 34  | LEU  | N-CA-C    | 8.04  | 119.82      | 111.14   |
| 1   | A3    | 34  | LEU  | N-CA-C    | 8.03  | 119.82      | 111.14   |
| 1   | A1    | 104 | LEU  | N-CA-C    | -7.96 | 103.71      | 113.50   |
| 1   | BL    | 104 | LEU  | N-CA-C    | -7.95 | 103.72      | 113.50   |
| 1   | CQ    | 104 | LEU  | N-CA-C    | -7.94 | 103.73      | 113.50   |
| 1   | AQ    | 104 | LEU  | N-CA-C    | -7.93 | 103.74      | 113.50   |
| 1   | CB    | 104 | LEU  | N-CA-C    | -7.93 | 103.74      | 113.50   |
| 1   | AG    | 104 | LEU  | N-CA-C    | -7.92 | 103.76      | 113.50   |
| 1   | BV    | 104 | LEU  | N-CA-C    | -7.92 | 103.76      | 113.50   |
| 1   | CV    | 104 | LEU  | N-CA-C    | -7.92 | 103.76      | 113.50   |
| 1   | BG    | 104 | LEU  | N-CA-C    | -7.92 | 103.76      | 113.50   |
| 1   | AB    | 104 | LEU  | N-CA-C    | -7.91 | 103.77      | 113.50   |
| 1   | CG    | 104 | LEU  | N-CA-C    | -7.91 | 103.77      | 113.50   |
| 1   | BB    | 104 | LEU  | N-CA-C    | -7.91 | 103.77      | 113.50   |
| 1   | AV    | 104 | LEU  | N-CA-C    | -7.91 | 103.78      | 113.50   |
| 1   | BQ    | 104 | LEU  | N-CA-C    | -7.91 | 103.78      | 113.50   |
| 1   | CL    | 104 | LEU  | N-CA-C    | -7.90 | 103.78      | 113.50   |
| 1   | AL    | 104 | LEU  | N-CA-C    | -7.90 | 103.79      | 113.50   |
| 1   | C1    | 104 | LEU  | N-CA-C    | -7.90 | 103.79      | 113.50   |
| 1   | B1    | 104 | LEU  | N-CA-C    | -7.89 | 103.80      | 113.50   |
| 1   | BC    | 105 | GLN  | CG-CD-NE2 | 7.19  | 127.18      | 116.40   |
| 1   | AW    | 105 | GLN  | CG-CD-NE2 | 7.19  | 127.18      | 116.40   |
| 1   | CR    | 105 | GLN  | CG-CD-NE2 | 7.19  | 127.18      | 116.40   |
| 1   | AH    | 105 | GLN  | CG-CD-NE2 | 7.17  | 127.16      | 116.40   |
| 1   | BW    | 105 | GLN  | CG-CD-NE2 | 7.17  | 127.16      | 116.40   |
| 1   | CC    | 105 | GLN  | CG-CD-NE2 | 7.17  | 127.16      | 116.40   |
| 1   | AR    | 105 | GLN  | CG-CD-NE2 | 7.17  | 127.16      | 116.40   |
| 1   | AC    | 105 | GLN  | CG-CD-NE2 | 7.17  | 127.15      | 116.40   |
| 1   | AM    | 105 | GLN  | CG-CD-NE2 | 7.17  | 127.15      | 116.40   |
| 1   | CW    | 105 | GLN  | CG-CD-NE2 | 7.16  | 127.14      | 116.40   |
| 1   | CH    | 105 | GLN  | CG-CD-NE2 | 7.16  | 127.14      | 116.40   |
| 1   | BH    | 105 | GLN  | CG-CD-NE2 | 7.16  | 127.13      | 116.40   |
| 1   | BM    | 105 | GLN  | CG-CD-NE2 | 7.16  | 127.13      | 116.40   |
| 1   | B2    | 105 | GLN  | CG-CD-NE2 | 7.15  | 127.13      | 116.40   |
| 1   | CM    | 105 | GLN  | CG-CD-NE2 | 7.15  | 127.13      | 116.40   |
| 1   | A2    | 105 | GLN  | CG-CD-NE2 | 7.15  | 127.13      | 116.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | BR    | 105 | GLN  | CG-CD-NE2 | 7.15  | 127.12      | 116.40   |
| 1   | C2    | 105 | GLN  | CG-CD-NE2 | 7.14  | 127.11      | 116.40   |
| 1   | AI    | 105 | GLN  | CG-CD-NE2 | 7.02  | 126.93      | 116.40   |
| 1   | BS    | 105 | GLN  | CG-CD-NE2 | 7.02  | 126.93      | 116.40   |
| 1   | B3    | 105 | GLN  | CG-CD-NE2 | 7.02  | 126.92      | 116.40   |
| 1   | CX    | 105 | GLN  | CG-CD-NE2 | 7.01  | 126.92      | 116.40   |
| 1   | AN    | 105 | GLN  | CG-CD-NE2 | 7.01  | 126.92      | 116.40   |
| 1   | CD    | 105 | GLN  | CG-CD-NE2 | 7.00  | 126.90      | 116.40   |
| 1   | CN    | 105 | GLN  | CG-CD-NE2 | 7.00  | 126.90      | 116.40   |
| 1   | AX    | 105 | GLN  | CG-CD-NE2 | 7.00  | 126.90      | 116.40   |
| 1   | C3    | 105 | GLN  | CG-CD-NE2 | 7.00  | 126.89      | 116.40   |
| 1   | AD    | 105 | GLN  | CG-CD-NE2 | 6.99  | 126.89      | 116.40   |
| 1   | BD    | 105 | GLN  | CG-CD-NE2 | 6.99  | 126.88      | 116.40   |
| 1   | CI    | 105 | GLN  | CG-CD-NE2 | 6.99  | 126.88      | 116.40   |
| 1   | BI    | 105 | GLN  | CG-CD-NE2 | 6.98  | 126.87      | 116.40   |
| 1   | AS    | 105 | GLN  | CG-CD-NE2 | 6.98  | 126.87      | 116.40   |
| 1   | A3    | 105 | GLN  | CG-CD-NE2 | 6.98  | 126.86      | 116.40   |
| 1   | CS    | 105 | GLN  | CG-CD-NE2 | 6.97  | 126.86      | 116.40   |
| 1   | BX    | 105 | GLN  | CG-CD-NE2 | 6.97  | 126.85      | 116.40   |
| 1   | BN    | 105 | GLN  | CG-CD-NE2 | 6.96  | 126.84      | 116.40   |
| 1   | BS    | 148 | LEU  | N-CA-C    | -6.78 | 95.23       | 107.98   |
| 1   | AX    | 148 | LEU  | N-CA-C    | -6.78 | 95.23       | 107.98   |
| 1   | CS    | 148 | LEU  | N-CA-C    | -6.78 | 95.24       | 107.98   |
| 1   | B3    | 148 | LEU  | N-CA-C    | -6.77 | 95.25       | 107.98   |
| 1   | CI    | 148 | LEU  | N-CA-C    | -6.77 | 95.25       | 107.98   |
| 1   | A3    | 148 | LEU  | N-CA-C    | -6.77 | 95.25       | 107.98   |
| 1   | BD    | 148 | LEU  | N-CA-C    | -6.77 | 95.25       | 107.98   |
| 1   | AD    | 148 | LEU  | N-CA-C    | -6.77 | 95.26       | 107.98   |
| 1   | BX    | 148 | LEU  | N-CA-C    | -6.76 | 95.27       | 107.98   |
| 1   | CN    | 148 | LEU  | N-CA-C    | -6.76 | 95.27       | 107.98   |
| 1   | AN    | 148 | LEU  | N-CA-C    | -6.76 | 95.27       | 107.98   |
| 1   | CX    | 148 | LEU  | N-CA-C    | -6.76 | 95.27       | 107.98   |
| 1   | AI    | 148 | LEU  | N-CA-C    | -6.76 | 95.28       | 107.98   |
| 1   | BI    | 148 | LEU  | N-CA-C    | -6.75 | 95.28       | 107.98   |
| 1   | CD    | 148 | LEU  | N-CA-C    | -6.75 | 95.28       | 107.98   |
| 1   | AS    | 148 | LEU  | N-CA-C    | -6.75 | 95.29       | 107.98   |
| 1   | C3    | 148 | LEU  | N-CA-C    | -6.75 | 95.29       | 107.98   |
| 1   | BN    | 148 | LEU  | N-CA-C    | -6.75 | 95.30       | 107.98   |
| 1   | BB    | 105 | GLN  | CG-CD-NE2 | 6.65  | 126.38      | 116.40   |
| 1   | AL    | 105 | GLN  | CG-CD-NE2 | 6.65  | 126.37      | 116.40   |
| 1   | BV    | 105 | GLN  | CG-CD-NE2 | 6.65  | 126.37      | 116.40   |
| 1   | CQ    | 105 | GLN  | CG-CD-NE2 | 6.64  | 126.36      | 116.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | AG    | 105 | GLN  | CG-CD-NE2 | 6.64  | 126.36      | 116.40   |
| 1   | BV    | 149 | SER  | N-CA-C    | 6.64  | 121.04      | 107.69   |
| 1   | CB    | 149 | SER  | N-CA-C    | 6.63  | 121.02      | 107.69   |
| 1   | CG    | 105 | GLN  | CG-CD-NE2 | 6.63  | 126.35      | 116.40   |
| 1   | BL    | 105 | GLN  | CG-CD-NE2 | 6.63  | 126.35      | 116.40   |
| 1   | AG    | 149 | SER  | N-CA-C    | 6.63  | 121.02      | 107.69   |
| 1   | BB    | 149 | SER  | N-CA-C    | 6.63  | 121.02      | 107.69   |
| 1   | C1    | 149 | SER  | N-CA-C    | 6.63  | 121.02      | 107.69   |
| 1   | BG    | 105 | GLN  | CG-CD-NE2 | 6.63  | 126.34      | 116.40   |
| 1   | CB    | 105 | GLN  | CG-CD-NE2 | 6.63  | 126.34      | 116.40   |
| 1   | BG    | 149 | SER  | N-CA-C    | 6.63  | 121.01      | 107.69   |
| 1   | BQ    | 105 | GLN  | CG-CD-NE2 | 6.63  | 126.34      | 116.40   |
| 1   | B1    | 149 | SER  | N-CA-C    | 6.62  | 121.00      | 107.69   |
| 1   | CL    | 149 | SER  | N-CA-C    | 6.62  | 121.01      | 107.69   |
| 1   | AB    | 149 | SER  | N-CA-C    | 6.62  | 121.00      | 107.69   |
| 1   | AV    | 149 | SER  | N-CA-C    | 6.62  | 121.00      | 107.69   |
| 1   | AB    | 105 | GLN  | CG-CD-NE2 | 6.62  | 126.33      | 116.40   |
| 1   | AL    | 149 | SER  | N-CA-C    | 6.62  | 121.00      | 107.69   |
| 1   | A1    | 149 | SER  | N-CA-C    | 6.62  | 121.00      | 107.69   |
| 1   | B1    | 105 | GLN  | CG-CD-NE2 | 6.62  | 126.33      | 116.40   |
| 1   | CV    | 105 | GLN  | CG-CD-NE2 | 6.62  | 126.33      | 116.40   |
| 1   | AV    | 105 | GLN  | CG-CD-NE2 | 6.62  | 126.33      | 116.40   |
| 1   | A1    | 105 | GLN  | CG-CD-NE2 | 6.62  | 126.33      | 116.40   |
| 1   | AQ    | 149 | SER  | N-CA-C    | 6.62  | 120.99      | 107.69   |
| 1   | BQ    | 149 | SER  | N-CA-C    | 6.62  | 120.98      | 107.69   |
| 1   | CL    | 105 | GLN  | CG-CD-NE2 | 6.62  | 126.32      | 116.40   |
| 1   | BL    | 149 | SER  | N-CA-C    | 6.61  | 120.98      | 107.69   |
| 1   | CV    | 149 | SER  | N-CA-C    | 6.61  | 120.97      | 107.69   |
| 1   | AQ    | 105 | GLN  | CG-CD-NE2 | 6.61  | 126.31      | 116.40   |
| 1   | CG    | 149 | SER  | N-CA-C    | 6.61  | 120.97      | 107.69   |
| 1   | CQ    | 149 | SER  | N-CA-C    | 6.60  | 120.96      | 107.69   |
| 1   | C1    | 105 | GLN  | CG-CD-NE2 | 6.59  | 126.29      | 116.40   |
| 1   | AJ    | 151 | HIS  | CA-CB-CG  | -6.58 | 107.22      | 113.80   |
| 1   | BJ    | 151 | HIS  | CA-CB-CG  | -6.56 | 107.24      | 113.80   |
| 1   | CO    | 151 | HIS  | CA-CB-CG  | -6.56 | 107.24      | 113.80   |
| 1   | B4    | 151 | HIS  | CA-CB-CG  | -6.56 | 107.24      | 113.80   |
| 1   | CY    | 151 | HIS  | CA-CB-CG  | -6.56 | 107.24      | 113.80   |
| 1   | A4    | 151 | HIS  | CA-CB-CG  | -6.55 | 107.25      | 113.80   |
| 1   | BY    | 151 | HIS  | CA-CB-CG  | -6.55 | 107.25      | 113.80   |
| 1   | BT    | 151 | HIS  | CA-CB-CG  | -6.55 | 107.25      | 113.80   |
| 1   | BO    | 151 | HIS  | CA-CB-CG  | -6.54 | 107.25      | 113.80   |
| 1   | CE    | 151 | HIS  | CA-CB-CG  | -6.54 | 107.25      | 113.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | AE    | 151 | HIS  | CA-CB-CG | -6.54 | 107.26      | 113.80   |
| 1   | AO    | 151 | HIS  | CA-CB-CG | -6.53 | 107.27      | 113.80   |
| 1   | CT    | 151 | HIS  | CA-CB-CG | -6.53 | 107.27      | 113.80   |
| 1   | BE    | 151 | HIS  | CA-CB-CG | -6.53 | 107.27      | 113.80   |
| 1   | AT    | 151 | HIS  | CA-CB-CG | -6.52 | 107.28      | 113.80   |
| 1   | AY    | 151 | HIS  | CA-CB-CG | -6.52 | 107.28      | 113.80   |
| 1   | CJ    | 151 | HIS  | CA-CB-CG | -6.52 | 107.28      | 113.80   |
| 1   | C4    | 151 | HIS  | CA-CB-CG | -6.51 | 107.28      | 113.80   |
| 1   | BL    | 151 | HIS  | CA-CB-CG | 6.31  | 120.11      | 113.80   |
| 1   | CL    | 151 | HIS  | CA-CB-CG | 6.30  | 120.10      | 113.80   |
| 1   | CQ    | 151 | HIS  | CA-CB-CG | 6.29  | 120.09      | 113.80   |
| 1   | BV    | 151 | HIS  | CA-CB-CG | 6.28  | 120.08      | 113.80   |
| 1   | A1    | 151 | HIS  | CA-CB-CG | 6.27  | 120.07      | 113.80   |
| 1   | AL    | 151 | HIS  | CA-CB-CG | 6.27  | 120.07      | 113.80   |
| 1   | AG    | 151 | HIS  | CA-CB-CG | 6.27  | 120.07      | 113.80   |
| 1   | AB    | 151 | HIS  | CA-CB-CG | 6.26  | 120.06      | 113.80   |
| 1   | BG    | 151 | HIS  | CA-CB-CG | 6.25  | 120.05      | 113.80   |
| 1   | AV    | 151 | HIS  | CA-CB-CG | 6.25  | 120.05      | 113.80   |
| 1   | B1    | 151 | HIS  | CA-CB-CG | 6.24  | 120.04      | 113.80   |
| 1   | BB    | 151 | HIS  | CA-CB-CG | 6.24  | 120.04      | 113.80   |
| 1   | CG    | 151 | HIS  | CA-CB-CG | 6.24  | 120.04      | 113.80   |
| 1   | AQ    | 151 | HIS  | CA-CB-CG | 6.23  | 120.03      | 113.80   |
| 1   | C1    | 151 | HIS  | CA-CB-CG | 6.23  | 120.03      | 113.80   |
| 1   | CV    | 151 | HIS  | CA-CB-CG | 6.23  | 120.03      | 113.80   |
| 1   | CB    | 151 | HIS  | CA-CB-CG | 6.23  | 120.03      | 113.80   |
| 1   | BQ    | 151 | HIS  | CA-CB-CG | 6.21  | 120.01      | 113.80   |
| 1   | BN    | 37  | LEU  | N-CA-C   | -6.15 | 104.12      | 111.69   |
| 1   | CS    | 37  | LEU  | N-CA-C   | -6.15 | 104.13      | 111.69   |
| 1   | BS    | 37  | LEU  | N-CA-C   | -6.15 | 104.13      | 111.69   |
| 1   | AI    | 37  | LEU  | N-CA-C   | -6.15 | 104.13      | 111.69   |
| 1   | BI    | 37  | LEU  | N-CA-C   | -6.14 | 104.14      | 111.69   |
| 1   | C3    | 37  | LEU  | N-CA-C   | -6.14 | 104.14      | 111.69   |
| 1   | AX    | 37  | LEU  | N-CA-C   | -6.13 | 104.15      | 111.69   |
| 1   | CX    | 37  | LEU  | N-CA-C   | -6.13 | 104.15      | 111.69   |
| 1   | B3    | 37  | LEU  | N-CA-C   | -6.13 | 104.16      | 111.69   |
| 1   | CN    | 37  | LEU  | N-CA-C   | -6.13 | 104.15      | 111.69   |
| 1   | AD    | 37  | LEU  | N-CA-C   | -6.12 | 104.16      | 111.69   |
| 1   | AS    | 37  | LEU  | N-CA-C   | -6.12 | 104.16      | 111.69   |
| 1   | AN    | 37  | LEU  | N-CA-C   | -6.12 | 104.17      | 111.69   |
| 1   | CD    | 37  | LEU  | N-CA-C   | -6.11 | 104.17      | 111.69   |
| 1   | A3    | 37  | LEU  | N-CA-C   | -6.11 | 104.18      | 111.69   |
| 1   | BD    | 37  | LEU  | N-CA-C   | -6.11 | 104.18      | 111.69   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | CI    | 37  | LEU  | N-CA-C  | -6.10 | 104.19      | 111.69   |
| 1   | BX    | 37  | LEU  | N-CA-C  | -6.08 | 104.21      | 111.69   |
| 1   | CL    | 42  | VAL  | N-CA-CB | 5.89  | 117.15      | 110.72   |
| 1   | AL    | 42  | VAL  | N-CA-CB | 5.89  | 117.14      | 110.72   |
| 1   | AQ    | 42  | VAL  | N-CA-CB | 5.89  | 117.14      | 110.72   |
| 1   | BV    | 42  | VAL  | N-CA-CB | 5.89  | 117.14      | 110.72   |
| 1   | C1    | 42  | VAL  | N-CA-CB | 5.88  | 117.13      | 110.72   |
| 1   | BB    | 42  | VAL  | N-CA-CB | 5.88  | 117.12      | 110.72   |
| 1   | AB    | 42  | VAL  | N-CA-CB | 5.87  | 117.12      | 110.72   |
| 1   | A1    | 42  | VAL  | N-CA-CB | 5.87  | 117.12      | 110.72   |
| 1   | BG    | 42  | VAL  | N-CA-CB | 5.87  | 117.12      | 110.72   |
| 1   | BQ    | 42  | VAL  | N-CA-CB | 5.87  | 117.12      | 110.72   |
| 1   | CG    | 42  | VAL  | N-CA-CB | 5.87  | 117.12      | 110.72   |
| 1   | AG    | 42  | VAL  | N-CA-CB | 5.87  | 117.11      | 110.72   |
| 1   | B1    | 42  | VAL  | N-CA-CB | 5.86  | 117.11      | 110.72   |
| 1   | AV    | 42  | VAL  | N-CA-CB | 5.86  | 117.10      | 110.72   |
| 1   | CQ    | 42  | VAL  | N-CA-CB | 5.86  | 117.11      | 110.72   |
| 1   | CV    | 42  | VAL  | N-CA-CB | 5.85  | 117.09      | 110.72   |
| 1   | BL    | 42  | VAL  | N-CA-CB | 5.84  | 117.09      | 110.72   |
| 1   | CB    | 42  | VAL  | N-CA-CB | 5.84  | 117.08      | 110.72   |
| 1   | C4    | 58  | ILE  | CB-CA-C | -5.68 | 101.02      | 111.36   |
| 1   | BE    | 58  | ILE  | CB-CA-C | -5.68 | 101.03      | 111.36   |
| 1   | BY    | 58  | ILE  | CB-CA-C | -5.67 | 101.03      | 111.36   |
| 1   | BJ    | 58  | ILE  | CB-CA-C | -5.67 | 101.04      | 111.36   |
| 1   | CO    | 58  | ILE  | CB-CA-C | -5.67 | 101.04      | 111.36   |
| 1   | AO    | 58  | ILE  | CB-CA-C | -5.67 | 101.05      | 111.36   |
| 1   | AN    | 31  | GLY  | N-CA-C  | -5.66 | 108.12      | 114.40   |
| 1   | AY    | 58  | ILE  | CB-CA-C | -5.66 | 101.06      | 111.36   |
| 1   | B4    | 58  | ILE  | CB-CA-C | -5.66 | 101.06      | 111.36   |
| 1   | CJ    | 58  | ILE  | CB-CA-C | -5.66 | 101.06      | 111.36   |
| 1   | CY    | 58  | ILE  | CB-CA-C | -5.66 | 101.06      | 111.36   |
| 1   | AT    | 58  | ILE  | CB-CA-C | -5.66 | 101.06      | 111.36   |
| 1   | AE    | 58  | ILE  | CB-CA-C | -5.66 | 101.07      | 111.36   |
| 1   | A4    | 58  | ILE  | CB-CA-C | -5.66 | 101.06      | 111.36   |
| 1   | CT    | 58  | ILE  | CB-CA-C | -5.66 | 101.07      | 111.36   |
| 1   | AJ    | 58  | ILE  | CB-CA-C | -5.65 | 101.07      | 111.36   |
| 1   | BT    | 58  | ILE  | CB-CA-C | -5.65 | 101.08      | 111.36   |
| 1   | C3    | 31  | GLY  | N-CA-C  | -5.65 | 108.13      | 114.40   |
| 1   | CE    | 58  | ILE  | CB-CA-C | -5.64 | 101.09      | 111.36   |
| 1   | BN    | 31  | GLY  | N-CA-C  | -5.63 | 108.14      | 114.40   |
| 1   | B3    | 31  | GLY  | N-CA-C  | -5.63 | 108.15      | 114.40   |
| 1   | A3    | 31  | GLY  | N-CA-C  | -5.63 | 108.15      | 114.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | BO    | 58  | ILE  | CB-CA-C | -5.63 | 101.12      | 111.36   |
| 1   | CX    | 31  | GLY  | N-CA-C  | -5.62 | 108.16      | 114.40   |
| 1   | AI    | 31  | GLY  | N-CA-C  | -5.62 | 108.17      | 114.40   |
| 1   | AX    | 31  | GLY  | N-CA-C  | -5.61 | 108.17      | 114.40   |
| 1   | BI    | 31  | GLY  | N-CA-C  | -5.61 | 108.17      | 114.40   |
| 1   | BX    | 31  | GLY  | N-CA-C  | -5.61 | 108.18      | 114.40   |
| 1   | AD    | 31  | GLY  | N-CA-C  | -5.60 | 108.18      | 114.40   |
| 1   | CI    | 31  | GLY  | N-CA-C  | -5.60 | 108.19      | 114.40   |
| 1   | BS    | 31  | GLY  | N-CA-C  | -5.59 | 108.20      | 114.40   |
| 1   | CN    | 31  | GLY  | N-CA-C  | -5.59 | 108.20      | 114.40   |
| 1   | CS    | 31  | GLY  | N-CA-C  | -5.59 | 108.20      | 114.40   |
| 1   | CD    | 31  | GLY  | N-CA-C  | -5.58 | 108.21      | 114.40   |
| 1   | BD    | 31  | GLY  | N-CA-C  | -5.58 | 108.21      | 114.40   |
| 1   | AS    | 31  | GLY  | N-CA-C  | -5.57 | 108.22      | 114.40   |
| 1   | AX    | 150 | LYS  | N-CA-C  | 5.54  | 117.31      | 111.28   |
| 1   | BS    | 150 | LYS  | N-CA-C  | 5.54  | 117.31      | 111.28   |
| 1   | BK    | 58  | ILE  | CB-CA-C | -5.53 | 101.29      | 111.36   |
| 1   | AP    | 58  | ILE  | CB-CA-C | -5.53 | 101.31      | 111.36   |
| 1   | CA    | 58  | ILE  | CB-CA-C | -5.52 | 101.31      | 111.36   |
| 1   | CU    | 58  | ILE  | CB-CA-C | -5.52 | 101.31      | 111.36   |
| 1   | BA    | 58  | ILE  | CB-CA-C | -5.52 | 101.31      | 111.36   |
| 1   | BZ    | 58  | ILE  | CB-CA-C | -5.52 | 101.31      | 111.36   |
| 1   | AK    | 58  | ILE  | CB-CA-C | -5.52 | 101.31      | 111.36   |
| 1   | BE    | 58  | ILE  | N-CA-C  | 5.52  | 120.80      | 108.88   |
| 1   | CP    | 58  | ILE  | CB-CA-C | -5.52 | 101.31      | 111.36   |
| 1   | BF    | 58  | ILE  | CB-CA-C | -5.52 | 101.32      | 111.36   |
| 1   | BU    | 58  | ILE  | CB-CA-C | -5.52 | 101.32      | 111.36   |
| 1   | CN    | 150 | LYS  | N-CA-C  | 5.52  | 117.29      | 111.28   |
| 1   | AA    | 58  | ILE  | CB-CA-C | -5.51 | 101.32      | 111.36   |
| 1   | AF    | 58  | ILE  | CB-CA-C | -5.51 | 101.32      | 111.36   |
| 1   | CT    | 58  | ILE  | N-CA-C  | 5.51  | 120.79      | 108.88   |
| 1   | CZ    | 58  | ILE  | CB-CA-C | -5.51 | 101.33      | 111.36   |
| 1   | BO    | 58  | ILE  | N-CA-C  | 5.51  | 120.79      | 108.88   |
| 1   | AU    | 58  | ILE  | CB-CA-C | -5.51 | 101.33      | 111.36   |
| 1   | BT    | 58  | ILE  | N-CA-C  | 5.51  | 120.78      | 108.88   |
| 1   | C4    | 58  | ILE  | N-CA-C  | 5.51  | 120.79      | 108.88   |
| 1   | BY    | 58  | ILE  | N-CA-C  | 5.51  | 120.78      | 108.88   |
| 1   | CJ    | 58  | ILE  | N-CA-C  | 5.51  | 120.78      | 108.88   |
| 1   | AY    | 58  | ILE  | N-CA-C  | 5.51  | 120.78      | 108.88   |
| 1   | BD    | 150 | LYS  | N-CA-C  | 5.51  | 117.28      | 111.28   |
| 1   | CK    | 58  | ILE  | CB-CA-C | -5.51 | 101.33      | 111.36   |
| 1   | AE    | 58  | ILE  | N-CA-C  | 5.51  | 120.78      | 108.88   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | AT    | 58  | ILE  | N-CA-C  | 5.51  | 120.77      | 108.88   |
| 1   | CE    | 58  | ILE  | N-CA-C  | 5.51  | 120.77      | 108.88   |
| 1   | A4    | 58  | ILE  | N-CA-C  | 5.50  | 120.76      | 108.88   |
| 1   | B4    | 58  | ILE  | N-CA-C  | 5.50  | 120.75      | 108.88   |
| 1   | AO    | 58  | ILE  | N-CA-C  | 5.50  | 120.75      | 108.88   |
| 1   | AZ    | 58  | ILE  | CB-CA-C | -5.50 | 101.36      | 111.36   |
| 1   | BP    | 58  | ILE  | CB-CA-C | -5.49 | 101.36      | 111.36   |
| 1   | CO    | 58  | ILE  | N-CA-C  | 5.49  | 120.74      | 108.88   |
| 1   | CY    | 58  | ILE  | N-CA-C  | 5.49  | 120.75      | 108.88   |
| 1   | AJ    | 58  | ILE  | N-CA-C  | 5.49  | 120.74      | 108.88   |
| 1   | BJ    | 58  | ILE  | N-CA-C  | 5.49  | 120.74      | 108.88   |
| 1   | C3    | 150 | LYS  | N-CA-C  | 5.49  | 117.26      | 111.28   |
| 1   | AD    | 150 | LYS  | N-CA-C  | 5.49  | 117.26      | 111.28   |
| 1   | CF    | 58  | ILE  | CB-CA-C | -5.49 | 101.38      | 111.36   |
| 1   | CS    | 150 | LYS  | N-CA-C  | 5.48  | 117.25      | 111.28   |
| 1   | CD    | 150 | LYS  | N-CA-C  | 5.48  | 117.25      | 111.28   |
| 1   | CI    | 150 | LYS  | N-CA-C  | 5.47  | 117.25      | 111.28   |
| 1   | B3    | 150 | LYS  | N-CA-C  | 5.47  | 117.24      | 111.28   |
| 1   | BI    | 150 | LYS  | N-CA-C  | 5.47  | 117.24      | 111.28   |
| 1   | BX    | 150 | LYS  | N-CA-C  | 5.47  | 117.24      | 111.28   |
| 1   | AI    | 150 | LYS  | N-CA-C  | 5.47  | 117.24      | 111.28   |
| 1   | A3    | 150 | LYS  | N-CA-C  | 5.47  | 117.24      | 111.28   |
| 1   | BN    | 150 | LYS  | N-CA-C  | 5.46  | 117.23      | 111.28   |
| 1   | AN    | 150 | LYS  | N-CA-C  | 5.46  | 117.22      | 111.28   |
| 1   | AS    | 150 | LYS  | N-CA-C  | 5.45  | 117.22      | 111.28   |
| 1   | AF    | 103 | SER  | N-CA-C  | -5.45 | 106.49      | 114.39   |
| 1   | BP    | 103 | SER  | N-CA-C  | -5.45 | 106.49      | 114.39   |
| 1   | CX    | 150 | LYS  | N-CA-C  | 5.45  | 117.22      | 111.28   |
| 1   | BF    | 103 | SER  | N-CA-C  | -5.45 | 106.49      | 114.39   |
| 1   | BK    | 103 | SER  | N-CA-C  | -5.45 | 106.49      | 114.39   |
| 1   | CA    | 103 | SER  | N-CA-C  | -5.45 | 106.49      | 114.39   |
| 1   | BZ    | 103 | SER  | N-CA-C  | -5.43 | 106.52      | 114.39   |
| 1   | BA    | 103 | SER  | N-CA-C  | -5.43 | 106.52      | 114.39   |
| 1   | AA    | 103 | SER  | N-CA-C  | -5.42 | 106.53      | 114.39   |
| 1   | CK    | 103 | SER  | N-CA-C  | -5.42 | 106.53      | 114.39   |
| 1   | CZ    | 103 | SER  | N-CA-C  | -5.42 | 106.53      | 114.39   |
| 1   | BU    | 103 | SER  | N-CA-C  | -5.42 | 106.53      | 114.39   |
| 1   | AZ    | 103 | SER  | N-CA-C  | -5.42 | 106.53      | 114.39   |
| 1   | AP    | 103 | SER  | N-CA-C  | -5.41 | 106.54      | 114.39   |
| 1   | AU    | 103 | SER  | N-CA-C  | -5.41 | 106.54      | 114.39   |
| 1   | AK    | 103 | SER  | N-CA-C  | -5.41 | 106.55      | 114.39   |
| 1   | CP    | 103 | SER  | N-CA-C  | -5.41 | 106.55      | 114.39   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | CU    | 103 | SER  | N-CA-C  | -5.40 | 106.56      | 114.39   |
| 1   | CF    | 103 | SER  | N-CA-C  | -5.39 | 106.57      | 114.39   |
| 1   | C4    | 108 | ILE  | N-CA-CB | 5.37  | 118.73      | 111.21   |
| 1   | CY    | 108 | ILE  | N-CA-CB | 5.36  | 118.72      | 111.21   |
| 1   | BO    | 108 | ILE  | N-CA-CB | 5.36  | 118.72      | 111.21   |
| 1   | AT    | 108 | ILE  | N-CA-CB | 5.36  | 118.72      | 111.21   |
| 1   | AO    | 108 | ILE  | N-CA-CB | 5.36  | 118.71      | 111.21   |
| 1   | BT    | 108 | ILE  | N-CA-CB | 5.35  | 118.70      | 111.21   |
| 1   | BJ    | 108 | ILE  | N-CA-CB | 5.35  | 118.70      | 111.21   |
| 1   | AJ    | 108 | ILE  | N-CA-CB | 5.35  | 118.70      | 111.21   |
| 1   | AE    | 108 | ILE  | N-CA-CB | 5.34  | 118.69      | 111.21   |
| 1   | BE    | 108 | ILE  | N-CA-CB | 5.34  | 118.69      | 111.21   |
| 1   | A4    | 108 | ILE  | N-CA-CB | 5.34  | 118.69      | 111.21   |
| 1   | AY    | 108 | ILE  | N-CA-CB | 5.34  | 118.69      | 111.21   |
| 1   | CE    | 108 | ILE  | N-CA-CB | 5.34  | 118.69      | 111.21   |
| 1   | CJ    | 108 | ILE  | N-CA-CB | 5.34  | 118.69      | 111.21   |
| 1   | CO    | 108 | ILE  | N-CA-CB | 5.34  | 118.68      | 111.21   |
| 1   | B4    | 108 | ILE  | N-CA-CB | 5.33  | 118.67      | 111.21   |
| 1   | CT    | 108 | ILE  | N-CA-CB | 5.33  | 118.67      | 111.21   |
| 1   | BY    | 108 | ILE  | N-CA-CB | 5.30  | 118.63      | 111.21   |
| 1   | AG    | 42  | VAL  | CB-CA-C | -5.28 | 104.37      | 110.91   |
| 1   | BQ    | 42  | VAL  | CB-CA-C | -5.28 | 104.37      | 110.91   |
| 1   | C1    | 42  | VAL  | CB-CA-C | -5.27 | 104.37      | 110.91   |
| 1   | CV    | 42  | VAL  | CB-CA-C | -5.27 | 104.38      | 110.91   |
| 1   | CG    | 42  | VAL  | CB-CA-C | -5.26 | 104.39      | 110.91   |
| 1   | AQ    | 42  | VAL  | CB-CA-C | -5.25 | 104.40      | 110.91   |
| 1   | CQ    | 42  | VAL  | CB-CA-C | -5.25 | 104.40      | 110.91   |
| 1   | AB    | 42  | VAL  | CB-CA-C | -5.24 | 104.42      | 110.91   |
| 1   | BB    | 42  | VAL  | CB-CA-C | -5.23 | 104.42      | 110.91   |
| 1   | BL    | 42  | VAL  | CB-CA-C | -5.23 | 104.43      | 110.91   |
| 1   | AV    | 42  | VAL  | CB-CA-C | -5.22 | 104.43      | 110.91   |
| 1   | A1    | 42  | VAL  | CB-CA-C | -5.22 | 104.44      | 110.91   |
| 1   | CB    | 42  | VAL  | CB-CA-C | -5.21 | 104.44      | 110.91   |
| 1   | AL    | 42  | VAL  | CB-CA-C | -5.21 | 104.45      | 110.91   |
| 1   | BV    | 42  | VAL  | CB-CA-C | -5.21 | 104.45      | 110.91   |
| 1   | B1    | 42  | VAL  | CB-CA-C | -5.21 | 104.45      | 110.91   |
| 1   | CL    | 42  | VAL  | CB-CA-C | -5.21 | 104.45      | 110.91   |
| 1   | BG    | 42  | VAL  | CB-CA-C | -5.20 | 104.46      | 110.91   |
| 1   | AO    | 103 | SER  | N-CA-C  | -5.14 | 106.93      | 114.39   |
| 1   | BY    | 103 | SER  | N-CA-C  | -5.13 | 106.95      | 114.39   |
| 1   | CT    | 103 | SER  | N-CA-C  | -5.13 | 106.95      | 114.39   |
| 1   | CY    | 103 | SER  | N-CA-C  | -5.13 | 106.95      | 114.39   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A4    | 103 | SER  | N-CA-C | -5.13 | 106.96      | 114.39   |
| 1   | AY    | 103 | SER  | N-CA-C | -5.12 | 106.96      | 114.39   |
| 1   | BE    | 103 | SER  | N-CA-C | -5.12 | 106.96      | 114.39   |
| 1   | BT    | 103 | SER  | N-CA-C | -5.12 | 106.96      | 114.39   |
| 1   | AJ    | 103 | SER  | N-CA-C | -5.12 | 106.97      | 114.39   |
| 1   | AE    | 103 | SER  | N-CA-C | -5.12 | 106.97      | 114.39   |
| 1   | AT    | 103 | SER  | N-CA-C | -5.11 | 106.98      | 114.39   |
| 1   | CO    | 103 | SER  | N-CA-C | -5.11 | 106.98      | 114.39   |
| 1   | C4    | 103 | SER  | N-CA-C | -5.10 | 106.99      | 114.39   |
| 1   | BJ    | 103 | SER  | N-CA-C | -5.10 | 106.99      | 114.39   |
| 1   | B4    | 103 | SER  | N-CA-C | -5.10 | 107.00      | 114.39   |
| 1   | BO    | 103 | SER  | N-CA-C | -5.09 | 107.00      | 114.39   |
| 1   | CJ    | 103 | SER  | N-CA-C | -5.09 | 107.01      | 114.39   |
| 1   | CE    | 103 | SER  | N-CA-C | -5.08 | 107.02      | 114.39   |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A1    | 99  | VAL  | Peptide |
| 1   | AB    | 99  | VAL  | Peptide |
| 1   | AG    | 99  | VAL  | Peptide |
| 1   | AL    | 99  | VAL  | Peptide |
| 1   | AQ    | 99  | VAL  | Peptide |
| 1   | AV    | 99  | VAL  | Peptide |
| 1   | B1    | 99  | VAL  | Peptide |
| 1   | BB    | 99  | VAL  | Peptide |
| 1   | BG    | 99  | VAL  | Peptide |
| 1   | BL    | 99  | VAL  | Peptide |
| 1   | BQ    | 99  | VAL  | Peptide |
| 1   | BV    | 99  | VAL  | Peptide |
| 1   | C1    | 99  | VAL  | Peptide |
| 1   | CB    | 99  | VAL  | Peptide |
| 1   | CG    | 99  | VAL  | Peptide |
| 1   | CL    | 99  | VAL  | Peptide |
| 1   | CQ    | 99  | VAL  | Peptide |
| 1   | CV    | 99  | VAL  | Peptide |

## 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   | A1    | 1129  | 0        | 1143     | 69      | 0            |
| 1   | A2    | 1132  | 0        | 1145     | 78      | 0            |
| 1   | A3    | 1132  | 0        | 1145     | 64      | 0            |
| 1   | A4    | 1132  | 0        | 1145     | 77      | 0            |
| 1   | AA    | 1129  | 0        | 1143     | 61      | 0            |
| 1   | AB    | 1129  | 0        | 1143     | 77      | 0            |
| 1   | AC    | 1132  | 0        | 1145     | 82      | 0            |
| 1   | AD    | 1132  | 0        | 1145     | 71      | 0            |
| 1   | AE    | 1132  | 0        | 1145     | 84      | 0            |
| 1   | AF    | 1129  | 0        | 1143     | 65      | 0            |
| 1   | AG    | 1129  | 0        | 1143     | 71      | 2            |
| 1   | AH    | 1132  | 0        | 1145     | 79      | 3            |
| 1   | AI    | 1132  | 0        | 1145     | 72      | 0            |
| 1   | AJ    | 1132  | 0        | 1145     | 82      | 0            |
| 1   | AK    | 1129  | 0        | 1143     | 65      | 0            |
| 1   | AL    | 1129  | 0        | 1143     | 68      | 0            |
| 1   | AM    | 1132  | 0        | 1145     | 79      | 0            |
| 1   | AN    | 1132  | 0        | 1145     | 65      | 0            |
| 1   | AO    | 1132  | 0        | 1145     | 82      | 0            |
| 1   | AP    | 1129  | 0        | 1143     | 61      | 0            |
| 1   | AQ    | 1129  | 0        | 1143     | 92      | 0            |
| 1   | AR    | 1132  | 0        | 1145     | 87      | 0            |
| 1   | AS    | 1132  | 0        | 1145     | 65      | 0            |
| 1   | AT    | 1132  | 0        | 1145     | 78      | 0            |
| 1   | AU    | 1129  | 0        | 1143     | 68      | 0            |
| 1   | AV    | 1129  | 0        | 1143     | 69      | 0            |
| 1   | AW    | 1132  | 0        | 1145     | 79      | 0            |
| 1   | AX    | 1132  | 0        | 1145     | 63      | 0            |
| 1   | AY    | 1132  | 0        | 1145     | 77      | 0            |
| 1   | AZ    | 1129  | 0        | 1143     | 57      | 0            |
| 1   | B1    | 1136  | 0        | 1149     | 75      | 0            |
| 1   | B2    | 1136  | 0        | 1149     | 83      | 0            |
| 1   | B3    | 1136  | 0        | 1149     | 61      | 0            |
| 1   | B4    | 1136  | 0        | 1149     | 76      | 0            |
| 1   | BA    | 1136  | 0        | 1149     | 55      | 0            |
| 1   | BB    | 1136  | 0        | 1149     | 84      | 0            |
| 1   | BC    | 1136  | 0        | 1149     | 91      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | BD    | 1136  | 0        | 1149     | 78      | 0            |
| 1   | BE    | 1136  | 0        | 1149     | 78      | 0            |
| 1   | BF    | 1136  | 0        | 1149     | 71      | 0            |
| 1   | BG    | 1136  | 0        | 1149     | 78      | 0            |
| 1   | BH    | 1136  | 0        | 1149     | 82      | 0            |
| 1   | BI    | 1136  | 0        | 1149     | 64      | 0            |
| 1   | BJ    | 1136  | 0        | 1149     | 81      | 1            |
| 1   | BK    | 1136  | 0        | 1149     | 60      | 0            |
| 1   | BL    | 1136  | 0        | 1149     | 75      | 3            |
| 1   | BM    | 1136  | 0        | 1149     | 81      | 0            |
| 1   | BN    | 1136  | 0        | 1149     | 66      | 0            |
| 1   | BO    | 1136  | 0        | 1149     | 77      | 0            |
| 1   | BP    | 1136  | 0        | 1149     | 58      | 0            |
| 1   | BQ    | 1136  | 0        | 1149     | 85      | 0            |
| 1   | BR    | 1136  | 0        | 1149     | 92      | 0            |
| 1   | BS    | 1136  | 0        | 1149     | 69      | 0            |
| 1   | BT    | 1136  | 0        | 1149     | 76      | 0            |
| 1   | BU    | 1136  | 0        | 1149     | 83      | 0            |
| 1   | BV    | 1136  | 0        | 1149     | 77      | 0            |
| 1   | BW    | 1136  | 0        | 1149     | 83      | 0            |
| 1   | BX    | 1136  | 0        | 1149     | 64      | 0            |
| 1   | BY    | 1136  | 0        | 1149     | 80      | 0            |
| 1   | BZ    | 1136  | 0        | 1149     | 57      | 0            |
| 1   | C1    | 1136  | 0        | 1149     | 75      | 0            |
| 1   | C2    | 1136  | 0        | 1149     | 94      | 0            |
| 1   | C3    | 1136  | 0        | 1149     | 76      | 0            |
| 1   | C4    | 1136  | 0        | 1149     | 78      | 1            |
| 1   | CA    | 1136  | 0        | 1149     | 64      | 0            |
| 1   | CB    | 1136  | 0        | 1149     | 79      | 2            |
| 1   | CC    | 1136  | 0        | 1149     | 98      | 2            |
| 1   | CD    | 1136  | 0        | 1149     | 75      | 0            |
| 1   | CE    | 1136  | 0        | 1149     | 78      | 0            |
| 1   | CF    | 1136  | 0        | 1149     | 72      | 0            |
| 1   | CG    | 1136  | 0        | 1149     | 86      | 3            |
| 1   | CH    | 1136  | 0        | 1149     | 87      | 3            |
| 1   | CI    | 1136  | 0        | 1149     | 69      | 0            |
| 1   | CJ    | 1136  | 0        | 1149     | 79      | 0            |
| 1   | CK    | 1136  | 0        | 1149     | 58      | 0            |
| 1   | CL    | 1136  | 0        | 1149     | 74      | 0            |
| 1   | CM    | 1136  | 0        | 1149     | 90      | 3            |
| 1   | CN    | 1136  | 0        | 1149     | 70      | 0            |
| 1   | CO    | 1136  | 0        | 1149     | 82      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CP    | 1136  | 0        | 1149     | 66      | 0            |
| 1   | CQ    | 1136  | 0        | 1149     | 81      | 0            |
| 1   | CR    | 1136  | 0        | 1149     | 98      | 0            |
| 1   | CS    | 1136  | 0        | 1149     | 72      | 0            |
| 1   | CT    | 1136  | 0        | 1149     | 85      | 0            |
| 1   | CU    | 1136  | 0        | 1149     | 68      | 0            |
| 1   | CV    | 1136  | 0        | 1149     | 80      | 0            |
| 1   | CW    | 1136  | 0        | 1149     | 94      | 0            |
| 1   | CX    | 1136  | 0        | 1149     | 70      | 0            |
| 1   | CY    | 1136  | 0        | 1149     | 76      | 1            |
| 1   | CZ    | 1136  | 0        | 1149     | 60      | 1            |
| 2   | A1    | 5     | 0        | 0        | 0       | 0            |
| 2   | A2    | 5     | 0        | 0        | 3       | 0            |
| 2   | A3    | 5     | 0        | 0        | 0       | 0            |
| 2   | A4    | 5     | 0        | 0        | 2       | 0            |
| 2   | AA    | 5     | 0        | 0        | 1       | 0            |
| 2   | AB    | 5     | 0        | 0        | 1       | 0            |
| 2   | AC    | 5     | 0        | 0        | 3       | 0            |
| 2   | AD    | 5     | 0        | 0        | 0       | 0            |
| 2   | AE    | 5     | 0        | 0        | 2       | 0            |
| 2   | AF    | 5     | 0        | 0        | 1       | 0            |
| 2   | AG    | 5     | 0        | 0        | 1       | 0            |
| 2   | AH    | 5     | 0        | 0        | 3       | 0            |
| 2   | AI    | 5     | 0        | 0        | 0       | 0            |
| 2   | AJ    | 5     | 0        | 0        | 2       | 0            |
| 2   | AK    | 5     | 0        | 0        | 1       | 0            |
| 2   | AL    | 5     | 0        | 0        | 0       | 0            |
| 2   | AM    | 5     | 0        | 0        | 3       | 0            |
| 2   | AN    | 5     | 0        | 0        | 0       | 0            |
| 2   | AO    | 5     | 0        | 0        | 2       | 0            |
| 2   | AP    | 5     | 0        | 0        | 1       | 0            |
| 2   | AQ    | 5     | 0        | 0        | 1       | 0            |
| 2   | AR    | 5     | 0        | 0        | 3       | 0            |
| 2   | AS    | 5     | 0        | 0        | 0       | 0            |
| 2   | AT    | 5     | 0        | 0        | 2       | 0            |
| 2   | AU    | 5     | 0        | 0        | 1       | 0            |
| 2   | AV    | 5     | 0        | 0        | 1       | 0            |
| 2   | AW    | 5     | 0        | 0        | 3       | 0            |
| 2   | AX    | 5     | 0        | 0        | 0       | 0            |
| 2   | AY    | 5     | 0        | 0        | 2       | 0            |
| 2   | AZ    | 5     | 0        | 0        | 1       | 0            |
| 2   | B1    | 5     | 0        | 0        | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B2    | 5     | 0        | 0        | 3       | 0            |
| 2   | B3    | 5     | 0        | 0        | 0       | 0            |
| 2   | B4    | 5     | 0        | 0        | 2       | 0            |
| 2   | BA    | 5     | 0        | 0        | 1       | 0            |
| 2   | BB    | 5     | 0        | 0        | 1       | 0            |
| 2   | BC    | 5     | 0        | 0        | 3       | 0            |
| 2   | BD    | 5     | 0        | 0        | 0       | 0            |
| 2   | BE    | 5     | 0        | 0        | 2       | 0            |
| 2   | BF    | 5     | 0        | 0        | 1       | 0            |
| 2   | BG    | 5     | 0        | 0        | 1       | 0            |
| 2   | BH    | 5     | 0        | 0        | 3       | 0            |
| 2   | BI    | 5     | 0        | 0        | 0       | 0            |
| 2   | BJ    | 5     | 0        | 0        | 2       | 0            |
| 2   | BK    | 5     | 0        | 0        | 1       | 0            |
| 2   | BL    | 5     | 0        | 0        | 1       | 0            |
| 2   | BM    | 5     | 0        | 0        | 3       | 0            |
| 2   | BN    | 5     | 0        | 0        | 0       | 0            |
| 2   | BO    | 5     | 0        | 0        | 2       | 0            |
| 2   | BP    | 5     | 0        | 0        | 1       | 0            |
| 2   | BQ    | 5     | 0        | 0        | 1       | 0            |
| 2   | BR    | 5     | 0        | 0        | 3       | 0            |
| 2   | BS    | 5     | 0        | 0        | 0       | 0            |
| 2   | BT    | 5     | 0        | 0        | 2       | 0            |
| 2   | BU    | 5     | 0        | 0        | 1       | 0            |
| 2   | BV    | 5     | 0        | 0        | 0       | 0            |
| 2   | BW    | 5     | 0        | 0        | 3       | 0            |
| 2   | BX    | 5     | 0        | 0        | 0       | 0            |
| 2   | BY    | 5     | 0        | 0        | 2       | 0            |
| 2   | BZ    | 5     | 0        | 0        | 1       | 0            |
| 2   | C1    | 5     | 0        | 0        | 1       | 0            |
| 2   | C2    | 5     | 0        | 0        | 3       | 0            |
| 2   | C3    | 5     | 0        | 0        | 0       | 0            |
| 2   | C4    | 5     | 0        | 0        | 2       | 0            |
| 2   | CA    | 5     | 0        | 0        | 1       | 0            |
| 2   | CB    | 5     | 0        | 0        | 1       | 0            |
| 2   | CC    | 5     | 0        | 0        | 3       | 0            |
| 2   | CD    | 5     | 0        | 0        | 0       | 0            |
| 2   | CE    | 5     | 0        | 0        | 2       | 0            |
| 2   | CF    | 5     | 0        | 0        | 1       | 0            |
| 2   | CG    | 5     | 0        | 0        | 1       | 0            |
| 2   | CH    | 5     | 0        | 0        | 3       | 0            |
| 2   | CI    | 5     | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | CJ    | 5      | 0        | 0        | 2       | 0            |
| 2   | CK    | 5      | 0        | 0        | 1       | 0            |
| 2   | CL    | 5      | 0        | 0        | 1       | 0            |
| 2   | CM    | 5      | 0        | 0        | 3       | 0            |
| 2   | CN    | 5      | 0        | 0        | 0       | 0            |
| 2   | CO    | 5      | 0        | 0        | 2       | 0            |
| 2   | CP    | 5      | 0        | 0        | 1       | 0            |
| 2   | CQ    | 5      | 0        | 0        | 0       | 0            |
| 2   | CR    | 5      | 0        | 0        | 3       | 0            |
| 2   | CS    | 5      | 0        | 0        | 0       | 0            |
| 2   | CT    | 5      | 0        | 0        | 2       | 0            |
| 2   | CU    | 5      | 0        | 0        | 1       | 0            |
| 2   | CV    | 5      | 0        | 0        | 0       | 0            |
| 2   | CW    | 5      | 0        | 0        | 3       | 0            |
| 2   | CX    | 5      | 0        | 0        | 0       | 0            |
| 2   | CY    | 5      | 0        | 0        | 2       | 0            |
| 2   | CZ    | 5      | 0        | 0        | 1       | 0            |
| All | All   | 102534 | 0        | 103266   | 5787    | 13           |

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 28.

All (5787) 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:CT:53:PRO:CG | 1:CT:57:GLU:HG3 | 1.49                     | 1.43              |
| 1:CJ:53:PRO:CG | 1:CJ:57:GLU:HG3 | 1.49                     | 1.42              |
| 1:AE:53:PRO:CG | 1:AE:57:GLU:HG3 | 1.49                     | 1.42              |
| 1:B4:53:PRO:CG | 1:B4:57:GLU:HG3 | 1.49                     | 1.42              |
| 1:C4:53:PRO:CG | 1:C4:57:GLU:HG3 | 1.49                     | 1.42              |
| 1:CY:53:PRO:CG | 1:CY:57:GLU:HG3 | 1.49                     | 1.42              |
| 1:A4:53:PRO:CG | 1:A4:57:GLU:HG3 | 1.49                     | 1.42              |
| 1:AJ:53:PRO:CG | 1:AJ:57:GLU:HG3 | 1.49                     | 1.41              |
| 1:AO:53:PRO:CG | 1:AO:57:GLU:HG3 | 1.49                     | 1.41              |
| 1:BJ:53:PRO:CG | 1:BJ:57:GLU:HG3 | 1.49                     | 1.41              |
| 1:BO:53:PRO:CG | 1:BO:57:GLU:HG3 | 1.49                     | 1.41              |
| 1:AT:53:PRO:CG | 1:AT:57:GLU:HG3 | 1.49                     | 1.41              |
| 1:BY:53:PRO:CG | 1:BY:57:GLU:HG3 | 1.49                     | 1.40              |
| 1:CE:53:PRO:CG | 1:CE:57:GLU:HG3 | 1.49                     | 1.40              |
| 1:CO:53:PRO:CG | 1:CO:57:GLU:HG3 | 1.49                     | 1.40              |
| 1:AY:53:PRO:CG | 1:AY:57:GLU:HG3 | 1.49                     | 1.39              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BT:53:PRO:CG    | 1:BT:57:GLU:HG3  | 1.49                     | 1.39              |
| 1:BE:53:PRO:CG    | 1:BE:57:GLU:HG3  | 1.49                     | 1.39              |
| 1:AQ:69:GLY:O     | 1:BU:10:THR:HG23 | 1.27                     | 1.33              |
| 1:CE:53:PRO:HG2   | 1:CE:57:GLU:CG   | 1.59                     | 1.32              |
| 1:CO:53:PRO:HG2   | 1:CO:57:GLU:CG   | 1.59                     | 1.32              |
| 1:CT:53:PRO:HG2   | 1:CT:57:GLU:CG   | 1.59                     | 1.32              |
| 1:AJ:53:PRO:HG2   | 1:AJ:57:GLU:CG   | 1.59                     | 1.32              |
| 1:CY:53:PRO:HG2   | 1:CY:57:GLU:CG   | 1.59                     | 1.32              |
| 1:AO:53:PRO:HG2   | 1:AO:57:GLU:CG   | 1.59                     | 1.31              |
| 1:AE:53:PRO:HG2   | 1:AE:57:GLU:CG   | 1.59                     | 1.31              |
| 1:AT:53:PRO:HG2   | 1:AT:57:GLU:CG   | 1.59                     | 1.31              |
| 1:CJ:53:PRO:HG2   | 1:CJ:57:GLU:CG   | 1.59                     | 1.31              |
| 1:BO:53:PRO:HG2   | 1:BO:57:GLU:CG   | 1.59                     | 1.30              |
| 1:A4:53:PRO:HG2   | 1:A4:57:GLU:CG   | 1.59                     | 1.30              |
| 1:BJ:53:PRO:HG2   | 1:BJ:57:GLU:CG   | 1.59                     | 1.30              |
| 1:BY:53:PRO:HG2   | 1:BY:57:GLU:CG   | 1.59                     | 1.30              |
| 1:B4:53:PRO:HG2   | 1:B4:57:GLU:CG   | 1.59                     | 1.30              |
| 1:C4:53:PRO:HG2   | 1:C4:57:GLU:CG   | 1.59                     | 1.30              |
| 1:BT:53:PRO:HG2   | 1:BT:57:GLU:CG   | 1.59                     | 1.29              |
| 1:BE:53:PRO:HG2   | 1:BE:57:GLU:CG   | 1.59                     | 1.29              |
| 1:AY:53:PRO:HG2   | 1:AY:57:GLU:CG   | 1.59                     | 1.29              |
| 1:AR:129:THR:HG22 | 1:AR:130:LYS:H   | 1.05                     | 1.20              |
| 1:BH:129:THR:HG22 | 1:BH:130:LYS:H   | 1.05                     | 1.20              |
| 1:C2:129:THR:HG22 | 1:C2:130:LYS:H   | 1.05                     | 1.19              |
| 1:AC:129:THR:HG22 | 1:AC:130:LYS:H   | 1.05                     | 1.17              |
| 1:CR:129:THR:HG22 | 1:CR:130:LYS:H   | 1.05                     | 1.17              |
| 1:B2:129:THR:HG22 | 1:B2:130:LYS:H   | 1.05                     | 1.16              |
| 1:BB:107:ASP:OD2  | 1:BC:64:LYS:NZ   | 1.76                     | 1.15              |
| 1:BM:129:THR:HG22 | 1:BM:130:LYS:H   | 1.05                     | 1.15              |
| 1:CM:129:THR:HG22 | 1:CM:130:LYS:H   | 1.05                     | 1.15              |
| 1:CW:129:THR:HG22 | 1:CW:130:LYS:H   | 1.05                     | 1.15              |
| 1:AM:129:THR:HG22 | 1:AM:130:LYS:H   | 1.05                     | 1.15              |
| 1:AG:104:LEU:HD21 | 1:AH:60:LEU:HA   | 1.30                     | 1.14              |
| 1:A2:129:THR:HG22 | 1:A2:130:LYS:H   | 1.05                     | 1.14              |
| 1:C1:107:ASP:OD2  | 1:C2:64:LYS:NZ   | 1.76                     | 1.14              |
| 1:BL:104:LEU:HD21 | 1:BM:60:LEU:HA   | 1.30                     | 1.14              |
| 1:BG:104:LEU:HD21 | 1:BH:60:LEU:HA   | 1.30                     | 1.13              |
| 1:A1:104:LEU:HD21 | 1:A2:60:LEU:HA   | 1.30                     | 1.12              |
| 1:CC:129:THR:HG22 | 1:CC:130:LYS:H   | 1.05                     | 1.12              |
| 1:CL:104:LEU:HD21 | 1:CM:60:LEU:HA   | 1.30                     | 1.12              |
| 1:AL:104:LEU:HD21 | 1:AM:60:LEU:HA   | 1.30                     | 1.12              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BV:104:LEU:HD21 | 1:BW:60:LEU:HA   | 1.30                     | 1.12              |
| 1:BW:129:THR:HG22 | 1:BW:130:LYS:H   | 1.05                     | 1.11              |
| 1:CV:107:ASP:OD2  | 1:CW:64:LYS:NZ   | 1.76                     | 1.11              |
| 1:BR:129:THR:HG22 | 1:BR:130:LYS:H   | 1.05                     | 1.11              |
| 1:AH:129:THR:HG22 | 1:AH:130:LYS:H   | 1.05                     | 1.11              |
| 1:AQ:13:LYS:NZ    | 1:BU:43:GLU:HG2  | 1.65                     | 1.11              |
| 1:AW:129:THR:HG22 | 1:AW:130:LYS:H   | 1.05                     | 1.11              |
| 1:CG:104:LEU:HD21 | 1:CH:60:LEU:HA   | 1.30                     | 1.10              |
| 1:B1:107:ASP:OD2  | 1:B2:64:LYS:NZ   | 1.76                     | 1.10              |
| 1:CV:104:LEU:HD21 | 1:CW:60:LEU:HA   | 1.30                     | 1.10              |
| 1:CB:107:ASP:OD2  | 1:CC:64:LYS:NZ   | 1.76                     | 1.09              |
| 1:AV:104:LEU:HD21 | 1:AW:60:LEU:HA   | 1.30                     | 1.09              |
| 1:CB:104:LEU:HD21 | 1:CC:60:LEU:HA   | 1.30                     | 1.09              |
| 1:AQ:104:LEU:HD21 | 1:AR:60:LEU:HA   | 1.30                     | 1.08              |
| 1:CH:129:THR:HG22 | 1:CH:130:LYS:H   | 1.05                     | 1.08              |
| 1:BV:107:ASP:OD2  | 1:BW:64:LYS:NZ   | 1.76                     | 1.07              |
| 1:B1:104:LEU:HD21 | 1:B2:60:LEU:HA   | 1.30                     | 1.07              |
| 1:CQ:107:ASP:OD2  | 1:CR:64:LYS:NZ   | 1.76                     | 1.07              |
| 1:BC:129:THR:HG22 | 1:BC:130:LYS:H   | 1.05                     | 1.07              |
| 1:BG:107:ASP:OD2  | 1:BH:64:LYS:NZ   | 1.76                     | 1.07              |
| 1:AB:104:LEU:HD21 | 1:AC:60:LEU:HA   | 1.30                     | 1.07              |
| 1:C1:104:LEU:HD21 | 1:C2:60:LEU:HA   | 1.30                     | 1.06              |
| 1:BQ:104:LEU:HD21 | 1:BR:60:LEU:HA   | 1.30                     | 1.06              |
| 1:AE:72:ASP:O     | 1:AE:150:LYS:HD3 | 1.56                     | 1.06              |
| 1:AO:72:ASP:O     | 1:AO:150:LYS:HD3 | 1.56                     | 1.05              |
| 1:BB:104:LEU:HD21 | 1:BC:60:LEU:HA   | 1.30                     | 1.05              |
| 1:BY:72:ASP:O     | 1:BY:150:LYS:HD3 | 1.56                     | 1.05              |
| 1:CJ:72:ASP:O     | 1:CJ:150:LYS:HD3 | 1.56                     | 1.05              |
| 1:CO:72:ASP:O     | 1:CO:150:LYS:HD3 | 1.56                     | 1.05              |
| 1:BD:11:GLY:HA3   | 1:CM:11:GLY:HA3  | 1.38                     | 1.05              |
| 1:CE:72:ASP:O     | 1:CE:150:LYS:HD3 | 1.56                     | 1.05              |
| 1:CL:107:ASP:OD2  | 1:CM:64:LYS:NZ   | 1.76                     | 1.05              |
| 1:AJ:72:ASP:O     | 1:AJ:150:LYS:HD3 | 1.56                     | 1.04              |
| 1:BE:72:ASP:O     | 1:BE:150:LYS:HD3 | 1.56                     | 1.04              |
| 1:BL:107:ASP:OD2  | 1:BM:64:LYS:NZ   | 1.76                     | 1.04              |
| 1:CQ:104:LEU:HD21 | 1:CR:60:LEU:HA   | 1.30                     | 1.04              |
| 1:AT:72:ASP:O     | 1:AT:150:LYS:HD3 | 1.56                     | 1.04              |
| 1:A4:72:ASP:O     | 1:A4:150:LYS:HD3 | 1.56                     | 1.04              |
| 1:BO:72:ASP:O     | 1:BO:150:LYS:HD3 | 1.56                     | 1.04              |
| 1:AY:72:ASP:O     | 1:AY:150:LYS:HD3 | 1.56                     | 1.03              |
| 1:CY:72:ASP:O     | 1:CY:150:LYS:HD3 | 1.56                     | 1.03              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BJ:72:ASP:O     | 1:BJ:150:LYS:HD3 | 1.56                     | 1.03              |
| 1:B4:72:ASP:O     | 1:B4:150:LYS:HD3 | 1.56                     | 1.03              |
| 1:BT:72:ASP:O     | 1:BT:150:LYS:HD3 | 1.56                     | 1.03              |
| 1:BI:107:ASP:O    | 1:BI:107:ASP:OD1 | 1.77                     | 1.02              |
| 1:C3:107:ASP:OD1  | 1:C3:107:ASP:O   | 1.77                     | 1.02              |
| 1:CT:72:ASP:O     | 1:CT:150:LYS:HD3 | 1.56                     | 1.02              |
| 1:AI:107:ASP:OD1  | 1:AI:107:ASP:O   | 1.77                     | 1.02              |
| 1:BN:107:ASP:O    | 1:BN:107:ASP:OD1 | 1.77                     | 1.02              |
| 1:CG:107:ASP:OD2  | 1:CH:64:LYS:NZ   | 1.76                     | 1.02              |
| 1:C4:72:ASP:O     | 1:C4:150:LYS:HD3 | 1.56                     | 1.02              |
| 1:AN:107:ASP:OD1  | 1:AN:107:ASP:O   | 1.77                     | 1.01              |
| 1:AV:96:ALA:C     | 1:AV:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:BB:96:ALA:C     | 1:BB:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:BL:96:ALA:C     | 1:BL:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:CI:107:ASP:OD1  | 1:CI:107:ASP:O   | 1.77                     | 1.01              |
| 1:CN:107:ASP:OD1  | 1:CN:107:ASP:O   | 1.77                     | 1.01              |
| 1:AD:107:ASP:O    | 1:AD:107:ASP:OD1 | 1.77                     | 1.01              |
| 1:A3:107:ASP:O    | 1:A3:107:ASP:OD1 | 1.77                     | 1.01              |
| 1:CB:96:ALA:C     | 1:CB:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:CL:96:ALA:C     | 1:CL:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:CQ:96:ALA:C     | 1:CQ:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:AL:96:ALA:C     | 1:AL:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:AQ:13:LYS:HZ1   | 1:BU:43:GLU:CG   | 1.73                     | 1.01              |
| 1:AQ:96:ALA:C     | 1:AQ:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:AX:107:ASP:O    | 1:AX:107:ASP:OD1 | 1.77                     | 1.01              |
| 1:BB:107:ASP:HB2  | 1:BB:152:TRP:CZ3 | 1.96                     | 1.01              |
| 1:BL:107:ASP:HB2  | 1:BL:152:TRP:CZ3 | 1.96                     | 1.01              |
| 1:B1:52:VAL:HG12  | 1:B1:61:ILE:HD12 | 1.43                     | 1.01              |
| 1:C1:96:ALA:C     | 1:C1:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:AB:96:ALA:C     | 1:AB:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:B1:96:ALA:C     | 1:B1:100:ALA:HB2 | 1.86                     | 1.01              |
| 1:CQ:107:ASP:HB2  | 1:CQ:152:TRP:CZ3 | 1.96                     | 1.01              |
| 1:CX:107:ASP:O    | 1:CX:107:ASP:OD1 | 1.77                     | 1.01              |
| 1:AQ:52:VAL:HG12  | 1:AQ:61:ILE:HD12 | 1.43                     | 1.00              |
| 1:BV:52:VAL:HG12  | 1:BV:61:ILE:HD12 | 1.43                     | 1.00              |
| 1:CD:107:ASP:OD1  | 1:CD:107:ASP:O   | 1.77                     | 1.00              |
| 1:CL:107:ASP:HB2  | 1:CL:152:TRP:CZ3 | 1.96                     | 1.00              |
| 1:CV:107:ASP:HB2  | 1:CV:152:TRP:CZ3 | 1.96                     | 1.00              |
| 1:BV:107:ASP:HB2  | 1:BV:152:TRP:CZ3 | 1.96                     | 1.00              |
| 1:CB:107:ASP:HB2  | 1:CB:152:TRP:CZ3 | 1.96                     | 1.00              |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:CD1 | 1.91                     | 1.00              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:CS:107:ASP:O   | 1:CS:107:ASP:OD1 | 1.77                     | 1.00              |
| 1:AG:96:ALA:C    | 1:AG:100:ALA:HB2 | 1.86                     | 1.00              |
| 1:BD:107:ASP:OD1 | 1:BD:107:ASP:O   | 1.77                     | 1.00              |
| 1:B1:107:ASP:HB2 | 1:B1:152:TRP:CZ3 | 1.96                     | 1.00              |
| 1:AG:52:VAL:HG12 | 1:AG:61:ILE:HD12 | 1.43                     | 1.00              |
| 1:AS:107:ASP:OD1 | 1:AS:107:ASP:O   | 1.77                     | 1.00              |
| 1:BX:107:ASP:OD1 | 1:BX:107:ASP:O   | 1.77                     | 1.00              |
| 1:CB:52:VAL:HG12 | 1:CB:61:ILE:HD12 | 1.43                     | 1.00              |
| 1:BG:96:ALA:C    | 1:BG:100:ALA:HB2 | 1.86                     | 1.00              |
| 1:BL:52:VAL:HG12 | 1:BL:61:ILE:HD12 | 1.43                     | 1.00              |
| 1:BQ:96:ALA:C    | 1:BQ:100:ALA:HB2 | 1.86                     | 1.00              |
| 1:BQ:107:ASP:OD2 | 1:BR:64:LYS:NZ   | 1.76                     | 1.00              |
| 1:BV:96:ALA:C    | 1:BV:100:ALA:HB2 | 1.86                     | 1.00              |
| 1:BG:107:ASP:HB2 | 1:BG:152:TRP:CZ3 | 1.96                     | 0.99              |
| 1:B3:107:ASP:OD1 | 1:B3:107:ASP:O   | 1.77                     | 0.99              |
| 1:CV:96:ALA:C    | 1:CV:100:ALA:HB2 | 1.86                     | 0.99              |
| 1:AQ:69:GLY:O    | 1:BU:10:THR:CG2  | 2.08                     | 0.99              |
| 1:BB:52:VAL:HG12 | 1:BB:61:ILE:HD12 | 1.43                     | 0.99              |
| 1:BQ:107:ASP:HB2 | 1:BQ:152:TRP:CZ3 | 1.96                     | 0.99              |
| 1:BS:107:ASP:OD1 | 1:BS:107:ASP:O   | 1.77                     | 0.99              |
| 1:AL:52:VAL:HG12 | 1:AL:61:ILE:HD12 | 1.43                     | 0.99              |
| 1:A1:96:ALA:C    | 1:A1:100:ALA:HB2 | 1.86                     | 0.99              |
| 1:C1:107:ASP:HB2 | 1:C1:152:TRP:CZ3 | 1.96                     | 0.99              |
| 1:CG:96:ALA:C    | 1:CG:100:ALA:HB2 | 1.86                     | 0.99              |
| 1:CG:107:ASP:HB2 | 1:CG:152:TRP:CZ3 | 1.96                     | 0.99              |
| 1:CQ:52:VAL:HG12 | 1:CQ:61:ILE:HD12 | 1.43                     | 0.99              |
| 1:A1:52:VAL:HG12 | 1:A1:61:ILE:HD12 | 1.43                     | 0.98              |
| 1:CL:52:VAL:HG12 | 1:CL:61:ILE:HD12 | 1.43                     | 0.98              |
| 1:C1:52:VAL:HG12 | 1:C1:61:ILE:HD12 | 1.43                     | 0.98              |
| 1:AQ:13:LYS:HZ1  | 1:BU:43:GLU:HG2  | 1.21                     | 0.98              |
| 1:CV:52:VAL:HG12 | 1:CV:61:ILE:HD12 | 1.43                     | 0.98              |
| 1:CG:52:VAL:HG12 | 1:CG:61:ILE:HD12 | 1.43                     | 0.97              |
| 1:BG:52:VAL:HG12 | 1:BG:61:ILE:HD12 | 1.43                     | 0.97              |
| 1:AB:52:VAL:HG12 | 1:AB:61:ILE:HD12 | 1.43                     | 0.97              |
| 1:AV:52:VAL:HG12 | 1:AV:61:ILE:HD12 | 1.43                     | 0.97              |
| 1:BQ:52:VAL:HG12 | 1:BQ:61:ILE:HD12 | 1.43                     | 0.97              |
| 1:AX:52:VAL:HG12 | 1:AX:61:ILE:HD12 | 1.49                     | 0.94              |
| 1:AD:52:VAL:HG12 | 1:AD:61:ILE:HD12 | 1.49                     | 0.94              |
| 1:AN:52:VAL:HG12 | 1:AN:61:ILE:HD12 | 1.49                     | 0.94              |
| 1:B3:52:VAL:HG12 | 1:B3:61:ILE:HD12 | 1.49                     | 0.94              |
| 1:BS:52:VAL:HG12 | 1:BS:61:ILE:HD12 | 1.49                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:CI:52:VAL:HG12 | 1:CI:61:ILE:HD12 | 1.49                     | 0.94              |
| 1:BJ:52:VAL:HG12 | 1:BJ:61:ILE:HD12 | 1.50                     | 0.94              |
| 1:BD:52:VAL:HG12 | 1:BD:61:ILE:HD12 | 1.49                     | 0.94              |
| 1:BX:52:VAL:HG12 | 1:BX:61:ILE:HD12 | 1.49                     | 0.93              |
| 1:BO:52:VAL:HG12 | 1:BO:61:ILE:HD12 | 1.50                     | 0.93              |
| 1:C3:52:VAL:HG12 | 1:C3:61:ILE:HD12 | 1.49                     | 0.93              |
| 1:AE:52:VAL:HG12 | 1:AE:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:AJ:52:VAL:HG12 | 1:AJ:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:AY:52:VAL:HG12 | 1:AY:61:ILE:HD12 | 1.50                     | 0.93              |
| 1:BY:52:VAL:HG12 | 1:BY:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:C4:52:VAL:HG12 | 1:C4:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:AS:52:VAL:HG12 | 1:AS:61:ILE:HD12 | 1.49                     | 0.93              |
| 1:B4:52:VAL:HG12 | 1:B4:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:AC:52:VAL:HG12 | 1:AC:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:AI:52:VAL:HG12 | 1:AI:61:ILE:HD12 | 1.49                     | 0.93              |
| 1:A3:52:VAL:HG12 | 1:A3:61:ILE:HD12 | 1.50                     | 0.93              |
| 1:A4:52:VAL:HG12 | 1:A4:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:CM:52:VAL:HG12 | 1:CM:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:BH:52:VAL:HG12 | 1:BH:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:BT:52:VAL:HG12 | 1:BT:61:ILE:HD12 | 1.50                     | 0.93              |
| 1:CE:52:VAL:HG12 | 1:CE:61:ILE:HD12 | 1.51                     | 0.93              |
| 1:BC:52:VAL:HG12 | 1:BC:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:AT:52:VAL:HG12 | 1:AT:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:BN:52:VAL:HG12 | 1:BN:61:ILE:HD12 | 1.49                     | 0.92              |
| 1:CN:52:VAL:HG12 | 1:CN:61:ILE:HD12 | 1.49                     | 0.92              |
| 1:AQ:13:LYS:HZ1  | 1:BU:43:GLU:CB   | 1.83                     | 0.92              |
| 1:AH:52:VAL:HG12 | 1:AH:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:AO:52:VAL:HG12 | 1:AO:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:CR:52:VAL:HG12 | 1:CR:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:AM:52:VAL:HG12 | 1:AM:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:A2:52:VAL:HG12 | 1:A2:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:AW:52:VAL:HG12 | 1:AW:61:ILE:HD12 | 1.52                     | 0.92              |
| 1:BE:52:VAL:HG12 | 1:BE:61:ILE:HD12 | 1.50                     | 0.92              |
| 1:BR:52:VAL:HG12 | 1:BR:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:CC:52:VAL:HG12 | 1:CC:61:ILE:HD12 | 1.51                     | 0.92              |
| 1:CS:52:VAL:HG12 | 1:CS:61:ILE:HD12 | 1.49                     | 0.92              |
| 1:CJ:52:VAL:HG12 | 1:CJ:61:ILE:HD12 | 1.51                     | 0.91              |
| 1:BI:52:VAL:HG12 | 1:BI:61:ILE:HD12 | 1.49                     | 0.91              |
| 1:CH:52:VAL:HG12 | 1:CH:61:ILE:HD12 | 1.51                     | 0.91              |
| 1:CX:52:VAL:HG12 | 1:CX:61:ILE:HD12 | 1.49                     | 0.91              |
| 1:B2:52:VAL:HG12 | 1:B2:61:ILE:HD12 | 1.51                     | 0.91              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BM:52:VAL:HG12  | 1:BM:61:ILE:HD12 | 1.51                     | 0.91              |
| 1:CD:52:VAL:HG12  | 1:CD:61:ILE:HD12 | 1.49                     | 0.91              |
| 1:BW:52:VAL:HG12  | 1:BW:61:ILE:HD12 | 1.51                     | 0.90              |
| 1:CO:52:VAL:HG12  | 1:CO:61:ILE:HD12 | 1.50                     | 0.90              |
| 1:AR:52:VAL:HG12  | 1:AR:61:ILE:HD12 | 1.51                     | 0.90              |
| 1:C2:52:VAL:HG12  | 1:C2:61:ILE:HD12 | 1.52                     | 0.90              |
| 1:BP:52:VAL:HG12  | 1:BP:61:ILE:HD12 | 1.54                     | 0.90              |
| 1:CW:52:VAL:HG12  | 1:CW:61:ILE:HD12 | 1.51                     | 0.90              |
| 1:CY:52:VAL:HG12  | 1:CY:61:ILE:HD12 | 1.51                     | 0.90              |
| 1:AP:52:VAL:HG12  | 1:AP:61:ILE:HD12 | 1.54                     | 0.90              |
| 1:CK:52:VAL:HG12  | 1:CK:61:ILE:HD12 | 1.54                     | 0.89              |
| 1:AU:52:VAL:HG12  | 1:AU:61:ILE:HD12 | 1.54                     | 0.89              |
| 1:CT:52:VAL:HG12  | 1:CT:61:ILE:HD12 | 1.51                     | 0.89              |
| 1:AF:52:VAL:HG12  | 1:AF:61:ILE:HD12 | 1.54                     | 0.89              |
| 1:CU:52:VAL:HG12  | 1:CU:61:ILE:HD12 | 1.54                     | 0.89              |
| 1:BO:52:VAL:HB    | 1:BO:53:PRO:HD2  | 1.55                     | 0.89              |
| 1:CT:52:VAL:HB    | 1:CT:53:PRO:HD2  | 1.55                     | 0.89              |
| 1:B4:52:VAL:HB    | 1:B4:53:PRO:HD2  | 1.55                     | 0.89              |
| 1:CJ:52:VAL:HB    | 1:CJ:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:CR:129:THR:HG22 | 1:CR:130:LYS:N   | 1.88                     | 0.88              |
| 1:AK:52:VAL:HG12  | 1:AK:61:ILE:HD12 | 1.54                     | 0.88              |
| 1:BT:52:VAL:HB    | 1:BT:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:BY:52:VAL:HB    | 1:BY:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:BF:52:VAL:HG12  | 1:BF:61:ILE:HD12 | 1.54                     | 0.88              |
| 1:BK:52:VAL:HG12  | 1:BK:61:ILE:HD12 | 1.54                     | 0.88              |
| 1:AJ:52:VAL:HB    | 1:AJ:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:AY:52:VAL:HB    | 1:AY:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:BA:52:VAL:HG12  | 1:BA:61:ILE:HD12 | 1.54                     | 0.88              |
| 1:BW:129:THR:HG22 | 1:BW:130:LYS:N   | 1.89                     | 0.88              |
| 1:AO:52:VAL:HB    | 1:AO:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:A4:52:VAL:HB    | 1:A4:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:BE:52:VAL:HB    | 1:BE:53:PRO:HD2  | 1.55                     | 0.88              |
| 1:CM:38:LYS:HZ2   | 1:CM:44:GLU:HG3  | 1.38                     | 0.88              |
| 1:AR:129:THR:HG22 | 1:AR:130:LYS:N   | 1.88                     | 0.88              |
| 1:CF:52:VAL:HG12  | 1:CF:61:ILE:HD12 | 1.54                     | 0.88              |
| 1:CA:52:VAL:HG12  | 1:CA:61:ILE:HD12 | 1.54                     | 0.88              |
| 1:CC:129:THR:HG22 | 1:CC:130:LYS:N   | 1.88                     | 0.88              |
| 1:AT:52:VAL:HB    | 1:AT:53:PRO:HD2  | 1.55                     | 0.87              |
| 1:BR:129:THR:HG22 | 1:BR:130:LYS:N   | 1.89                     | 0.87              |
| 1:CM:129:THR:HG22 | 1:CM:130:LYS:N   | 1.88                     | 0.87              |
| 1:C4:52:VAL:HB    | 1:C4:53:PRO:HD2  | 1.55                     | 0.87              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BZ:52:VAL:HG12  | 1:BZ:61:ILE:HD12 | 1.54                     | 0.87              |
| 1:CP:52:VAL:HG12  | 1:CP:61:ILE:HD12 | 1.54                     | 0.87              |
| 1:AH:129:THR:HG22 | 1:AH:130:LYS:N   | 1.89                     | 0.87              |
| 1:AW:129:THR:HG22 | 1:AW:130:LYS:N   | 1.88                     | 0.87              |
| 1:CO:52:VAL:HB    | 1:CO:53:PRO:HD2  | 1.55                     | 0.87              |
| 1:CE:52:VAL:HB    | 1:CE:53:PRO:HD2  | 1.55                     | 0.87              |
| 1:BC:129:THR:HG21 | 1:BS:120:ILE:CD1 | 2.05                     | 0.86              |
| 1:C2:129:THR:HG22 | 1:C2:130:LYS:N   | 1.88                     | 0.86              |
| 1:AW:129:THR:CG2  | 1:AW:130:LYS:H   | 1.89                     | 0.86              |
| 1:BU:52:VAL:HG12  | 1:BU:61:ILE:HD12 | 1.54                     | 0.86              |
| 1:A2:129:THR:HG22 | 1:A2:130:LYS:N   | 1.88                     | 0.86              |
| 1:AE:52:VAL:HB    | 1:AE:53:PRO:HD2  | 1.55                     | 0.86              |
| 1:BH:129:THR:HG22 | 1:BH:130:LYS:N   | 1.89                     | 0.86              |
| 1:CY:52:VAL:HB    | 1:CY:53:PRO:HD2  | 1.55                     | 0.86              |
| 1:AA:52:VAL:HG12  | 1:AA:61:ILE:HD12 | 1.54                     | 0.86              |
| 1:BJ:52:VAL:HB    | 1:BJ:53:PRO:HD2  | 1.55                     | 0.86              |
| 1:BM:129:THR:HG22 | 1:BM:130:LYS:N   | 1.88                     | 0.86              |
| 1:AM:129:THR:HG22 | 1:AM:130:LYS:N   | 1.88                     | 0.85              |
| 1:B2:129:THR:HG22 | 1:B2:130:LYS:N   | 1.88                     | 0.85              |
| 1:AZ:52:VAL:HG12  | 1:AZ:61:ILE:HD12 | 1.54                     | 0.85              |
| 1:CZ:52:VAL:HG12  | 1:CZ:61:ILE:HD12 | 1.54                     | 0.85              |
| 1:C1:55:ALA:HB1   | 1:C1:95:VAL:HG21 | 1.59                     | 0.85              |
| 1:CQ:55:ALA:HB1   | 1:CQ:95:VAL:HG21 | 1.59                     | 0.85              |
| 1:CV:55:ALA:HB1   | 1:CV:95:VAL:HG21 | 1.59                     | 0.85              |
| 1:BC:129:THR:CG2  | 1:BC:130:LYS:H   | 1.89                     | 0.85              |
| 1:AM:129:THR:CG2  | 1:AM:130:LYS:H   | 1.89                     | 0.85              |
| 1:A1:55:ALA:HB1   | 1:A1:95:VAL:HG21 | 1.59                     | 0.85              |
| 1:BG:55:ALA:HB1   | 1:BG:95:VAL:HG21 | 1.59                     | 0.85              |
| 1:C2:129:THR:CG2  | 1:C2:130:LYS:H   | 1.89                     | 0.85              |
| 1:AB:55:ALA:HB1   | 1:AB:95:VAL:HG21 | 1.59                     | 0.85              |
| 1:B1:55:ALA:HB1   | 1:B1:95:VAL:HG21 | 1.59                     | 0.84              |
| 1:BB:55:ALA:HB1   | 1:BB:95:VAL:HG21 | 1.59                     | 0.84              |
| 1:BC:129:THR:HG22 | 1:BC:130:LYS:N   | 1.88                     | 0.84              |
| 1:CB:55:ALA:HB1   | 1:CB:95:VAL:HG21 | 1.59                     | 0.84              |
| 1:AG:55:ALA:HB1   | 1:AG:95:VAL:HG21 | 1.59                     | 0.84              |
| 1:CM:129:THR:CG2  | 1:CM:130:LYS:H   | 1.89                     | 0.84              |
| 1:AO:72:ASP:C     | 1:AO:150:LYS:HD3 | 2.03                     | 0.84              |
| 1:AY:72:ASP:C     | 1:AY:150:LYS:HD3 | 2.03                     | 0.84              |
| 1:BT:124:ILE:O    | 1:BT:129:THR:OG1 | 1.96                     | 0.84              |
| 1:CH:129:THR:CG2  | 1:CH:130:LYS:H   | 1.89                     | 0.84              |
| 1:AT:72:ASP:C     | 1:AT:150:LYS:HD3 | 2.03                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AO:124:ILE:O    | 1:AO:129:THR:OG1 | 1.96                     | 0.84              |
| 1:BO:124:ILE:O    | 1:BO:129:THR:OG1 | 1.96                     | 0.84              |
| 1:BV:55:ALA:HB1   | 1:BV:95:VAL:HG21 | 1.59                     | 0.84              |
| 1:CE:72:ASP:C     | 1:CE:150:LYS:HD3 | 2.03                     | 0.84              |
| 1:BO:72:ASP:C     | 1:BO:150:LYS:HD3 | 2.03                     | 0.84              |
| 1:AY:124:ILE:O    | 1:AY:129:THR:OG1 | 1.96                     | 0.83              |
| 1:CJ:72:ASP:C     | 1:CJ:150:LYS:HD3 | 2.03                     | 0.83              |
| 1:CT:124:ILE:O    | 1:CT:129:THR:OG1 | 1.96                     | 0.83              |
| 1:A4:124:ILE:O    | 1:A4:129:THR:OG1 | 1.96                     | 0.83              |
| 1:BY:124:ILE:O    | 1:BY:129:THR:OG1 | 1.96                     | 0.83              |
| 1:AV:55:ALA:HB1   | 1:AV:95:VAL:HG21 | 1.59                     | 0.83              |
| 1:AJ:108:ILE:HG12 | 1:AJ:150:LYS:HE3 | 1.61                     | 0.83              |
| 1:CO:124:ILE:O    | 1:CO:129:THR:OG1 | 1.96                     | 0.83              |
| 1:BT:108:ILE:HG12 | 1:BT:150:LYS:HE3 | 1.61                     | 0.83              |
| 1:CO:108:ILE:HG12 | 1:CO:150:LYS:HE3 | 1.61                     | 0.83              |
| 1:CY:124:ILE:O    | 1:CY:129:THR:OG1 | 1.96                     | 0.83              |
| 1:AJ:124:ILE:O    | 1:AJ:129:THR:OG1 | 1.96                     | 0.83              |
| 1:BE:124:ILE:O    | 1:BE:129:THR:OG1 | 1.96                     | 0.83              |
| 1:BL:55:ALA:HB1   | 1:BL:95:VAL:HG21 | 1.59                     | 0.83              |
| 1:B2:129:THR:CG2  | 1:B2:130:LYS:H   | 1.89                     | 0.83              |
| 1:CT:72:ASP:C     | 1:CT:150:LYS:HD3 | 2.03                     | 0.83              |
| 1:BO:108:ILE:HG12 | 1:BO:150:LYS:HE3 | 1.61                     | 0.83              |
| 1:BQ:55:ALA:HB1   | 1:BQ:95:VAL:HG21 | 1.59                     | 0.83              |
| 1:CH:129:THR:HG22 | 1:CH:130:LYS:N   | 1.88                     | 0.83              |
| 1:AQ:55:ALA:HB1   | 1:AQ:95:VAL:HG21 | 1.59                     | 0.83              |
| 1:AT:108:ILE:HG12 | 1:AT:150:LYS:HE3 | 1.61                     | 0.83              |
| 1:BD:11:GLY:HA3   | 1:CM:11:GLY:CA   | 2.09                     | 0.83              |
| 1:BT:72:ASP:C     | 1:BT:150:LYS:HD3 | 2.03                     | 0.83              |
| 1:CL:55:ALA:HB1   | 1:CL:95:VAL:HG21 | 1.59                     | 0.83              |
| 1:AC:129:THR:HG22 | 1:AC:130:LYS:N   | 1.88                     | 0.83              |
| 1:BE:72:ASP:C     | 1:BE:150:LYS:HD3 | 2.03                     | 0.83              |
| 1:BJ:124:ILE:O    | 1:BJ:129:THR:OG1 | 1.96                     | 0.83              |
| 1:CG:55:ALA:HB1   | 1:CG:95:VAL:HG21 | 1.59                     | 0.83              |
| 1:CO:72:ASP:C     | 1:CO:150:LYS:HD3 | 2.03                     | 0.82              |
| 1:AE:108:ILE:HG12 | 1:AE:150:LYS:HE3 | 1.61                     | 0.82              |
| 1:BE:108:ILE:HG12 | 1:BE:150:LYS:HE3 | 1.61                     | 0.82              |
| 1:CR:129:THR:CG2  | 1:CR:130:LYS:H   | 1.89                     | 0.82              |
| 1:AO:108:ILE:HG12 | 1:AO:150:LYS:HE3 | 1.61                     | 0.82              |
| 1:B4:72:ASP:C     | 1:B4:150:LYS:HD3 | 2.03                     | 0.82              |
| 1:CE:124:ILE:O    | 1:CE:129:THR:OG1 | 1.96                     | 0.82              |
| 1:CY:108:ILE:HG12 | 1:CY:150:LYS:HE3 | 1.61                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C4:72:ASP:C     | 1:C4:150:LYS:HD3  | 2.03                     | 0.82              |
| 1:AE:124:ILE:O    | 1:AE:129:THR:OG1  | 1.96                     | 0.82              |
| 1:AJ:72:ASP:C     | 1:AJ:150:LYS:HD3  | 2.03                     | 0.82              |
| 1:AL:55:ALA:HB1   | 1:AL:95:VAL:HG21  | 1.59                     | 0.82              |
| 1:BJ:108:ILE:HG12 | 1:BJ:150:LYS:HE3  | 1.61                     | 0.82              |
| 1:AE:72:ASP:C     | 1:AE:150:LYS:HD3  | 2.03                     | 0.82              |
| 1:AY:108:ILE:HG12 | 1:AY:150:LYS:HE3  | 1.61                     | 0.82              |
| 1:BJ:72:ASP:C     | 1:BJ:150:LYS:HD3  | 2.03                     | 0.82              |
| 1:B4:108:ILE:HG12 | 1:B4:150:LYS:HE3  | 1.61                     | 0.82              |
| 1:CJ:124:ILE:O    | 1:CJ:129:THR:OG1  | 1.96                     | 0.82              |
| 1:CY:72:ASP:C     | 1:CY:150:LYS:HD3  | 2.03                     | 0.82              |
| 1:A4:72:ASP:C     | 1:A4:150:LYS:HD3  | 2.03                     | 0.82              |
| 1:BY:72:ASP:C     | 1:BY:150:LYS:HD3  | 2.03                     | 0.82              |
| 1:B4:124:ILE:O    | 1:B4:129:THR:OG1  | 1.96                     | 0.82              |
| 1:CW:129:THR:HG22 | 1:CW:130:LYS:N    | 1.88                     | 0.82              |
| 1:AT:124:ILE:O    | 1:AT:129:THR:OG1  | 1.96                     | 0.82              |
| 1:CJ:108:ILE:HG12 | 1:CJ:150:LYS:HE3  | 1.61                     | 0.82              |
| 1:C4:124:ILE:O    | 1:C4:129:THR:OG1  | 1.96                     | 0.82              |
| 1:C4:108:ILE:HG12 | 1:C4:150:LYS:HE3  | 1.61                     | 0.81              |
| 1:A4:108:ILE:HG12 | 1:A4:150:LYS:HE3  | 1.61                     | 0.81              |
| 1:CE:108:ILE:HG12 | 1:CE:150:LYS:HE3  | 1.61                     | 0.81              |
| 1:AR:129:THR:CG2  | 1:AR:130:LYS:H    | 1.89                     | 0.81              |
| 1:BY:108:ILE:HG12 | 1:BY:150:LYS:HE3  | 1.61                     | 0.81              |
| 1:B2:7:LEU:HD11   | 1:B2:140:VAL:HG13 | 1.63                     | 0.81              |
| 1:AR:7:LEU:HD11   | 1:AR:140:VAL:HG13 | 1.63                     | 0.81              |
| 1:BM:7:LEU:HD11   | 1:BM:140:VAL:HG13 | 1.63                     | 0.81              |
| 1:BR:7:LEU:HD11   | 1:BR:140:VAL:HG13 | 1.63                     | 0.81              |
| 1:CT:108:ILE:HG12 | 1:CT:150:LYS:HE3  | 1.61                     | 0.81              |
| 1:CW:7:LEU:HD11   | 1:CW:140:VAL:HG13 | 1.63                     | 0.80              |
| 1:BD:11:GLY:CA    | 1:CM:11:GLY:HA3   | 2.11                     | 0.80              |
| 1:BM:129:THR:CG2  | 1:BM:130:LYS:H    | 1.89                     | 0.80              |
| 1:BN:18:VAL:HG12  | 1:BN:77:LEU:HB2   | 1.63                     | 0.80              |
| 1:B3:18:VAL:HG12  | 1:B3:77:LEU:HB2   | 1.64                     | 0.80              |
| 1:AD:18:VAL:HG12  | 1:AD:77:LEU:HB2   | 1.64                     | 0.80              |
| 1:CC:7:LEU:HD11   | 1:CC:140:VAL:HG13 | 1.63                     | 0.80              |
| 1:AH:7:LEU:HD11   | 1:AH:140:VAL:HG13 | 1.63                     | 0.80              |
| 1:AS:18:VAL:HG12  | 1:AS:77:LEU:HB2   | 1.64                     | 0.80              |
| 1:AX:18:VAL:HG12  | 1:AX:77:LEU:HB2   | 1.63                     | 0.80              |
| 1:AL:7:LEU:HD11   | 1:AL:140:VAL:HG13 | 1.64                     | 0.80              |
| 1:BD:18:VAL:HG12  | 1:BD:77:LEU:HB2   | 1.64                     | 0.80              |
| 1:AB:7:LEU:HD11   | 1:AB:140:VAL:HG13 | 1.64                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:7:LEU:HD11   | 1:AC:140:VAL:HG13 | 1.63                     | 0.80              |
| 1:CM:7:LEU:HD11   | 1:CM:140:VAL:HG13 | 1.63                     | 0.80              |
| 1:A2:7:LEU:HD11   | 1:A2:140:VAL:HG13 | 1.63                     | 0.80              |
| 1:CB:7:LEU:HD11   | 1:CB:140:VAL:HG13 | 1.64                     | 0.80              |
| 1:CR:7:LEU:HD11   | 1:CR:140:VAL:HG13 | 1.63                     | 0.80              |
| 1:CW:129:THR:CG2  | 1:CW:130:LYS:H    | 1.89                     | 0.80              |
| 1:CG:7:LEU:HD11   | 1:CG:140:VAL:HG13 | 1.64                     | 0.79              |
| 1:AW:7:LEU:HD11   | 1:AW:140:VAL:HG13 | 1.63                     | 0.79              |
| 1:BX:18:VAL:HG12  | 1:BX:77:LEU:HB2   | 1.64                     | 0.79              |
| 1:CQ:7:LEU:HD11   | 1:CQ:140:VAL:HG13 | 1.64                     | 0.79              |
| 1:BB:7:LEU:HD11   | 1:BB:140:VAL:HG13 | 1.64                     | 0.79              |
| 1:BI:18:VAL:HG12  | 1:BI:77:LEU:HB2   | 1.64                     | 0.79              |
| 1:CL:7:LEU:HD11   | 1:CL:140:VAL:HG13 | 1.64                     | 0.79              |
| 1:BH:7:LEU:HD11   | 1:BH:140:VAL:HG13 | 1.63                     | 0.79              |
| 1:BW:7:LEU:HD11   | 1:BW:140:VAL:HG13 | 1.63                     | 0.79              |
| 1:CI:18:VAL:HG12  | 1:CI:77:LEU:HB2   | 1.63                     | 0.79              |
| 1:CX:18:VAL:HG12  | 1:CX:77:LEU:HB2   | 1.64                     | 0.79              |
| 1:AC:129:THR:CG2  | 1:AC:130:LYS:H    | 1.89                     | 0.79              |
| 1:BD:120:ILE:CD1  | 1:BR:129:THR:HG21 | 2.12                     | 0.79              |
| 1:BH:34:LEU:HD22  | 1:BH:38:LYS:HE2   | 1.65                     | 0.79              |
| 1:BH:129:THR:CG2  | 1:BH:130:LYS:H    | 1.89                     | 0.79              |
| 1:BS:18:VAL:HG12  | 1:BS:77:LEU:HB2   | 1.63                     | 0.79              |
| 1:CN:18:VAL:HG12  | 1:CN:77:LEU:HB2   | 1.64                     | 0.79              |
| 1:CS:18:VAL:HG12  | 1:CS:77:LEU:HB2   | 1.63                     | 0.79              |
| 1:CW:34:LEU:HD22  | 1:CW:38:LYS:HE2   | 1.65                     | 0.79              |
| 1:C2:7:LEU:HD11   | 1:C2:140:VAL:HG13 | 1.63                     | 0.79              |
| 1:CV:7:LEU:HD11   | 1:CV:140:VAL:HG13 | 1.64                     | 0.79              |
| 1:C2:82:ARG:HH11  | 1:C2:82:ARG:HG3   | 1.49                     | 0.79              |
| 1:AH:82:ARG:HH11  | 1:AH:82:ARG:HG3   | 1.48                     | 0.78              |
| 1:AV:7:LEU:HD11   | 1:AV:140:VAL:HG13 | 1.64                     | 0.78              |
| 1:BR:82:ARG:HH11  | 1:BR:82:ARG:HG3   | 1.48                     | 0.78              |
| 1:B1:7:LEU:HD11   | 1:B1:140:VAL:HG13 | 1.64                     | 0.78              |
| 1:B2:34:LEU:HD22  | 1:B2:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:CR:82:ARG:HH11  | 1:CR:82:ARG:HG3   | 1.49                     | 0.78              |
| 1:AR:34:LEU:HD22  | 1:AR:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:A3:18:VAL:HG12  | 1:A3:77:LEU:HB2   | 1.64                     | 0.78              |
| 1:BC:7:LEU:HD11   | 1:BC:140:VAL:HG13 | 1.63                     | 0.78              |
| 1:BC:82:ARG:HG3   | 1:BC:82:ARG:HH11  | 1.49                     | 0.78              |
| 1:BH:82:ARG:HH11  | 1:BH:82:ARG:HG3   | 1.49                     | 0.78              |
| 1:BW:119:THR:HG22 | 1:BW:121:GLU:H    | 1.49                     | 0.78              |
| 1:BW:129:THR:CG2  | 1:BW:130:LYS:H    | 1.89                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CD:18:VAL:HG12  | 1:CD:77:LEU:HB2   | 1.64                     | 0.78              |
| 1:AN:18:VAL:HG12  | 1:AN:77:LEU:HB2   | 1.64                     | 0.78              |
| 1:AW:82:ARG:HH11  | 1:AW:82:ARG:HG3   | 1.49                     | 0.78              |
| 1:BW:82:ARG:HG3   | 1:BW:82:ARG:HH11  | 1.49                     | 0.78              |
| 1:AD:120:ILE:CD1  | 1:AR:129:THR:HG21 | 2.14                     | 0.78              |
| 1:BR:119:THR:HG22 | 1:BR:121:GLU:H    | 1.49                     | 0.78              |
| 1:AC:34:LEU:HD22  | 1:AC:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:AM:7:LEU:HD11   | 1:AM:140:VAL:HG13 | 1.63                     | 0.78              |
| 1:BL:7:LEU:HD11   | 1:BL:140:VAL:HG13 | 1.64                     | 0.78              |
| 1:BM:119:THR:HG22 | 1:BM:121:GLU:H    | 1.49                     | 0.78              |
| 1:A2:34:LEU:HD22  | 1:A2:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:BG:7:LEU:HD11   | 1:BG:140:VAL:HG13 | 1.64                     | 0.78              |
| 1:B2:119:THR:HG22 | 1:B2:121:GLU:H    | 1.49                     | 0.78              |
| 1:CM:119:THR:HG22 | 1:CM:121:GLU:H    | 1.49                     | 0.78              |
| 1:C3:18:VAL:HG12  | 1:C3:77:LEU:HB2   | 1.64                     | 0.78              |
| 1:AI:18:VAL:HG12  | 1:AI:77:LEU:HB2   | 1.64                     | 0.78              |
| 1:BC:119:THR:HG22 | 1:BC:121:GLU:H    | 1.49                     | 0.78              |
| 1:BI:16:VAL:HG12  | 1:BI:75:ILE:HB    | 1.66                     | 0.78              |
| 1:CW:82:ARG:HH11  | 1:CW:82:ARG:HG3   | 1.49                     | 0.78              |
| 1:AR:119:THR:HG22 | 1:AR:121:GLU:H    | 1.49                     | 0.78              |
| 1:A2:82:ARG:HH11  | 1:A2:82:ARG:HG3   | 1.48                     | 0.78              |
| 1:BM:34:LEU:HD22  | 1:BM:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:CW:119:THR:HG22 | 1:CW:121:GLU:H    | 1.49                     | 0.78              |
| 1:AW:119:THR:HG22 | 1:AW:121:GLU:H    | 1.49                     | 0.78              |
| 1:BC:34:LEU:HD22  | 1:BC:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:BM:82:ARG:HH11  | 1:BM:82:ARG:HG3   | 1.49                     | 0.78              |
| 1:BR:34:LEU:HD22  | 1:BR:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:CH:34:LEU:HD22  | 1:CH:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:C2:119:THR:HG22 | 1:C2:121:GLU:H    | 1.49                     | 0.78              |
| 1:AH:34:LEU:HD22  | 1:AH:38:LYS:HE2   | 1.65                     | 0.78              |
| 1:AX:16:VAL:HG12  | 1:AX:75:ILE:HB    | 1.66                     | 0.78              |
| 1:BD:16:VAL:HG12  | 1:BD:75:ILE:HB    | 1.66                     | 0.78              |
| 1:CR:38:LYS:HZ2   | 1:CR:44:GLU:HG3   | 1.48                     | 0.78              |
| 1:CX:16:VAL:HG12  | 1:CX:75:ILE:HB    | 1.66                     | 0.78              |
| 1:C1:7:LEU:HD11   | 1:C1:140:VAL:HG13 | 1.64                     | 0.78              |
| 1:C3:16:VAL:HG12  | 1:C3:75:ILE:HB    | 1.66                     | 0.78              |
| 1:AM:119:THR:HG22 | 1:AM:121:GLU:H    | 1.49                     | 0.77              |
| 1:CC:34:LEU:HD22  | 1:CC:38:LYS:HE2   | 1.65                     | 0.77              |
| 1:CC:82:ARG:HH11  | 1:CC:82:ARG:HG3   | 1.48                     | 0.77              |
| 1:CC:119:THR:HG22 | 1:CC:121:GLU:H    | 1.49                     | 0.77              |
| 1:CH:7:LEU:HD11   | 1:CH:140:VAL:HG13 | 1.63                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CS:16:VAL:HG12  | 1:CS:75:ILE:HB    | 1.66                     | 0.77              |
| 1:AN:16:VAL:HG12  | 1:AN:75:ILE:HB    | 1.66                     | 0.77              |
| 1:BQ:7:LEU:HD11   | 1:BQ:140:VAL:HG13 | 1.64                     | 0.77              |
| 1:AM:38:LYS:HZ2   | 1:AM:44:GLU:HG3   | 1.50                     | 0.77              |
| 1:AQ:13:LYS:NZ    | 1:BU:43:GLU:CG    | 2.39                     | 0.77              |
| 1:AY:18:VAL:HG12  | 1:AY:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:BO:18:VAL:HG12  | 1:BO:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:BY:18:VAL:HG12  | 1:BY:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:CR:34:LEU:HD22  | 1:CR:38:LYS:HE2   | 1.65                     | 0.77              |
| 1:CY:18:VAL:HG12  | 1:CY:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:AM:82:ARG:HG3   | 1:AM:82:ARG:HH11  | 1.49                     | 0.77              |
| 1:A3:16:VAL:HG12  | 1:A3:75:ILE:HB    | 1.66                     | 0.77              |
| 1:AQ:7:LEU:HD11   | 1:AQ:140:VAL:HG13 | 1.64                     | 0.77              |
| 1:AW:34:LEU:HD22  | 1:AW:38:LYS:HE2   | 1.65                     | 0.77              |
| 1:BT:18:VAL:HG12  | 1:BT:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:AC:82:ARG:HH11  | 1:AC:82:ARG:HG3   | 1.49                     | 0.77              |
| 1:AO:18:VAL:HG12  | 1:AO:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:BG:104:LEU:HD13 | 1:BH:102:LEU:HD22 | 1.67                     | 0.77              |
| 1:BW:34:LEU:HD22  | 1:BW:38:LYS:HE2   | 1.65                     | 0.77              |
| 1:CN:16:VAL:HG12  | 1:CN:75:ILE:HB    | 1.66                     | 0.77              |
| 1:AC:119:THR:HG22 | 1:AC:121:GLU:H    | 1.49                     | 0.77              |
| 1:BV:7:LEU:HD11   | 1:BV:140:VAL:HG13 | 1.64                     | 0.77              |
| 1:BV:104:LEU:HD13 | 1:BW:102:LEU:HD22 | 1.67                     | 0.77              |
| 1:BX:16:VAL:HG12  | 1:BX:75:ILE:HB    | 1.66                     | 0.77              |
| 1:CB:104:LEU:HD13 | 1:CC:102:LEU:HD22 | 1.67                     | 0.77              |
| 1:CM:82:ARG:HH11  | 1:CM:82:ARG:HG3   | 1.49                     | 0.77              |
| 1:AE:18:VAL:HG12  | 1:AE:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:BC:38:LYS:HZ2   | 1:BC:44:GLU:HG3   | 1.50                     | 0.77              |
| 1:BS:16:VAL:HG12  | 1:BS:75:ILE:HB    | 1.66                     | 0.77              |
| 1:C1:104:LEU:HD13 | 1:C2:102:LEU:HD22 | 1.67                     | 0.77              |
| 1:AD:16:VAL:HG12  | 1:AD:75:ILE:HB    | 1.66                     | 0.77              |
| 1:AJ:18:VAL:HG12  | 1:AJ:77:LEU:HB2   | 1.67                     | 0.77              |
| 1:AS:16:VAL:HG12  | 1:AS:75:ILE:HB    | 1.66                     | 0.77              |
| 1:B1:104:LEU:HD13 | 1:B2:102:LEU:HD22 | 1.67                     | 0.77              |
| 1:CV:104:LEU:HD13 | 1:CW:102:LEU:HD22 | 1.67                     | 0.77              |
| 1:C2:34:LEU:HD22  | 1:C2:38:LYS:HE2   | 1.65                     | 0.77              |
| 1:AH:119:THR:HG22 | 1:AH:121:GLU:H    | 1.49                     | 0.76              |
| 1:AH:129:THR:CG2  | 1:AH:130:LYS:H    | 1.89                     | 0.76              |
| 1:AM:34:LEU:HD22  | 1:AM:38:LYS:HE2   | 1.65                     | 0.76              |
| 1:BO:109:PRO:HD2  | 1:BO:150:LYS:HD2  | 1.67                     | 0.76              |
| 1:CC:7:LEU:HD23   | 1:CR:40:HIS:CE1   | 2.20                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CJ:109:PRO:HD2  | 1:CJ:150:LYS:HD2  | 1.67                     | 0.76              |
| 1:CQ:104:LEU:HD13 | 1:CR:102:LEU:HD22 | 1.67                     | 0.76              |
| 1:AG:7:LEU:HD11   | 1:AG:140:VAL:HG13 | 1.64                     | 0.76              |
| 1:AI:16:VAL:HG12  | 1:AI:75:ILE:HB    | 1.66                     | 0.76              |
| 1:A1:104:LEU:HD13 | 1:A2:102:LEU:HD22 | 1.67                     | 0.76              |
| 1:A2:119:THR:HG22 | 1:A2:121:GLU:H    | 1.49                     | 0.76              |
| 1:CM:34:LEU:HD22  | 1:CM:38:LYS:HE2   | 1.65                     | 0.76              |
| 1:CO:18:VAL:HG12  | 1:CO:77:LEU:HB2   | 1.67                     | 0.76              |
| 1:A1:7:LEU:HD11   | 1:A1:140:VAL:HG13 | 1.64                     | 0.76              |
| 1:B4:109:PRO:HD2  | 1:B4:150:LYS:HD2  | 1.68                     | 0.76              |
| 1:AQ:104:LEU:HD13 | 1:AR:102:LEU:HD22 | 1.67                     | 0.76              |
| 1:B3:16:VAL:HG12  | 1:B3:75:ILE:HB    | 1.66                     | 0.76              |
| 1:CE:18:VAL:HG12  | 1:CE:77:LEU:HB2   | 1.67                     | 0.76              |
| 1:CY:109:PRO:HD2  | 1:CY:150:LYS:HD2  | 1.68                     | 0.76              |
| 1:AJ:109:PRO:HD2  | 1:AJ:150:LYS:HD2  | 1.67                     | 0.76              |
| 1:AR:68:SER:O     | 1:AR:70:LYS:HG2   | 1.86                     | 0.76              |
| 1:AW:68:SER:O     | 1:AW:70:LYS:HG2   | 1.86                     | 0.76              |
| 1:A4:109:PRO:HD2  | 1:A4:150:LYS:HD2  | 1.67                     | 0.76              |
| 1:BB:104:LEU:HD13 | 1:BC:102:LEU:HD22 | 1.67                     | 0.76              |
| 1:BE:18:VAL:HG12  | 1:BE:77:LEU:HB2   | 1.67                     | 0.76              |
| 1:CH:119:THR:HG22 | 1:CH:121:GLU:H    | 1.49                     | 0.76              |
| 1:AH:68:SER:O     | 1:AH:70:LYS:HG2   | 1.86                     | 0.76              |
| 1:AO:109:PRO:HD2  | 1:AO:150:LYS:HD2  | 1.68                     | 0.76              |
| 1:AL:104:LEU:HD13 | 1:AM:102:LEU:HD22 | 1.67                     | 0.76              |
| 1:CD:107:ASP:O    | 1:CD:107:ASP:CG   | 2.29                     | 0.76              |
| 1:AN:107:ASP:O    | 1:AN:107:ASP:CG   | 2.29                     | 0.76              |
| 1:BE:109:PRO:HD2  | 1:BE:150:LYS:HD2  | 1.67                     | 0.76              |
| 1:BH:68:SER:O     | 1:BH:70:LYS:HG2   | 1.86                     | 0.76              |
| 1:BJ:18:VAL:HG12  | 1:BJ:77:LEU:HB2   | 1.67                     | 0.76              |
| 1:BY:109:PRO:HD2  | 1:BY:150:LYS:HD2  | 1.67                     | 0.76              |
| 1:CC:68:SER:O     | 1:CC:70:LYS:HG2   | 1.86                     | 0.76              |
| 1:CC:129:THR:CG2  | 1:CC:130:LYS:H    | 1.89                     | 0.76              |
| 1:CE:109:PRO:HD2  | 1:CE:150:LYS:HD2  | 1.68                     | 0.76              |
| 1:CJ:18:VAL:HG12  | 1:CJ:77:LEU:HB2   | 1.67                     | 0.76              |
| 1:AR:82:ARG:HG3   | 1:AR:82:ARG:HH11  | 1.48                     | 0.76              |
| 1:AT:18:VAL:HG12  | 1:AT:77:LEU:HB2   | 1.67                     | 0.76              |
| 1:A2:129:THR:CG2  | 1:A2:130:LYS:H    | 1.89                     | 0.76              |
| 1:BJ:109:PRO:HD2  | 1:BJ:150:LYS:HD2  | 1.68                     | 0.76              |
| 1:CH:38:LYS:HZ2   | 1:CH:44:GLU:HG3   | 1.50                     | 0.76              |
| 1:CK:55:ALA:HB1   | 1:CK:95:VAL:HG21  | 1.68                     | 0.76              |
| 1:CR:68:SER:O     | 1:CR:70:LYS:HG2   | 1.86                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C3:107:ASP:O    | 1:C3:107:ASP:CG   | 2.29                     | 0.76              |
| 1:AX:107:ASP:O    | 1:AX:107:ASP:CG   | 2.29                     | 0.76              |
| 1:BH:119:THR:HG22 | 1:BH:121:GLU:H    | 1.49                     | 0.76              |
| 1:CF:125:GLU:HA   | 1:CF:129:THR:OG1  | 1.87                     | 0.76              |
| 1:CR:119:THR:HG22 | 1:CR:121:GLU:H    | 1.49                     | 0.76              |
| 1:C4:18:VAL:HG12  | 1:C4:77:LEU:HB2   | 1.67                     | 0.76              |
| 1:AA:55:ALA:HB1   | 1:AA:95:VAL:HG21  | 1.68                     | 0.75              |
| 1:AB:104:LEU:HD13 | 1:AC:102:LEU:HD22 | 1.67                     | 0.75              |
| 1:AI:107:ASP:O    | 1:AI:107:ASP:CG   | 2.29                     | 0.75              |
| 1:BK:125:GLU:HA   | 1:BK:129:THR:OG1  | 1.87                     | 0.75              |
| 1:BN:16:VAL:HG12  | 1:BN:75:ILE:HB    | 1.66                     | 0.75              |
| 1:BN:107:ASP:O    | 1:BN:107:ASP:CG   | 2.29                     | 0.75              |
| 1:BP:125:GLU:HA   | 1:BP:129:THR:OG1  | 1.87                     | 0.75              |
| 1:B2:68:SER:O     | 1:B2:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:CN:107:ASP:O    | 1:CN:107:ASP:CG   | 2.29                     | 0.75              |
| 1:CO:109:PRO:HD2  | 1:CO:150:LYS:HD2  | 1.67                     | 0.75              |
| 1:AK:152:TRP:CG   | 1:AK:153:ALA:H    | 2.05                     | 0.75              |
| 1:AU:55:ALA:HB1   | 1:AU:95:VAL:HG21  | 1.68                     | 0.75              |
| 1:AU:125:GLU:HA   | 1:AU:129:THR:OG1  | 1.87                     | 0.75              |
| 1:BA:152:TRP:CG   | 1:BA:153:ALA:H    | 2.04                     | 0.75              |
| 1:BH:38:LYS:HZ2   | 1:BH:44:GLU:HG3   | 1.50                     | 0.75              |
| 1:BM:68:SER:O     | 1:BM:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:BS:107:ASP:O    | 1:BS:107:ASP:CG   | 2.29                     | 0.75              |
| 1:BW:68:SER:O     | 1:BW:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:B4:18:VAL:HG12  | 1:B4:77:LEU:HB2   | 1.67                     | 0.75              |
| 1:CD:16:VAL:HG12  | 1:CD:75:ILE:HB    | 1.66                     | 0.75              |
| 1:CG:104:LEU:HD13 | 1:CH:102:LEU:HD22 | 1.67                     | 0.75              |
| 1:AD:107:ASP:O    | 1:AD:107:ASP:CG   | 2.29                     | 0.75              |
| 1:AE:109:PRO:HD2  | 1:AE:150:LYS:HD2  | 1.68                     | 0.75              |
| 1:AP:152:TRP:CG   | 1:AP:153:ALA:H    | 2.05                     | 0.75              |
| 1:BU:152:TRP:CG   | 1:BU:153:ALA:H    | 2.05                     | 0.75              |
| 1:B2:82:ARG:HH11  | 1:B2:82:ARG:HG3   | 1.49                     | 0.75              |
| 1:CI:16:VAL:HG12  | 1:CI:75:ILE:HB    | 1.66                     | 0.75              |
| 1:CP:125:GLU:HA   | 1:CP:129:THR:OG1  | 1.87                     | 0.75              |
| 1:BA:55:ALA:HB1   | 1:BA:95:VAL:HG21  | 1.68                     | 0.75              |
| 1:BA:125:GLU:HA   | 1:BA:129:THR:OG1  | 1.87                     | 0.75              |
| 1:B3:107:ASP:O    | 1:B3:107:ASP:CG   | 2.29                     | 0.75              |
| 1:CL:104:LEU:HD13 | 1:CM:102:LEU:HD22 | 1.67                     | 0.75              |
| 1:A4:18:VAL:HG12  | 1:A4:77:LEU:HB2   | 1.67                     | 0.75              |
| 1:BZ:152:TRP:CG   | 1:BZ:153:ALA:H    | 2.05                     | 0.75              |
| 1:CZ:152:TRP:CG   | 1:CZ:153:ALA:H    | 2.05                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AV:104:LEU:HD13 | 1:AW:102:LEU:HD22 | 1.67                     | 0.75              |
| 1:A2:68:SER:O     | 1:A2:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:BA:119:THR:HG22 | 1:BA:121:GLU:H    | 1.52                     | 0.75              |
| 1:BK:152:TRP:CG   | 1:BK:153:ALA:H    | 2.05                     | 0.75              |
| 1:BZ:55:ALA:HB1   | 1:BZ:95:VAL:HG21  | 1.68                     | 0.75              |
| 1:BZ:125:GLU:HA   | 1:BZ:129:THR:OG1  | 1.87                     | 0.75              |
| 1:CH:82:ARG:HG3   | 1:CH:82:ARG:HH11  | 1.48                     | 0.75              |
| 1:CT:119:THR:HG22 | 1:CT:121:GLU:H    | 1.52                     | 0.75              |
| 1:CZ:55:ALA:HB1   | 1:CZ:95:VAL:HG21  | 1.68                     | 0.75              |
| 1:AG:104:LEU:HD13 | 1:AH:102:LEU:HD22 | 1.67                     | 0.75              |
| 1:AM:68:SER:O     | 1:AM:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:AU:119:THR:HG22 | 1:AU:121:GLU:H    | 1.52                     | 0.75              |
| 1:BC:68:SER:O     | 1:BC:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:BO:119:THR:HG22 | 1:BO:121:GLU:H    | 1.52                     | 0.75              |
| 1:BU:119:THR:HG22 | 1:BU:121:GLU:H    | 1.52                     | 0.75              |
| 1:CM:68:SER:O     | 1:CM:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:CU:125:GLU:HA   | 1:CU:129:THR:OG1  | 1.86                     | 0.75              |
| 1:AZ:55:ALA:HB1   | 1:AZ:95:VAL:HG21  | 1.68                     | 0.75              |
| 1:AZ:152:TRP:CG   | 1:AZ:153:ALA:H    | 2.05                     | 0.75              |
| 1:BI:107:ASP:O    | 1:BI:107:ASP:CG   | 2.29                     | 0.75              |
| 1:BL:104:LEU:HD13 | 1:BM:102:LEU:HD22 | 1.67                     | 0.75              |
| 1:BR:68:SER:O     | 1:BR:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:CA:125:GLU:HA   | 1:CA:129:THR:OG1  | 1.87                     | 0.75              |
| 1:CA:152:TRP:CG   | 1:CA:153:ALA:H    | 2.05                     | 0.75              |
| 1:CF:119:THR:HG22 | 1:CF:121:GLU:H    | 1.52                     | 0.75              |
| 1:CH:68:SER:O     | 1:CH:70:LYS:HG2   | 1.86                     | 0.75              |
| 1:CO:119:THR:HG22 | 1:CO:121:GLU:H    | 1.52                     | 0.75              |
| 1:CY:119:THR:HG22 | 1:CY:121:GLU:H    | 1.52                     | 0.75              |
| 1:CZ:125:GLU:HA   | 1:CZ:129:THR:OG1  | 1.87                     | 0.75              |
| 1:BX:107:ASP:O    | 1:BX:107:ASP:CG   | 2.29                     | 0.75              |
| 1:CI:107:ASP:O    | 1:CI:107:ASP:CG   | 2.29                     | 0.75              |
| 1:CK:119:THR:HG22 | 1:CK:121:GLU:H    | 1.52                     | 0.75              |
| 1:CT:18:VAL:HG12  | 1:CT:77:LEU:HB2   | 1.67                     | 0.75              |
| 1:CU:152:TRP:CG   | 1:CU:153:ALA:H    | 2.05                     | 0.75              |
| 1:AC:68:SER:O     | 1:AC:70:LYS:HG2   | 1.86                     | 0.74              |
| 1:AF:125:GLU:HA   | 1:AF:129:THR:OG1  | 1.87                     | 0.74              |
| 1:BU:55:ALA:HB1   | 1:BU:95:VAL:HG21  | 1.68                     | 0.74              |
| 1:BZ:119:THR:HG22 | 1:BZ:121:GLU:H    | 1.52                     | 0.74              |
| 1:CT:109:PRO:HD2  | 1:CT:150:LYS:HD2  | 1.68                     | 0.74              |
| 1:AA:119:THR:HG22 | 1:AA:121:GLU:H    | 1.52                     | 0.74              |
| 1:BF:125:GLU:HA   | 1:BF:129:THR:OG1  | 1.87                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BF:152:TRP:CG   | 1:BF:153:ALA:H   | 2.05                     | 0.74              |
| 1:BP:119:THR:HG22 | 1:BP:121:GLU:H   | 1.52                     | 0.74              |
| 1:BT:119:THR:HG22 | 1:BT:121:GLU:H   | 1.52                     | 0.74              |
| 1:CF:152:TRP:CG   | 1:CF:153:ALA:H   | 2.05                     | 0.74              |
| 1:CU:55:ALA:HB1   | 1:CU:95:VAL:HG21 | 1.68                     | 0.74              |
| 1:CU:119:THR:HG22 | 1:CU:121:GLU:H   | 1.52                     | 0.74              |
| 1:CW:68:SER:O     | 1:CW:70:LYS:HG2  | 1.86                     | 0.74              |
| 1:BA:76:THR:HG22  | 1:BA:111:ILE:O   | 1.88                     | 0.74              |
| 1:CX:107:ASP:O    | 1:CX:107:ASP:CG  | 2.29                     | 0.74              |
| 1:AF:152:TRP:CG   | 1:AF:153:ALA:H   | 2.05                     | 0.74              |
| 1:AK:76:THR:HG22  | 1:AK:111:ILE:O   | 1.88                     | 0.74              |
| 1:AR:38:LYS:HZ2   | 1:AR:44:GLU:HG3  | 1.51                     | 0.74              |
| 1:AT:109:PRO:HD2  | 1:AT:150:LYS:HD2 | 1.67                     | 0.74              |
| 1:CZ:119:THR:HG22 | 1:CZ:121:GLU:H   | 1.52                     | 0.74              |
| 1:C2:68:SER:O     | 1:C2:70:LYS:HG2  | 1.86                     | 0.74              |
| 1:A3:107:ASP:O    | 1:A3:107:ASP:CG  | 2.29                     | 0.74              |
| 1:BJ:119:THR:HG22 | 1:BJ:121:GLU:H   | 1.52                     | 0.74              |
| 1:BU:125:GLU:HA   | 1:BU:129:THR:OG1 | 1.87                     | 0.74              |
| 1:CA:119:THR:HG22 | 1:CA:121:GLU:H   | 1.52                     | 0.74              |
| 1:CF:39:ARG:O     | 1:CQ:7:LEU:HB3   | 1.87                     | 0.74              |
| 1:CZ:76:THR:HG22  | 1:CZ:111:ILE:O   | 1.88                     | 0.74              |
| 1:AA:125:GLU:HA   | 1:AA:129:THR:OG1 | 1.87                     | 0.74              |
| 1:AC:38:LYS:HZ2   | 1:AC:44:GLU:HG3  | 1.53                     | 0.74              |
| 1:AU:152:TRP:CG   | 1:AU:153:ALA:H   | 2.05                     | 0.74              |
| 1:AZ:125:GLU:HA   | 1:AZ:129:THR:OG1 | 1.87                     | 0.74              |
| 1:BB:144:GLU:CD   | 1:BU:39:ARG:HH22 | 1.95                     | 0.74              |
| 1:BF:55:ALA:HB1   | 1:BF:95:VAL:HG21 | 1.68                     | 0.74              |
| 1:BF:76:THR:HG22  | 1:BF:111:ILE:O   | 1.88                     | 0.74              |
| 1:CP:152:TRP:CG   | 1:CP:153:ALA:H   | 2.05                     | 0.74              |
| 1:C4:119:THR:HG22 | 1:C4:121:GLU:H   | 1.52                     | 0.74              |
| 1:AZ:119:THR:HG22 | 1:AZ:121:GLU:H   | 1.52                     | 0.74              |
| 1:BD:107:ASP:O    | 1:BD:107:ASP:CG  | 2.29                     | 0.74              |
| 1:BP:76:THR:HG22  | 1:BP:111:ILE:O   | 1.88                     | 0.74              |
| 1:BZ:76:THR:HG22  | 1:BZ:111:ILE:O   | 1.88                     | 0.74              |
| 1:CA:76:THR:HG22  | 1:CA:111:ILE:O   | 1.88                     | 0.74              |
| 1:CE:119:THR:HG22 | 1:CE:121:GLU:H   | 1.52                     | 0.74              |
| 1:CU:76:THR:HG22  | 1:CU:111:ILE:O   | 1.88                     | 0.74              |
| 1:AK:55:ALA:HB1   | 1:AK:95:VAL:HG21 | 1.68                     | 0.74              |
| 1:AP:55:ALA:HB1   | 1:AP:95:VAL:HG21 | 1.68                     | 0.74              |
| 1:AP:125:GLU:HA   | 1:AP:129:THR:OG1 | 1.87                     | 0.74              |
| 1:AS:107:ASP:O    | 1:AS:107:ASP:CG  | 2.29                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BK:55:ALA:HB1   | 1:BK:95:VAL:HG21  | 1.68                     | 0.74              |
| 1:BK:76:THR:HG22  | 1:BK:111:ILE:O    | 1.88                     | 0.74              |
| 1:CF:76:THR:HG22  | 1:CF:111:ILE:O    | 1.88                     | 0.74              |
| 1:AE:119:THR:HG22 | 1:AE:121:GLU:H    | 1.52                     | 0.74              |
| 1:AT:119:THR:HG22 | 1:AT:121:GLU:H    | 1.52                     | 0.74              |
| 1:AY:119:THR:HG22 | 1:AY:121:GLU:H    | 1.52                     | 0.74              |
| 1:BQ:104:LEU:HD13 | 1:BR:102:LEU:HD22 | 1.67                     | 0.74              |
| 1:BT:109:PRO:HD2  | 1:BT:150:LYS:HD2  | 1.67                     | 0.74              |
| 1:AA:152:TRP:CG   | 1:AA:153:ALA:H    | 2.05                     | 0.74              |
| 1:AF:76:THR:HG22  | 1:AF:111:ILE:O    | 1.88                     | 0.74              |
| 1:AY:109:PRO:HD2  | 1:AY:150:LYS:HD2  | 1.68                     | 0.74              |
| 1:AZ:76:THR:HG22  | 1:AZ:111:ILE:O    | 1.88                     | 0.74              |
| 1:BU:76:THR:HG22  | 1:BU:111:ILE:O    | 1.88                     | 0.74              |
| 1:CA:55:ALA:HB1   | 1:CA:95:VAL:HG21  | 1.68                     | 0.74              |
| 1:CK:152:TRP:CG   | 1:CK:153:ALA:H    | 2.05                     | 0.74              |
| 1:CP:76:THR:HG22  | 1:CP:111:ILE:O    | 1.88                     | 0.74              |
| 1:CG:144:GLU:CD   | 1:CU:39:ARG:HH22  | 1.96                     | 0.73              |
| 1:CT:40:HIS:CE1   | 1:C3:7:LEU:HD23   | 2.23                     | 0.73              |
| 1:AK:125:GLU:HA   | 1:AK:129:THR:OG1  | 1.87                     | 0.73              |
| 1:B4:119:THR:HG22 | 1:B4:121:GLU:H    | 1.52                     | 0.73              |
| 1:A4:119:THR:HG22 | 1:A4:121:GLU:H    | 1.52                     | 0.73              |
| 1:C4:109:PRO:HD2  | 1:C4:150:LYS:HD2  | 1.68                     | 0.73              |
| 1:BF:119:THR:HG22 | 1:BF:121:GLU:H    | 1.52                     | 0.73              |
| 1:CF:55:ALA:HB1   | 1:CF:95:VAL:HG21  | 1.68                     | 0.73              |
| 1:CK:76:THR:HG22  | 1:CK:111:ILE:O    | 1.88                     | 0.73              |
| 1:CK:125:GLU:HA   | 1:CK:129:THR:OG1  | 1.87                     | 0.73              |
| 1:CP:119:THR:HG22 | 1:CP:121:GLU:H    | 1.52                     | 0.73              |
| 1:BP:152:TRP:CG   | 1:BP:153:ALA:H    | 2.05                     | 0.73              |
| 1:CP:55:ALA:HB1   | 1:CP:95:VAL:HG21  | 1.68                     | 0.73              |
| 1:CS:107:ASP:O    | 1:CS:107:ASP:CG   | 2.29                     | 0.73              |
| 1:AA:76:THR:HG22  | 1:AA:111:ILE:O    | 1.88                     | 0.73              |
| 1:AJ:119:THR:HG22 | 1:AJ:121:GLU:H    | 1.52                     | 0.73              |
| 1:AF:119:THR:HG22 | 1:AF:121:GLU:H    | 1.52                     | 0.73              |
| 1:AK:119:THR:HG22 | 1:AK:121:GLU:H    | 1.52                     | 0.73              |
| 1:BE:119:THR:HG22 | 1:BE:121:GLU:H    | 1.52                     | 0.73              |
| 1:BP:55:ALA:HB1   | 1:BP:95:VAL:HG21  | 1.68                     | 0.73              |
| 1:CG:40:HIS:CE1   | 1:CU:7:LEU:HD23   | 2.23                     | 0.73              |
| 1:AF:55:ALA:HB1   | 1:AF:95:VAL:HG21  | 1.68                     | 0.72              |
| 1:BB:7:LEU:HB3    | 1:BU:39:ARG:O     | 1.89                     | 0.72              |
| 1:BW:38:LYS:HZ2   | 1:BW:44:GLU:HG3   | 1.53                     | 0.72              |
| 1:CJ:119:THR:HG22 | 1:CJ:121:GLU:H    | 1.52                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CL:96:ALA:C     | 1:CL:100:ALA:CB   | 2.63                     | 0.72              |
| 1:AW:38:LYS:HZ2   | 1:AW:44:GLU:HG3   | 1.54                     | 0.72              |
| 1:AU:76:THR:HG22  | 1:AU:111:ILE:O    | 1.88                     | 0.72              |
| 1:BB:40:HIS:CE1   | 1:BU:7:LEU:HD23   | 2.23                     | 0.72              |
| 1:BK:119:THR:HG22 | 1:BK:121:GLU:H    | 1.52                     | 0.72              |
| 1:AB:96:ALA:C     | 1:AB:100:ALA:CB   | 2.62                     | 0.72              |
| 1:BY:119:THR:HG22 | 1:BY:121:GLU:H    | 1.52                     | 0.72              |
| 1:AP:76:THR:HG22  | 1:AP:111:ILE:O    | 1.88                     | 0.72              |
| 1:AP:119:THR:HG22 | 1:AP:121:GLU:H    | 1.52                     | 0.72              |
| 1:BG:96:ALA:C     | 1:BG:100:ALA:CB   | 2.62                     | 0.72              |
| 1:C1:96:ALA:C     | 1:C1:100:ALA:CB   | 2.62                     | 0.72              |
| 1:CQ:96:ALA:C     | 1:CQ:100:ALA:CB   | 2.63                     | 0.72              |
| 1:AO:119:THR:HG22 | 1:AO:121:GLU:H    | 1.52                     | 0.72              |
| 1:A1:96:ALA:C     | 1:A1:100:ALA:CB   | 2.62                     | 0.72              |
| 1:AQ:96:ALA:C     | 1:AQ:100:ALA:CB   | 2.63                     | 0.72              |
| 1:AB:104:LEU:CD2  | 1:AC:60:LEU:HA    | 2.17                     | 0.72              |
| 1:CV:96:ALA:C     | 1:CV:100:ALA:CB   | 2.63                     | 0.72              |
| 1:AI:149:SER:O    | 1:AI:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:AX:149:SER:O    | 1:AX:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:A1:119:THR:HG22 | 1:A1:121:GLU:H    | 1.55                     | 0.71              |
| 1:BN:149:SER:O    | 1:BN:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:B1:104:LEU:CD2  | 1:B2:60:LEU:HA    | 2.17                     | 0.71              |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:HD13 | 1.72                     | 0.71              |
| 1:AV:119:THR:HG22 | 1:AV:121:GLU:H    | 1.55                     | 0.71              |
| 1:A3:149:SER:O    | 1:A3:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:BG:119:THR:HG22 | 1:BG:121:GLU:H    | 1.55                     | 0.71              |
| 1:BQ:96:ALA:C     | 1:BQ:100:ALA:CB   | 2.62                     | 0.71              |
| 1:BQ:119:THR:HG22 | 1:BQ:121:GLU:H    | 1.55                     | 0.71              |
| 1:BX:149:SER:O    | 1:BX:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:CN:149:SER:O    | 1:CN:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:AG:96:ALA:C     | 1:AG:100:ALA:CB   | 2.62                     | 0.71              |
| 1:AQ:104:LEU:CD2  | 1:AR:60:LEU:HA    | 2.17                     | 0.71              |
| 1:AS:149:SER:O    | 1:AS:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:AV:96:ALA:C     | 1:AV:100:ALA:CB   | 2.62                     | 0.71              |
| 1:BD:149:SER:O    | 1:BD:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:BM:38:LYS:HZ2   | 1:BM:44:GLU:HG3   | 1.54                     | 0.71              |
| 1:CC:38:LYS:HZ2   | 1:CC:44:GLU:HG3   | 1.55                     | 0.71              |
| 1:CL:119:THR:HG22 | 1:CL:121:GLU:H    | 1.55                     | 0.71              |
| 1:CQ:119:THR:HG22 | 1:CQ:121:GLU:H    | 1.55                     | 0.71              |
| 1:C3:149:SER:O    | 1:C3:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:BB:119:THR:HG22 | 1:BB:121:GLU:H    | 1.55                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BS:149:SER:O    | 1:BS:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:AN:149:SER:O    | 1:AN:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:BI:149:SER:O    | 1:BI:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:BV:119:THR:HG22 | 1:BV:121:GLU:H    | 1.55                     | 0.71              |
| 1:B3:149:SER:O    | 1:B3:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:CB:119:THR:HG22 | 1:CB:121:GLU:H    | 1.55                     | 0.71              |
| 1:CD:28:LYS:NZ    | 1:CF:28:LYS:HZ2   | 1.87                     | 0.71              |
| 1:CV:119:THR:HG22 | 1:CV:121:GLU:H    | 1.55                     | 0.71              |
| 1:AD:149:SER:O    | 1:AD:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:BC:129:THR:HG21 | 1:BS:120:ILE:HD11 | 1.73                     | 0.71              |
| 1:CI:149:SER:O    | 1:CI:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:CS:149:SER:O    | 1:CS:152:TRP:CZ2  | 2.43                     | 0.71              |
| 1:AL:119:THR:HG22 | 1:AL:121:GLU:H    | 1.55                     | 0.71              |
| 1:BF:7:LEU:HD23   | 1:BQ:40:HIS:CE1   | 2.26                     | 0.71              |
| 1:AB:119:THR:HG22 | 1:AB:121:GLU:H    | 1.55                     | 0.71              |
| 1:B1:96:ALA:C     | 1:B1:100:ALA:CB   | 2.62                     | 0.71              |
| 1:BL:96:ALA:C     | 1:BL:100:ALA:CB   | 2.63                     | 0.71              |
| 1:C2:38:LYS:HZ2   | 1:C2:44:GLU:HG3   | 1.54                     | 0.71              |
| 1:A2:38:LYS:HZ2   | 1:A2:44:GLU:HG3   | 1.56                     | 0.70              |
| 1:BR:38:LYS:HZ2   | 1:BR:44:GLU:HG3   | 1.56                     | 0.70              |
| 1:CW:38:LYS:HZ2   | 1:CW:44:GLU:HG3   | 1.56                     | 0.70              |
| 1:AL:96:ALA:C     | 1:AL:100:ALA:CB   | 2.62                     | 0.70              |
| 1:BL:119:THR:HG22 | 1:BL:121:GLU:H    | 1.55                     | 0.70              |
| 1:CX:149:SER:O    | 1:CX:152:TRP:CZ2  | 2.43                     | 0.70              |
| 1:AL:104:LEU:CD2  | 1:AM:60:LEU:HA    | 2.17                     | 0.70              |
| 1:AG:119:THR:HG22 | 1:AG:121:GLU:H    | 1.55                     | 0.70              |
| 1:CD:149:SER:O    | 1:CD:152:TRP:CZ2  | 2.43                     | 0.70              |
| 1:B2:38:LYS:HZ2   | 1:B2:44:GLU:HG3   | 1.56                     | 0.70              |
| 1:CF:39:ARG:HH22  | 1:CQ:144:GLU:CD   | 2.00                     | 0.70              |
| 1:CG:96:ALA:C     | 1:CG:100:ALA:CB   | 2.63                     | 0.70              |
| 1:CG:104:LEU:CD2  | 1:CH:60:LEU:HA    | 2.17                     | 0.70              |
| 1:CE:107:ASP:CG   | 1:CE:107:ASP:O    | 2.35                     | 0.70              |
| 1:AE:107:ASP:CG   | 1:AE:107:ASP:O    | 2.35                     | 0.70              |
| 1:BU:124:ILE:O    | 1:BU:129:THR:OG1  | 2.10                     | 0.70              |
| 1:CG:119:THR:HG22 | 1:CG:121:GLU:H    | 1.55                     | 0.70              |
| 1:CQ:104:LEU:CD2  | 1:CR:60:LEU:HA    | 2.17                     | 0.70              |
| 1:A1:104:LEU:CD2  | 1:A2:60:LEU:HA    | 2.17                     | 0.69              |
| 1:BE:16:VAL:HG12  | 1:BE:75:ILE:HB    | 1.74                     | 0.69              |
| 1:BG:104:LEU:CD2  | 1:BH:60:LEU:HA    | 2.17                     | 0.69              |
| 1:BL:104:LEU:CD2  | 1:BM:60:LEU:HA    | 2.17                     | 0.69              |
| 1:CE:16:VAL:HG12  | 1:CE:75:ILE:HB    | 1.74                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AE:16:VAL:HG12  | 1:AE:75:ILE:HB   | 1.75                     | 0.69              |
| 1:AJ:16:VAL:HG12  | 1:AJ:75:ILE:HB   | 1.75                     | 0.69              |
| 1:AQ:119:THR:HG22 | 1:AQ:121:GLU:H   | 1.55                     | 0.69              |
| 1:A4:16:VAL:HG12  | 1:A4:75:ILE:HB   | 1.74                     | 0.69              |
| 1:BB:104:LEU:CD2  | 1:BC:60:LEU:HA   | 2.17                     | 0.69              |
| 1:BT:107:ASP:CG   | 1:BT:107:ASP:O   | 2.35                     | 0.69              |
| 1:BB:96:ALA:C     | 1:BB:100:ALA:CB  | 2.62                     | 0.69              |
| 1:BJ:107:ASP:CG   | 1:BJ:107:ASP:O   | 2.35                     | 0.69              |
| 1:BY:107:ASP:O    | 1:BY:107:ASP:CG  | 2.35                     | 0.69              |
| 1:CT:107:ASP:CG   | 1:CT:107:ASP:O   | 2.35                     | 0.69              |
| 1:CY:16:VAL:HG12  | 1:CY:75:ILE:HB   | 1.74                     | 0.69              |
| 1:CZ:124:ILE:O    | 1:CZ:129:THR:OG1 | 2.10                     | 0.69              |
| 1:C1:119:THR:HG22 | 1:C1:121:GLU:H   | 1.55                     | 0.69              |
| 1:CA:124:ILE:O    | 1:CA:129:THR:OG1 | 2.10                     | 0.69              |
| 1:CU:124:ILE:O    | 1:CU:129:THR:OG1 | 2.10                     | 0.69              |
| 1:B1:119:THR:HG22 | 1:B1:121:GLU:H   | 1.55                     | 0.69              |
| 1:CT:16:VAL:HG12  | 1:CT:75:ILE:HB   | 1.74                     | 0.69              |
| 1:A4:107:ASP:CG   | 1:A4:107:ASP:O   | 2.35                     | 0.69              |
| 1:BR:129:THR:CG2  | 1:BR:130:LYS:H   | 1.89                     | 0.69              |
| 1:BY:16:VAL:HG12  | 1:BY:75:ILE:HB   | 1.75                     | 0.69              |
| 1:B4:16:VAL:HG12  | 1:B4:75:ILE:HB   | 1.74                     | 0.69              |
| 1:CY:107:ASP:CG   | 1:CY:107:ASP:O   | 2.35                     | 0.69              |
| 1:AA:124:ILE:O    | 1:AA:129:THR:OG1 | 2.10                     | 0.69              |
| 1:AM:106:THR:O    | 1:AM:107:ASP:CB  | 2.41                     | 0.69              |
| 1:BY:109:PRO:HG3  | 1:BY:149:SER:OG  | 1.93                     | 0.69              |
| 1:CJ:16:VAL:HG12  | 1:CJ:75:ILE:HB   | 1.75                     | 0.69              |
| 1:CR:106:THR:O    | 1:CR:107:ASP:CB  | 2.41                     | 0.69              |
| 1:AO:109:PRO:HG3  | 1:AO:149:SER:OG  | 1.93                     | 0.69              |
| 1:BJ:109:PRO:HG3  | 1:BJ:149:SER:OG  | 1.93                     | 0.69              |
| 1:BV:96:ALA:C     | 1:BV:100:ALA:CB  | 2.63                     | 0.69              |
| 1:CC:106:THR:O    | 1:CC:107:ASP:CB  | 2.41                     | 0.69              |
| 1:CY:109:PRO:HG3  | 1:CY:149:SER:OG  | 1.93                     | 0.69              |
| 1:C4:107:ASP:CG   | 1:C4:107:ASP:O   | 2.35                     | 0.69              |
| 1:BO:16:VAL:HG12  | 1:BO:75:ILE:HB   | 1.75                     | 0.69              |
| 1:BR:106:THR:O    | 1:BR:107:ASP:CB  | 2.41                     | 0.69              |
| 1:BT:16:VAL:HG12  | 1:BT:75:ILE:HB   | 1.75                     | 0.69              |
| 1:CJ:109:PRO:HG3  | 1:CJ:149:SER:OG  | 1.93                     | 0.69              |
| 1:AJ:107:ASP:CG   | 1:AJ:107:ASP:O   | 2.35                     | 0.69              |
| 1:AO:107:ASP:O    | 1:AO:107:ASP:CG  | 2.35                     | 0.69              |
| 1:BJ:16:VAL:HG12  | 1:BJ:75:ILE:HB   | 1.75                     | 0.69              |
| 1:CB:96:ALA:C     | 1:CB:100:ALA:CB  | 2.63                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C2:106:THR:O   | 1:C2:107:ASP:CB  | 2.41                     | 0.69              |
| 1:AY:16:VAL:HG12 | 1:AY:75:ILE:HB   | 1.75                     | 0.68              |
| 1:BW:106:THR:O   | 1:BW:107:ASP:CB  | 2.41                     | 0.68              |
| 1:AO:16:VAL:HG12 | 1:AO:75:ILE:HB   | 1.74                     | 0.68              |
| 1:A4:109:PRO:HG3 | 1:A4:149:SER:OG  | 1.93                     | 0.68              |
| 1:BT:109:PRO:HG3 | 1:BT:149:SER:OG  | 1.93                     | 0.68              |
| 1:CO:109:PRO:HG3 | 1:CO:149:SER:OG  | 1.93                     | 0.68              |
| 1:C4:109:PRO:HG3 | 1:C4:149:SER:OG  | 1.93                     | 0.68              |
| 1:AT:107:ASP:CG  | 1:AT:107:ASP:O   | 2.35                     | 0.68              |
| 1:AW:106:THR:O   | 1:AW:107:ASP:CB  | 2.41                     | 0.68              |
| 1:BO:109:PRO:HG3 | 1:BO:149:SER:OG  | 1.93                     | 0.68              |
| 1:BV:104:LEU:CD2 | 1:BW:60:LEU:HA   | 2.17                     | 0.68              |
| 1:B4:107:ASP:CG  | 1:B4:107:ASP:O   | 2.35                     | 0.68              |
| 1:CE:109:PRO:HG3 | 1:CE:149:SER:OG  | 1.93                     | 0.68              |
| 1:AF:124:ILE:O   | 1:AF:129:THR:OG1 | 2.10                     | 0.68              |
| 1:AY:109:PRO:HG3 | 1:AY:149:SER:OG  | 1.93                     | 0.68              |
| 1:BA:124:ILE:O   | 1:BA:129:THR:OG1 | 2.10                     | 0.68              |
| 1:AH:38:LYS:HZ2  | 1:AH:44:GLU:HG3  | 1.59                     | 0.68              |
| 1:AT:109:PRO:HG3 | 1:AT:149:SER:OG  | 1.93                     | 0.68              |
| 1:BE:109:PRO:HG3 | 1:BE:149:SER:OG  | 1.93                     | 0.68              |
| 1:B2:106:THR:O   | 1:B2:107:ASP:CB  | 2.41                     | 0.68              |
| 1:CJ:107:ASP:O   | 1:CJ:107:ASP:CG  | 2.35                     | 0.68              |
| 1:AJ:109:PRO:HG3 | 1:AJ:149:SER:OG  | 1.93                     | 0.68              |
| 1:A4:17:VAL:HG12 | 1:A4:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:BE:107:ASP:CG  | 1:BE:107:ASP:O   | 2.35                     | 0.68              |
| 1:BK:56:PHE:CZ   | 1:BO:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:BO:107:ASP:CG  | 1:BO:107:ASP:O   | 2.35                     | 0.68              |
| 1:BU:56:PHE:CZ   | 1:BY:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:CO:107:ASP:CG  | 1:CO:107:ASP:O   | 2.35                     | 0.68              |
| 1:CU:56:PHE:CZ   | 1:CY:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:AN:17:VAL:HG12 | 1:AN:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:AT:17:VAL:HG12 | 1:AT:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:AY:107:ASP:CG  | 1:AY:107:ASP:O   | 2.35                     | 0.68              |
| 1:BP:56:PHE:CZ   | 1:BT:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:B4:17:VAL:HG12 | 1:B4:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:CK:124:ILE:O   | 1:CK:129:THR:OG1 | 2.10                     | 0.68              |
| 1:CM:106:THR:O   | 1:CM:107:ASP:CB  | 2.41                     | 0.68              |
| 1:CQ:30:LEU:HA   | 1:CQ:77:LEU:HD23 | 1.76                     | 0.68              |
| 1:AE:17:VAL:HG12 | 1:AE:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:AT:16:VAL:HG12 | 1:AT:75:ILE:HB   | 1.75                     | 0.68              |
| 1:CJ:17:VAL:HG12 | 1:CJ:50:ALA:HB3  | 1.76                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:CN:17:VAL:HG12 | 1:CN:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:CZ:56:PHE:CZ   | 1:C4:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:C3:17:VAL:HG12 | 1:C3:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:C4:16:VAL:HG12 | 1:C4:75:ILE:HB   | 1.75                     | 0.68              |
| 1:AE:109:PRO:HG3 | 1:AE:149:SER:OG  | 1.93                     | 0.68              |
| 1:AP:56:PHE:CZ   | 1:AT:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:AU:152:TRP:CG  | 1:AU:153:ALA:N   | 2.62                     | 0.68              |
| 1:BF:152:TRP:CG  | 1:BF:153:ALA:N   | 2.62                     | 0.68              |
| 1:BG:30:LEU:HA   | 1:BG:77:LEU:HD23 | 1.76                     | 0.68              |
| 1:BJ:17:VAL:HG12 | 1:BJ:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:BP:152:TRP:CG  | 1:BP:153:ALA:N   | 2.62                     | 0.68              |
| 1:BZ:56:PHE:CZ   | 1:B4:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:B1:30:LEU:HA   | 1:B1:77:LEU:HD23 | 1.76                     | 0.68              |
| 1:B4:109:PRO:HG3 | 1:B4:149:SER:OG  | 1.93                     | 0.68              |
| 1:CL:30:LEU:HA   | 1:CL:77:LEU:HD23 | 1.76                     | 0.68              |
| 1:AF:56:PHE:CZ   | 1:AJ:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:AK:56:PHE:CZ   | 1:AO:100:ALA:HB2 | 2.29                     | 0.68              |
| 1:AQ:30:LEU:HA   | 1:AQ:77:LEU:HD23 | 1.76                     | 0.68              |
| 1:BD:17:VAL:HG12 | 1:BD:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:BE:37:LEU:HG   | 1:BE:139:ALA:HB1 | 1.77                     | 0.68              |
| 1:BQ:104:LEU:CD2 | 1:BR:60:LEU:HA   | 2.17                     | 0.68              |
| 1:CO:17:VAL:HG12 | 1:CO:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:CT:109:PRO:HG3 | 1:CT:149:SER:OG  | 1.93                     | 0.68              |
| 1:C1:30:LEU:HA   | 1:C1:77:LEU:HD23 | 1.76                     | 0.68              |
| 1:C4:17:VAL:HG12 | 1:C4:50:ALA:HB3  | 1.76                     | 0.68              |
| 1:AP:124:ILE:O   | 1:AP:129:THR:OG1 | 2.10                     | 0.67              |
| 1:AX:17:VAL:HG12 | 1:AX:50:ALA:HB3  | 1.76                     | 0.67              |
| 1:AX:151:HIS:CB  | 1:AY:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:BB:30:LEU:HA   | 1:BB:77:LEU:HD23 | 1.76                     | 0.67              |
| 1:CA:56:PHE:CZ   | 1:CE:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:CK:56:PHE:CZ   | 1:CO:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:CP:124:ILE:O   | 1:CP:129:THR:OG1 | 2.10                     | 0.67              |
| 1:AF:7:LEU:HD23  | 1:AQ:40:HIS:CE1  | 2.28                     | 0.67              |
| 1:AF:152:TRP:CG  | 1:AF:153:ALA:N   | 2.62                     | 0.67              |
| 1:AG:104:LEU:CD2 | 1:AH:60:LEU:HA   | 2.17                     | 0.67              |
| 1:AO:37:LEU:HG   | 1:AO:139:ALA:HB1 | 1.77                     | 0.67              |
| 1:AR:106:THR:O   | 1:AR:107:ASP:CB  | 2.41                     | 0.67              |
| 1:AU:56:PHE:CZ   | 1:AY:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:BF:56:PHE:CZ   | 1:BJ:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:BI:151:HIS:CB  | 1:BJ:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:BK:124:ILE:O   | 1:BK:129:THR:OG1 | 2.10                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BS:151:HIS:CB   | 1:BT:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:CF:56:PHE:CZ    | 1:CJ:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:AA:152:TRP:CG   | 1:AA:153:ALA:N   | 2.62                     | 0.67              |
| 1:AB:30:LEU:HA    | 1:AB:77:LEU:HD23 | 1.76                     | 0.67              |
| 1:AT:37:LEU:HG    | 1:AT:139:ALA:HB1 | 1.77                     | 0.67              |
| 1:BB:124:ILE:HD11 | 1:BV:24:PHE:CE2  | 2.29                     | 0.67              |
| 1:BD:151:HIS:CB   | 1:BE:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:BY:17:VAL:HG12  | 1:BY:50:ALA:HB3  | 1.76                     | 0.67              |
| 1:B3:151:HIS:CB   | 1:B4:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:CS:151:HIS:CB   | 1:CT:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:CT:17:VAL:HG12  | 1:CT:50:ALA:HB3  | 1.76                     | 0.67              |
| 1:CX:151:HIS:CB   | 1:CY:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:C3:151:HIS:CB   | 1:C4:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:AD:151:HIS:CB   | 1:AE:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:AF:39:ARG:HH22  | 1:AQ:144:GLU:CD  | 2.02                     | 0.67              |
| 1:AI:151:HIS:CB   | 1:AJ:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:AP:152:TRP:CG   | 1:AP:153:ALA:N   | 2.62                     | 0.67              |
| 1:A3:151:HIS:CB   | 1:A4:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:BM:106:THR:O    | 1:BM:107:ASP:CB  | 2.41                     | 0.67              |
| 1:BO:17:VAL:HG12  | 1:BO:50:ALA:HB3  | 1.76                     | 0.67              |
| 1:BX:151:HIS:CB   | 1:BY:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:BZ:124:ILE:O    | 1:BZ:129:THR:OG1 | 2.10                     | 0.67              |
| 1:B4:37:LEU:HG    | 1:B4:139:ALA:HB1 | 1.77                     | 0.67              |
| 1:CB:104:LEU:CD2  | 1:CC:60:LEU:HA   | 2.17                     | 0.67              |
| 1:CG:30:LEU:HA    | 1:CG:77:LEU:HD23 | 1.76                     | 0.67              |
| 1:CP:56:PHE:CZ    | 1:CT:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:A1:30:LEU:HA    | 1:A1:77:LEU:HD23 | 1.76                     | 0.67              |
| 1:BC:106:THR:O    | 1:BC:107:ASP:CB  | 2.41                     | 0.67              |
| 1:BN:151:HIS:CB   | 1:BO:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:CW:106:THR:O    | 1:CW:107:ASP:CB  | 2.41                     | 0.67              |
| 1:AK:152:TRP:CG   | 1:AK:153:ALA:N   | 2.62                     | 0.67              |
| 1:CL:104:LEU:CD2  | 1:CM:60:LEU:HA   | 2.17                     | 0.67              |
| 1:CN:151:HIS:CB   | 1:CO:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:AA:56:PHE:CZ    | 1:AE:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:AD:17:VAL:HG12  | 1:AD:50:ALA:HB3  | 1.76                     | 0.67              |
| 1:AE:37:LEU:HG    | 1:AE:139:ALA:HB1 | 1.77                     | 0.67              |
| 1:BO:37:LEU:HG    | 1:BO:139:ALA:HB1 | 1.77                     | 0.67              |
| 1:BV:30:LEU:HA    | 1:BV:77:LEU:HD23 | 1.76                     | 0.67              |
| 1:AC:106:THR:O    | 1:AC:107:ASP:CB  | 2.41                     | 0.67              |
| 1:AG:30:LEU:HA    | 1:AG:77:LEU:HD23 | 1.76                     | 0.67              |
| 1:AJ:17:VAL:HG12  | 1:AJ:50:ALA:HB3  | 1.76                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AS:151:HIS:CB   | 1:AT:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:BA:56:PHE:CZ    | 1:BE:100:ALA:HB2 | 2.29                     | 0.67              |
| 1:BZ:152:TRP:CG   | 1:BZ:153:ALA:N   | 2.62                     | 0.67              |
| 1:CK:152:TRP:CG   | 1:CK:153:ALA:N   | 2.62                     | 0.67              |
| 1:CW:7:LEU:HB3    | 1:C2:39:ARG:O    | 1.94                     | 0.67              |
| 1:AZ:152:TRP:CG   | 1:AZ:153:ALA:N   | 2.62                     | 0.67              |
| 1:A1:148:LEU:HD13 | 1:A2:61:ILE:CD1  | 2.25                     | 0.67              |
| 1:A3:17:VAL:HG12  | 1:A3:50:ALA:HB3  | 1.76                     | 0.67              |
| 1:BX:17:VAL:HG12  | 1:BX:50:ALA:HB3  | 1.76                     | 0.67              |
| 1:CT:37:LEU:HG    | 1:CT:139:ALA:HB1 | 1.77                     | 0.67              |
| 1:CY:37:LEU:HG    | 1:CY:139:ALA:HB1 | 1.77                     | 0.67              |
| 1:AN:151:HIS:CB   | 1:AO:64:LYS:HB3  | 2.25                     | 0.67              |
| 1:BL:30:LEU:HA    | 1:BL:77:LEU:HD23 | 1.76                     | 0.67              |
| 1:BT:55:ALA:HB1   | 1:BT:95:VAL:HG21 | 1.77                     | 0.67              |
| 1:CQ:148:LEU:HD13 | 1:CR:61:ILE:CD1  | 2.25                     | 0.67              |
| 1:C1:104:LEU:CD2  | 1:C2:60:LEU:HA   | 2.17                     | 0.67              |
| 1:AG:148:LEU:HD13 | 1:AH:61:ILE:CD1  | 2.25                     | 0.66              |
| 1:A2:106:THR:O    | 1:A2:107:ASP:CB  | 2.41                     | 0.66              |
| 1:B4:55:ALA:HB1   | 1:B4:95:VAL:HG21 | 1.77                     | 0.66              |
| 1:CD:151:HIS:CB   | 1:CE:64:LYS:HB3  | 2.25                     | 0.66              |
| 1:CO:16:VAL:HG12  | 1:CO:75:ILE:HB   | 1.74                     | 0.66              |
| 1:AL:30:LEU:HA    | 1:AL:77:LEU:HD23 | 1.76                     | 0.66              |
| 1:AV:148:LEU:HD13 | 1:AW:61:ILE:CD1  | 2.26                     | 0.66              |
| 1:AZ:56:PHE:CZ    | 1:A4:100:ALA:HB2 | 2.29                     | 0.66              |
| 1:BL:148:LEU:HD13 | 1:BM:61:ILE:CD1  | 2.25                     | 0.66              |
| 1:CB:148:LEU:HD13 | 1:CC:61:ILE:CD1  | 2.25                     | 0.66              |
| 1:AM:106:THR:O    | 1:AM:107:ASP:HB3 | 1.96                     | 0.66              |
| 1:AU:124:ILE:O    | 1:AU:129:THR:OG1 | 2.10                     | 0.66              |
| 1:AY:55:ALA:HB1   | 1:AY:95:VAL:HG21 | 1.77                     | 0.66              |
| 1:BA:152:TRP:CG   | 1:BA:153:ALA:N   | 2.62                     | 0.66              |
| 1:BB:148:LEU:HD13 | 1:BC:61:ILE:CD1  | 2.25                     | 0.66              |
| 1:B2:106:THR:O    | 1:B2:107:ASP:HB3 | 1.96                     | 0.66              |
| 1:CI:17:VAL:HG12  | 1:CI:50:ALA:HB3  | 1.76                     | 0.66              |
| 1:CS:17:VAL:HG12  | 1:CS:50:ALA:HB3  | 1.76                     | 0.66              |
| 1:CV:30:LEU:HA    | 1:CV:77:LEU:HD23 | 1.76                     | 0.66              |
| 1:CV:148:LEU:HD13 | 1:CW:61:ILE:CD1  | 2.26                     | 0.66              |
| 1:AT:55:ALA:HB1   | 1:AT:95:VAL:HG21 | 1.77                     | 0.66              |
| 1:AZ:124:ILE:O    | 1:AZ:129:THR:OG1 | 2.10                     | 0.66              |
| 1:BG:148:LEU:HD13 | 1:BH:61:ILE:CD1  | 2.25                     | 0.66              |
| 1:B1:148:LEU:HD13 | 1:B2:61:ILE:CD1  | 2.25                     | 0.66              |
| 1:CD:17:VAL:HG12  | 1:CD:50:ALA:HB3  | 1.76                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C1:148:LEU:HD13 | 1:C2:61:ILE:CD1   | 2.25                     | 0.66              |
| 1:AC:106:THR:O    | 1:AC:107:ASP:HB3  | 1.96                     | 0.66              |
| 1:AE:55:ALA:HB1   | 1:AE:95:VAL:HG21  | 1.77                     | 0.66              |
| 1:AV:104:LEU:CD2  | 1:AW:60:LEU:HA    | 2.17                     | 0.66              |
| 1:A4:55:ALA:HB1   | 1:A4:95:VAL:HG21  | 1.77                     | 0.66              |
| 1:BR:106:THR:O    | 1:BR:107:ASP:HB3  | 1.96                     | 0.66              |
| 1:BS:17:VAL:HG12  | 1:BS:50:ALA:HB3   | 1.76                     | 0.66              |
| 1:CT:55:ALA:HB1   | 1:CT:95:VAL:HG21  | 1.78                     | 0.66              |
| 1:C4:37:LEU:HG    | 1:C4:139:ALA:HB1  | 1.77                     | 0.66              |
| 1:AR:106:THR:O    | 1:AR:107:ASP:HB3  | 1.96                     | 0.66              |
| 1:AS:17:VAL:HG12  | 1:AS:50:ALA:HB3   | 1.76                     | 0.66              |
| 1:AY:37:LEU:HG    | 1:AY:139:ALA:HB1  | 1.77                     | 0.66              |
| 1:BH:106:THR:O    | 1:BH:107:ASP:CB   | 2.41                     | 0.66              |
| 1:BI:17:VAL:HG12  | 1:BI:50:ALA:HB3   | 1.76                     | 0.66              |
| 1:BT:17:VAL:HG12  | 1:BT:50:ALA:HB3   | 1.76                     | 0.66              |
| 1:CE:17:VAL:HG12  | 1:CE:50:ALA:HB3   | 1.76                     | 0.66              |
| 1:AC:7:LEU:HB3    | 1:AR:39:ARG:O     | 1.96                     | 0.66              |
| 1:AD:120:ILE:HD11 | 1:AR:129:THR:HG21 | 1.76                     | 0.66              |
| 1:BE:17:VAL:HG12  | 1:BE:50:ALA:HB3   | 1.76                     | 0.66              |
| 1:BQ:148:LEU:HD13 | 1:BR:61:ILE:CD1   | 2.25                     | 0.66              |
| 1:CW:106:THR:O    | 1:CW:107:ASP:HB3  | 1.96                     | 0.66              |
| 1:AV:30:LEU:HA    | 1:AV:77:LEU:HD23  | 1.76                     | 0.66              |
| 1:A4:37:LEU:HG    | 1:A4:139:ALA:HB1  | 1.77                     | 0.66              |
| 1:B2:38:LYS:NZ    | 1:B2:44:GLU:HG3   | 2.11                     | 0.66              |
| 1:CA:152:TRP:CG   | 1:CA:153:ALA:N    | 2.62                     | 0.66              |
| 1:CG:148:LEU:HD13 | 1:CH:61:ILE:CD1   | 2.26                     | 0.66              |
| 1:CI:151:HIS:CB   | 1:CJ:64:LYS:HB3   | 2.25                     | 0.66              |
| 1:CJ:55:ALA:HB1   | 1:CJ:95:VAL:HG21  | 1.77                     | 0.66              |
| 1:CW:38:LYS:NZ    | 1:CW:44:GLU:HG3   | 2.11                     | 0.66              |
| 1:AE:75:ILE:HG22  | 1:AE:77:LEU:HD13  | 1.78                     | 0.66              |
| 1:AJ:55:ALA:HB1   | 1:AJ:95:VAL:HG21  | 1.77                     | 0.66              |
| 1:AK:124:ILE:O    | 1:AK:129:THR:OG1  | 2.10                     | 0.66              |
| 1:AO:58:ILE:HG22  | 1:AO:58:ILE:O     | 1.96                     | 0.66              |
| 1:BK:152:TRP:CG   | 1:BK:153:ALA:N    | 2.62                     | 0.66              |
| 1:BM:38:LYS:NZ    | 1:BM:44:GLU:HG3   | 2.11                     | 0.66              |
| 1:BP:124:ILE:O    | 1:BP:129:THR:OG1  | 2.10                     | 0.66              |
| 1:BR:38:LYS:NZ    | 1:BR:44:GLU:HG3   | 2.11                     | 0.66              |
| 1:BW:38:LYS:NZ    | 1:BW:44:GLU:HG3   | 2.11                     | 0.66              |
| 1:CH:106:THR:O    | 1:CH:107:ASP:CB   | 2.41                     | 0.66              |
| 1:CL:148:LEU:HD13 | 1:CM:61:ILE:CD1   | 2.26                     | 0.66              |
| 1:CV:104:LEU:CD2  | 1:CW:60:LEU:HA    | 2.17                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:CW:128:GLY:O    | 1:C3:22:ASN:HA   | 1.96                     | 0.66              |
| 1:AB:148:LEU:HD13 | 1:AC:61:ILE:CD1  | 2.25                     | 0.66              |
| 1:AG:96:ALA:O     | 1:AG:100:ALA:CB  | 2.44                     | 0.66              |
| 1:BH:106:THR:O    | 1:BH:107:ASP:HB3 | 1.96                     | 0.66              |
| 1:BQ:4:GLU:HG2    | 1:BR:51:TRP:HD1  | 1.61                     | 0.66              |
| 1:BT:37:LEU:HG    | 1:BT:139:ALA:HB1 | 1.77                     | 0.66              |
| 1:CC:38:LYS:NZ    | 1:CC:44:GLU:HG3  | 2.11                     | 0.66              |
| 1:CJ:75:ILE:HG22  | 1:CJ:77:LEU:HD13 | 1.78                     | 0.66              |
| 1:CO:58:ILE:O     | 1:CO:58:ILE:HG22 | 1.96                     | 0.66              |
| 1:CR:106:THR:O    | 1:CR:107:ASP:HB3 | 1.96                     | 0.66              |
| 1:C4:75:ILE:HG22  | 1:C4:77:LEU:HD13 | 1.78                     | 0.66              |
| 1:AH:106:THR:O    | 1:AH:107:ASP:HB3 | 1.96                     | 0.65              |
| 1:AJ:37:LEU:HG    | 1:AJ:139:ALA:HB1 | 1.77                     | 0.65              |
| 1:AW:38:LYS:NZ    | 1:AW:44:GLU:HG3  | 2.11                     | 0.65              |
| 1:AY:17:VAL:HG12  | 1:AY:50:ALA:HB3  | 1.76                     | 0.65              |
| 1:BC:38:LYS:NZ    | 1:BC:44:GLU:HG3  | 2.11                     | 0.65              |
| 1:BL:96:ALA:O     | 1:BL:100:ALA:CB  | 2.45                     | 0.65              |
| 1:BT:75:ILE:HG22  | 1:BT:77:LEU:HD13 | 1.78                     | 0.65              |
| 1:BV:4:GLU:HG2    | 1:BW:51:TRP:HD1  | 1.61                     | 0.65              |
| 1:B3:17:VAL:HG12  | 1:B3:50:ALA:HB3  | 1.76                     | 0.65              |
| 1:CF:124:ILE:O    | 1:CF:129:THR:OG1 | 2.10                     | 0.65              |
| 1:CO:37:LEU:HG    | 1:CO:139:ALA:HB1 | 1.77                     | 0.65              |
| 1:CY:17:VAL:HG12  | 1:CY:50:ALA:HB3  | 1.76                     | 0.65              |
| 1:AK:53:PRO:HD2   | 1:AK:57:GLU:HB2  | 1.79                     | 0.65              |
| 1:AL:148:LEU:HD13 | 1:AM:61:ILE:CD1  | 2.26                     | 0.65              |
| 1:AO:75:ILE:HG22  | 1:AO:77:LEU:HD13 | 1.78                     | 0.65              |
| 1:AQ:96:ALA:O     | 1:AQ:100:ALA:CB  | 2.45                     | 0.65              |
| 1:BA:53:PRO:HD2   | 1:BA:57:GLU:HB2  | 1.79                     | 0.65              |
| 1:BE:55:ALA:HB1   | 1:BE:95:VAL:HG21 | 1.77                     | 0.65              |
| 1:BG:96:ALA:O     | 1:BG:100:ALA:CB  | 2.44                     | 0.65              |
| 1:BJ:58:ILE:O     | 1:BJ:58:ILE:HG22 | 1.96                     | 0.65              |
| 1:BY:55:ALA:HB1   | 1:BY:95:VAL:HG21 | 1.77                     | 0.65              |
| 1:B4:75:ILE:HG22  | 1:B4:77:LEU:HD13 | 1.78                     | 0.65              |
| 1:CP:152:TRP:CG   | 1:CP:153:ALA:N   | 2.62                     | 0.65              |
| 1:CX:17:VAL:HG12  | 1:CX:50:ALA:HB3  | 1.76                     | 0.65              |
| 1:AC:38:LYS:NZ    | 1:AC:44:GLU:HG3  | 2.11                     | 0.65              |
| 1:AH:38:LYS:NZ    | 1:AH:44:GLU:HG3  | 2.11                     | 0.65              |
| 1:AI:17:VAL:HG12  | 1:AI:50:ALA:HB3  | 1.76                     | 0.65              |
| 1:AO:17:VAL:HG12  | 1:AO:50:ALA:HB3  | 1.76                     | 0.65              |
| 1:AR:38:LYS:NZ    | 1:AR:44:GLU:HG3  | 2.11                     | 0.65              |
| 1:AT:58:ILE:O     | 1:AT:58:ILE:HG22 | 1.96                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BB:96:ALA:O     | 1:BB:100:ALA:CB   | 2.45                     | 0.65              |
| 1:CP:39:ARG:O     | 1:CV:7:LEU:HB3    | 1.96                     | 0.65              |
| 1:AL:96:ALA:O     | 1:AL:100:ALA:CB   | 2.45                     | 0.65              |
| 1:AQ:148:LEU:HD13 | 1:AR:61:ILE:CD1   | 2.26                     | 0.65              |
| 1:A2:106:THR:O    | 1:A2:107:ASP:HB3  | 1.96                     | 0.65              |
| 1:A4:75:ILE:HG22  | 1:A4:77:LEU:HD13  | 1.78                     | 0.65              |
| 1:BJ:55:ALA:HB1   | 1:BJ:95:VAL:HG21  | 1.77                     | 0.65              |
| 1:BN:17:VAL:HG12  | 1:BN:50:ALA:HB3   | 1.76                     | 0.65              |
| 1:BQ:96:ALA:O     | 1:BQ:100:ALA:CB   | 2.45                     | 0.65              |
| 1:CE:37:LEU:HG    | 1:CE:139:ALA:HB1  | 1.77                     | 0.65              |
| 1:CG:96:ALA:O     | 1:CG:100:ALA:CB   | 2.45                     | 0.65              |
| 1:CL:4:GLU:HG2    | 1:CM:51:TRP:HD1   | 1.61                     | 0.65              |
| 1:CO:55:ALA:HB1   | 1:CO:95:VAL:HG21  | 1.77                     | 0.65              |
| 1:CU:152:TRP:CG   | 1:CU:153:ALA:N    | 2.62                     | 0.65              |
| 1:CY:75:ILE:HG22  | 1:CY:77:LEU:HD13  | 1.78                     | 0.65              |
| 1:AZ:53:PRO:HD2   | 1:AZ:57:GLU:HB2   | 1.79                     | 0.65              |
| 1:A1:96:ALA:O     | 1:A1:100:ALA:CB   | 2.45                     | 0.65              |
| 1:BL:100:ALA:HA   | 1:BM:56:PHE:HZ    | 1.62                     | 0.65              |
| 1:BO:58:ILE:O     | 1:BO:58:ILE:HG22  | 1.96                     | 0.65              |
| 1:BQ:4:GLU:HG2    | 1:BR:51:TRP:CD1   | 2.32                     | 0.65              |
| 1:BV:96:ALA:O     | 1:BV:100:ALA:CB   | 2.45                     | 0.65              |
| 1:BV:148:LEU:HD13 | 1:BW:61:ILE:CD1   | 2.26                     | 0.65              |
| 1:CB:30:LEU:HA    | 1:CB:77:LEU:HD23  | 1.76                     | 0.65              |
| 1:CU:53:PRO:HD2   | 1:CU:57:GLU:HB2   | 1.79                     | 0.65              |
| 1:C1:4:GLU:HG2    | 1:C2:51:TRP:HD1   | 1.61                     | 0.65              |
| 1:C1:96:ALA:O     | 1:C1:100:ALA:CB   | 2.44                     | 0.65              |
| 1:C2:106:THR:O    | 1:C2:107:ASP:HB3  | 1.96                     | 0.65              |
| 1:C4:55:ALA:HB1   | 1:C4:95:VAL:HG21  | 1.77                     | 0.65              |
| 1:AB:7:LEU:HB3    | 1:AU:39:ARG:O     | 1.97                     | 0.65              |
| 1:AC:129:THR:HG21 | 1:AS:120:ILE:CD1  | 2.27                     | 0.65              |
| 1:AM:38:LYS:NZ    | 1:AM:44:GLU:HG3   | 2.11                     | 0.65              |
| 1:BF:53:PRO:HD2   | 1:BF:57:GLU:HB2   | 1.79                     | 0.65              |
| 1:BJ:37:LEU:HG    | 1:BJ:139:ALA:HB1  | 1.77                     | 0.65              |
| 1:BK:7:LEU:HD11   | 1:BK:140:VAL:HG13 | 1.79                     | 0.65              |
| 1:BW:106:THR:O    | 1:BW:107:ASP:HB3  | 1.96                     | 0.65              |
| 1:BY:37:LEU:HG    | 1:BY:139:ALA:HB1  | 1.77                     | 0.65              |
| 1:CC:40:HIS:CE1   | 1:CR:7:LEU:HD23   | 2.32                     | 0.65              |
| 1:CQ:96:ALA:O     | 1:CQ:100:ALA:CB   | 2.45                     | 0.65              |
| 1:CT:75:ILE:HG22  | 1:CT:77:LEU:HD13  | 1.78                     | 0.65              |
| 1:CZ:53:PRO:HD2   | 1:CZ:57:GLU:HB2   | 1.79                     | 0.65              |
| 1:C1:4:GLU:HG2    | 1:C2:51:TRP:CD1   | 2.32                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AP:7:LEU:HD11  | 1:AP:140:VAL:HG13 | 1.79                     | 0.65              |
| 1:AU:53:PRO:HD2  | 1:AU:57:GLU:HB2   | 1.79                     | 0.65              |
| 1:BA:7:LEU:HD11  | 1:BA:140:VAL:HG13 | 1.79                     | 0.65              |
| 1:BJ:75:ILE:HG22 | 1:BJ:77:LEU:HD13  | 1.78                     | 0.65              |
| 1:BL:4:GLU:HG2   | 1:BM:51:TRP:HD1   | 1.61                     | 0.65              |
| 1:B1:96:ALA:O    | 1:B1:100:ALA:CB   | 2.45                     | 0.65              |
| 1:CB:4:GLU:HG2   | 1:CC:51:TRP:HD1   | 1.61                     | 0.65              |
| 1:CE:55:ALA:HB1  | 1:CE:95:VAL:HG21  | 1.77                     | 0.65              |
| 1:CJ:37:LEU:HG   | 1:CJ:139:ALA:HB1  | 1.77                     | 0.65              |
| 1:CU:7:LEU:HD11  | 1:CU:140:VAL:HG13 | 1.79                     | 0.65              |
| 1:AW:106:THR:O   | 1:AW:107:ASP:HB3  | 1.96                     | 0.65              |
| 1:BB:4:GLU:HG2   | 1:BC:51:TRP:HD1   | 1.61                     | 0.65              |
| 1:BB:100:ALA:HA  | 1:BC:56:PHE:HZ    | 1.62                     | 0.65              |
| 1:BL:4:GLU:HG2   | 1:BM:51:TRP:CD1   | 2.32                     | 0.65              |
| 1:BO:75:ILE:HG22 | 1:BO:77:LEU:HD13  | 1.78                     | 0.65              |
| 1:BQ:30:LEU:HA   | 1:BQ:77:LEU:HD23  | 1.76                     | 0.65              |
| 1:BZ:7:LEU:HD11  | 1:BZ:140:VAL:HG13 | 1.79                     | 0.65              |
| 1:CB:96:ALA:O    | 1:CB:100:ALA:CB   | 2.45                     | 0.65              |
| 1:CF:7:LEU:HD11  | 1:CF:140:VAL:HG13 | 1.79                     | 0.65              |
| 1:CV:96:ALA:O    | 1:CV:100:ALA:CB   | 2.45                     | 0.65              |
| 1:AB:100:ALA:HA  | 1:AC:56:PHE:HZ    | 1.62                     | 0.65              |
| 1:BE:75:ILE:HG22 | 1:BE:77:LEU:HD13  | 1.78                     | 0.65              |
| 1:BV:107:ASP:HB2 | 1:BV:152:TRP:HZ3  | 1.62                     | 0.65              |
| 1:CD:28:LYS:NZ   | 1:CF:28:LYS:NZ    | 2.43                     | 0.65              |
| 1:CE:58:ILE:HG22 | 1:CE:58:ILE:O     | 1.96                     | 0.65              |
| 1:CK:53:PRO:HD2  | 1:CK:57:GLU:HB2   | 1.79                     | 0.65              |
| 1:CL:4:GLU:HG2   | 1:CM:51:TRP:CD1   | 2.32                     | 0.65              |
| 1:CQ:4:GLU:HG2   | 1:CR:51:TRP:HD1   | 1.62                     | 0.65              |
| 1:CT:58:ILE:O    | 1:CT:58:ILE:HG22  | 1.96                     | 0.65              |
| 1:CX:120:ILE:CD1 | 1:C2:129:THR:HG21 | 2.27                     | 0.65              |
| 1:AG:100:ALA:HA  | 1:AH:56:PHE:HZ    | 1.62                     | 0.65              |
| 1:AK:7:LEU:HD11  | 1:AK:140:VAL:HG13 | 1.79                     | 0.65              |
| 1:BC:106:THR:O   | 1:BC:107:ASP:HB3  | 1.96                     | 0.65              |
| 1:BF:124:ILE:O   | 1:BF:129:THR:OG1  | 2.10                     | 0.65              |
| 1:BG:4:GLU:HG2   | 1:BH:51:TRP:CD1   | 2.32                     | 0.65              |
| 1:BO:55:ALA:HB1  | 1:BO:95:VAL:HG21  | 1.77                     | 0.65              |
| 1:BS:100:ALA:HB2 | 1:BT:56:PHE:CZ    | 2.32                     | 0.65              |
| 1:BU:53:PRO:HD2  | 1:BU:57:GLU:HB2   | 1.79                     | 0.65              |
| 1:BY:58:ILE:HG22 | 1:BY:58:ILE:O     | 1.96                     | 0.65              |
| 1:B1:100:ALA:HA  | 1:B2:56:PHE:HZ    | 1.62                     | 0.65              |
| 1:CB:100:ALA:HA  | 1:CC:56:PHE:HZ    | 1.62                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CB:107:ASP:HB2  | 1:CB:152:TRP:HZ3  | 1.61                     | 0.65              |
| 1:CL:96:ALA:O     | 1:CL:100:ALA:CB   | 2.45                     | 0.65              |
| 1:CN:100:ALA:HB2  | 1:CO:56:PHE:CZ    | 2.32                     | 0.65              |
| 1:CQ:100:ALA:HA   | 1:CR:56:PHE:HZ    | 1.62                     | 0.65              |
| 1:CV:4:GLU:HG2    | 1:CW:51:TRP:CD1   | 2.32                     | 0.65              |
| 1:CY:55:ALA:HB1   | 1:CY:95:VAL:HG21  | 1.77                     | 0.65              |
| 1:CZ:152:TRP:CG   | 1:CZ:153:ALA:N    | 2.62                     | 0.65              |
| 1:C1:100:ALA:HA   | 1:C2:56:PHE:HZ    | 1.62                     | 0.65              |
| 1:AD:100:ALA:HB2  | 1:AE:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:AN:100:ALA:HB2  | 1:AO:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:AV:100:ALA:HA   | 1:AW:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:A1:96:ALA:HB2   | 1:A1:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:BF:39:ARG:HH22  | 1:BQ:144:GLU:CD   | 2.05                     | 0.64              |
| 1:BI:100:ALA:HB2  | 1:BJ:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:BI:149:SER:O    | 1:BI:152:TRP:CE2  | 2.50                     | 0.64              |
| 1:BN:100:ALA:HB2  | 1:BO:56:PHE:CZ    | 2.33                     | 0.64              |
| 1:BU:7:LEU:HD11   | 1:BU:140:VAL:HG13 | 1.79                     | 0.64              |
| 1:BX:149:SER:O    | 1:BX:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:BY:75:ILE:HG22  | 1:BY:77:LEU:HD13  | 1.78                     | 0.64              |
| 1:B3:149:SER:O    | 1:B3:152:TRP:CE2  | 2.50                     | 0.64              |
| 1:CS:149:SER:O    | 1:CS:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:C3:100:ALA:HB2  | 1:C4:56:PHE:CZ    | 2.33                     | 0.64              |
| 1:AA:7:LEU:HD11   | 1:AA:140:VAL:HG13 | 1.79                     | 0.64              |
| 1:AH:106:THR:O    | 1:AH:107:ASP:CB   | 2.41                     | 0.64              |
| 1:AP:53:PRO:HD2   | 1:AP:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:AY:75:ILE:HG22  | 1:AY:77:LEU:HD13  | 1.78                     | 0.64              |
| 1:BB:4:GLU:HG2    | 1:BC:51:TRP:CD1   | 2.32                     | 0.64              |
| 1:BD:149:SER:O    | 1:BD:152:TRP:CE2  | 2.50                     | 0.64              |
| 1:BG:96:ALA:HB2   | 1:BG:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:BH:38:LYS:NZ    | 1:BH:44:GLU:HG3   | 2.11                     | 0.64              |
| 1:CD:100:ALA:HB2  | 1:CE:56:PHE:CZ    | 2.33                     | 0.64              |
| 1:CG:96:ALA:HB2   | 1:CG:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:CI:100:ALA:HB2  | 1:CJ:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:CR:38:LYS:NZ    | 1:CR:44:GLU:HG3   | 2.11                     | 0.64              |
| 1:AJ:75:ILE:HG22  | 1:AJ:77:LEU:HD13  | 1.78                     | 0.64              |
| 1:AN:149:SER:O    | 1:AN:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:AT:75:ILE:HG22  | 1:AT:77:LEU:HD13  | 1.78                     | 0.64              |
| 1:AV:96:ALA:O     | 1:AV:100:ALA:CB   | 2.45                     | 0.64              |
| 1:AX:100:ALA:HB2  | 1:AY:56:PHE:CZ    | 2.33                     | 0.64              |
| 1:BB:98:GLY:HA2   | 1:BB:102:LEU:HD23 | 1.80                     | 0.64              |
| 1:BD:119:THR:HG22 | 1:BD:121:GLU:H    | 1.63                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BD:120:ILE:HD11 | 1:BR:129:THR:HG21 | 1.79                     | 0.64              |
| 1:BE:58:ILE:O     | 1:BE:58:ILE:HG22  | 1.96                     | 0.64              |
| 1:BK:53:PRO:HD2   | 1:BK:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:BP:53:PRO:HD2   | 1:BP:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:BQ:96:ALA:HB2   | 1:BQ:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:BV:96:ALA:HB2   | 1:BV:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:CC:106:THR:O    | 1:CC:107:ASP:HB3  | 1.96                     | 0.64              |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:CG1  | 2.27                     | 0.64              |
| 1:CE:75:ILE:HG22  | 1:CE:77:LEU:HD13  | 1.78                     | 0.64              |
| 1:CF:7:LEU:HD23   | 1:CQ:40:HIS:CE1   | 2.32                     | 0.64              |
| 1:CG:4:GLU:HG2    | 1:CH:51:TRP:CD1   | 2.32                     | 0.64              |
| 1:CG:98:GLY:HA2   | 1:CG:102:LEU:HD23 | 1.80                     | 0.64              |
| 1:CH:38:LYS:NZ    | 1:CH:44:GLU:HG3   | 2.11                     | 0.64              |
| 1:CH:106:THR:O    | 1:CH:107:ASP:HB3  | 1.96                     | 0.64              |
| 1:CM:38:LYS:NZ    | 1:CM:44:GLU:HG3   | 2.11                     | 0.64              |
| 1:CO:75:ILE:HG22  | 1:CO:77:LEU:HD13  | 1.78                     | 0.64              |
| 1:CY:58:ILE:HG22  | 1:CY:58:ILE:O     | 1.96                     | 0.64              |
| 1:C1:96:ALA:HB2   | 1:C1:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:AA:53:PRO:HD2   | 1:AA:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:AQ:100:ALA:HA   | 1:AR:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:A2:38:LYS:NZ    | 1:A2:44:GLU:HG3   | 2.11                     | 0.64              |
| 1:BM:106:THR:O    | 1:BM:107:ASP:HB3  | 1.96                     | 0.64              |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:HD11 | 1.75                     | 0.64              |
| 1:CI:149:SER:O    | 1:CI:152:TRP:CE2  | 2.50                     | 0.64              |
| 1:CL:98:GLY:O     | 1:CL:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:CL:100:ALA:HA   | 1:CM:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:CS:100:ALA:HB2  | 1:CT:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:CX:119:THR:HG22 | 1:CX:121:GLU:H    | 1.63                     | 0.64              |
| 1:C3:119:THR:HG22 | 1:C3:121:GLU:H    | 1.63                     | 0.64              |
| 1:AE:58:ILE:O     | 1:AE:58:ILE:HG22  | 1.96                     | 0.64              |
| 1:AI:149:SER:O    | 1:AI:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:AX:119:THR:HG22 | 1:AX:121:GLU:H    | 1.63                     | 0.64              |
| 1:BF:7:LEU:HD11   | 1:BF:140:VAL:HG13 | 1.79                     | 0.64              |
| 1:BI:119:THR:HG22 | 1:BI:121:GLU:H    | 1.63                     | 0.64              |
| 1:BL:98:GLY:O     | 1:BL:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:BQ:18:VAL:HG22  | 1:BQ:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:BX:100:ALA:HB2  | 1:BY:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:BX:119:THR:HG22 | 1:BX:121:GLU:H    | 1.63                     | 0.64              |
| 1:B1:4:GLU:HG2    | 1:B2:51:TRP:HD1   | 1.61                     | 0.64              |
| 1:B1:96:ALA:HB2   | 1:B1:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:B3:100:ALA:HB2  | 1:B4:56:PHE:CZ    | 2.33                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B4:58:ILE:O     | 1:B4:58:ILE:HG22  | 1.96                     | 0.64              |
| 1:CF:152:TRP:CG   | 1:CF:153:ALA:N    | 2.62                     | 0.64              |
| 1:CI:119:THR:HG22 | 1:CI:121:GLU:H    | 1.63                     | 0.64              |
| 1:CM:106:THR:O    | 1:CM:107:ASP:HB3  | 1.96                     | 0.64              |
| 1:CQ:98:GLY:O     | 1:CQ:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:AB:98:GLY:O     | 1:AB:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:AG:98:GLY:O     | 1:AG:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:AL:98:GLY:O     | 1:AL:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:A3:149:SER:O    | 1:A3:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:BB:98:GLY:O     | 1:BB:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:BG:98:GLY:O     | 1:BG:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:BG:100:ALA:HA   | 1:BH:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:CB:4:GLU:HG2    | 1:CC:51:TRP:CD1   | 2.32                     | 0.64              |
| 1:CG:100:ALA:HA   | 1:CH:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:CV:4:GLU:HG2    | 1:CW:51:TRP:HD1   | 1.61                     | 0.64              |
| 1:CV:96:ALA:HB2   | 1:CV:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:AD:149:SER:O    | 1:AD:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:AS:149:SER:O    | 1:AS:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:AY:58:ILE:O     | 1:AY:58:ILE:HG22  | 1.96                     | 0.64              |
| 1:BB:18:VAL:HG22  | 1:BB:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:BN:149:SER:O    | 1:BN:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:BU:152:TRP:CG   | 1:BU:153:ALA:N    | 2.62                     | 0.64              |
| 1:BV:98:GLY:O     | 1:BV:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:BV:100:ALA:HA   | 1:BW:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:CB:98:GLY:O     | 1:CB:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:CG:4:GLU:HG2    | 1:CH:51:TRP:HD1   | 1.61                     | 0.64              |
| 1:CL:98:GLY:HA2   | 1:CL:102:LEU:HD23 | 1.80                     | 0.64              |
| 1:CQ:4:GLU:HG2    | 1:CR:51:TRP:CD1   | 2.32                     | 0.64              |
| 1:C1:98:GLY:O     | 1:C1:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:C3:149:SER:O    | 1:C3:152:TRP:CE2  | 2.50                     | 0.64              |
| 1:AB:96:ALA:O     | 1:AB:100:ALA:CB   | 2.45                     | 0.64              |
| 1:AG:96:ALA:HB2   | 1:AG:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:AI:100:ALA:HB2  | 1:AJ:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:AL:96:ALA:HB2   | 1:AL:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:AV:96:ALA:HB2   | 1:AV:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:BL:96:ALA:HB2   | 1:BL:112:PHE:CZ   | 2.33                     | 0.64              |
| 1:BQ:100:ALA:HA   | 1:BR:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:BR:82:ARG:HH11  | 1:BR:82:ARG:CG    | 2.11                     | 0.64              |
| 1:BV:4:GLU:HG2    | 1:BW:51:TRP:CD1   | 2.32                     | 0.64              |
| 1:B1:98:GLY:HA2   | 1:B1:102:LEU:HD23 | 1.80                     | 0.64              |
| 1:CB:96:ALA:HB2   | 1:CB:112:PHE:CZ   | 2.33                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CV:98:GLY:O     | 1:CV:102:LEU:HB3  | 1.98                     | 0.64              |
| 1:AF:7:LEU:HD11   | 1:AF:140:VAL:HG13 | 1.79                     | 0.64              |
| 1:AJ:58:ILE:HG22  | 1:AJ:58:ILE:O     | 1.96                     | 0.64              |
| 1:AL:100:ALA:HA   | 1:AM:56:PHE:HZ    | 1.62                     | 0.64              |
| 1:AS:100:ALA:HB2  | 1:AT:56:PHE:CZ    | 2.33                     | 0.64              |
| 1:CP:53:PRO:HD2   | 1:CP:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:CT:7:LEU:HB3    | 1:C3:39:ARG:O     | 1.98                     | 0.64              |
| 1:CV:98:GLY:HA2   | 1:CV:102:LEU:HD23 | 1.80                     | 0.64              |
| 1:CX:100:ALA:HB2  | 1:CY:56:PHE:CZ    | 2.32                     | 0.64              |
| 1:CX:149:SER:O    | 1:CX:152:TRP:CE2  | 2.51                     | 0.64              |
| 1:C1:18:VAL:HG22  | 1:C1:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:AF:53:PRO:HD2   | 1:AF:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:AL:18:VAL:HG22  | 1:AL:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:AQ:18:VAL:HG22  | 1:AQ:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:AV:18:VAL:HG22  | 1:AV:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:BZ:53:PRO:HD2   | 1:BZ:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:B1:18:VAL:HG22  | 1:B1:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:CF:53:PRO:HD2   | 1:CF:57:GLU:HB2   | 1.79                     | 0.64              |
| 1:CG:18:VAL:HG22  | 1:CG:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:CQ:18:VAL:HG22  | 1:CQ:77:LEU:HB2   | 1.80                     | 0.64              |
| 1:CU:34:LEU:HD11  | 1:CU:38:LYS:HD2   | 1.80                     | 0.64              |
| 1:C1:98:GLY:HA2   | 1:C1:102:LEU:HD23 | 1.80                     | 0.64              |
| 1:C2:38:LYS:NZ    | 1:C2:44:GLU:HG3   | 2.11                     | 0.64              |
| 1:AC:82:ARG:HH11  | 1:AC:82:ARG:CG    | 2.11                     | 0.63              |
| 1:AG:18:VAL:HG22  | 1:AG:77:LEU:HB2   | 1.80                     | 0.63              |
| 1:AI:119:THR:HG22 | 1:AI:121:GLU:H    | 1.63                     | 0.63              |
| 1:AU:34:LEU:HD11  | 1:AU:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:A3:100:ALA:HB2  | 1:A4:56:PHE:CZ    | 2.33                     | 0.63              |
| 1:BP:34:LEU:HD11  | 1:BP:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:BS:119:THR:HG22 | 1:BS:121:GLU:H    | 1.63                     | 0.63              |
| 1:BT:58:ILE:HG22  | 1:BT:58:ILE:O     | 1.96                     | 0.63              |
| 1:CN:119:THR:HG22 | 1:CN:121:GLU:H    | 1.63                     | 0.63              |
| 1:CN:149:SER:O    | 1:CN:152:TRP:CE2  | 2.50                     | 0.63              |
| 1:CQ:96:ALA:HB2   | 1:CQ:112:PHE:CZ   | 2.33                     | 0.63              |
| 1:CZ:34:LEU:HD11  | 1:CZ:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:AB:96:ALA:HB2   | 1:AB:112:PHE:CZ   | 2.33                     | 0.63              |
| 1:AI:39:ARG:O     | 1:AO:7:LEU:HB3    | 1.99                     | 0.63              |
| 1:AO:55:ALA:HB1   | 1:AO:95:VAL:HG21  | 1.77                     | 0.63              |
| 1:AW:82:ARG:HH11  | 1:AW:82:ARG:CG    | 2.11                     | 0.63              |
| 1:A1:100:ALA:HA   | 1:A2:56:PHE:HZ    | 1.62                     | 0.63              |
| 1:A4:58:ILE:HG22  | 1:A4:58:ILE:O     | 1.96                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BB:96:ALA:HB2   | 1:BB:112:PHE:CZ   | 2.33                     | 0.63              |
| 1:BC:82:ARG:HH11  | 1:BC:82:ARG:CG    | 2.11                     | 0.63              |
| 1:BD:100:ALA:HB2  | 1:BE:56:PHE:CZ    | 2.32                     | 0.63              |
| 1:BQ:98:GLY:HA2   | 1:BQ:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:CA:7:LEU:HD11   | 1:CA:140:VAL:HG13 | 1.79                     | 0.63              |
| 1:CK:7:LEU:HD11   | 1:CK:140:VAL:HG13 | 1.79                     | 0.63              |
| 1:CL:18:VAL:HG22  | 1:CL:77:LEU:HB2   | 1.80                     | 0.63              |
| 1:AB:18:VAL:HG22  | 1:AB:77:LEU:HB2   | 1.80                     | 0.63              |
| 1:AQ:96:ALA:HB2   | 1:AQ:112:PHE:CZ   | 2.33                     | 0.63              |
| 1:AX:149:SER:O    | 1:AX:152:TRP:CE2  | 2.51                     | 0.63              |
| 1:AZ:7:LEU:HD11   | 1:AZ:140:VAL:HG13 | 1.79                     | 0.63              |
| 1:BF:34:LEU:HD11  | 1:BF:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:BV:18:VAL:HG22  | 1:BV:77:LEU:HB2   | 1.80                     | 0.63              |
| 1:B1:4:GLU:HG2    | 1:B2:51:TRP:CD1   | 2.32                     | 0.63              |
| 1:CA:34:LEU:HD11  | 1:CA:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:CQ:98:GLY:HA2   | 1:CQ:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:CV:100:ALA:HA   | 1:CW:56:PHE:HZ    | 1.62                     | 0.63              |
| 1:AQ:98:GLY:HA2   | 1:AQ:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:A1:98:GLY:HA2   | 1:A1:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:A1:98:GLY:O     | 1:A1:102:LEU:HB3  | 1.98                     | 0.63              |
| 1:BG:4:GLU:HG2    | 1:BH:51:TRP:HD1   | 1.61                     | 0.63              |
| 1:BG:98:GLY:HA2   | 1:BG:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:BS:149:SER:O    | 1:BS:152:TRP:CE2  | 2.50                     | 0.63              |
| 1:CA:53:PRO:HD2   | 1:CA:57:GLU:HB2   | 1.79                     | 0.63              |
| 1:CC:82:ARG:HH11  | 1:CC:82:ARG:CG    | 2.11                     | 0.63              |
| 1:CD:149:SER:O    | 1:CD:152:TRP:CE2  | 2.51                     | 0.63              |
| 1:CL:96:ALA:HB2   | 1:CL:112:PHE:CZ   | 2.33                     | 0.63              |
| 1:C4:58:ILE:HG22  | 1:C4:58:ILE:O     | 1.96                     | 0.63              |
| 1:AZ:34:LEU:HD11  | 1:AZ:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:A2:82:ARG:HH11  | 1:A2:82:ARG:CG    | 2.11                     | 0.63              |
| 1:A3:119:THR:HG22 | 1:A3:121:GLU:H    | 1.63                     | 0.63              |
| 1:BA:34:LEU:HD11  | 1:BA:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:BP:7:LEU:HD11   | 1:BP:140:VAL:HG13 | 1.79                     | 0.63              |
| 1:BQ:98:GLY:O     | 1:BQ:102:LEU:HB3  | 1.98                     | 0.63              |
| 1:CD:119:THR:HG22 | 1:CD:121:GLU:H    | 1.63                     | 0.63              |
| 1:CG:7:LEU:HB3    | 1:CU:39:ARG:O     | 1.98                     | 0.63              |
| 1:CP:7:LEU:HD11   | 1:CP:140:VAL:HG13 | 1.79                     | 0.63              |
| 1:CW:82:ARG:HH11  | 1:CW:82:ARG:CG    | 2.11                     | 0.63              |
| 1:CZ:7:LEU:HD11   | 1:CZ:140:VAL:HG13 | 1.79                     | 0.63              |
| 1:AF:34:LEU:HD11  | 1:AF:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:AQ:98:GLY:O     | 1:AQ:102:LEU:HB3  | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AV:98:GLY:O     | 1:AV:102:LEU:HB3  | 1.98                     | 0.63              |
| 1:BV:98:GLY:HA2   | 1:BV:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:AG:98:GLY:HA2   | 1:AG:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:AM:82:ARG:HH11  | 1:AM:82:ARG:CG    | 2.11                     | 0.63              |
| 1:BD:40:HIS:CE1   | 1:BJ:7:LEU:HD23   | 2.34                     | 0.63              |
| 1:B1:98:GLY:O     | 1:B1:102:LEU:HB3  | 1.98                     | 0.63              |
| 1:CJ:58:ILE:HG22  | 1:CJ:58:ILE:O     | 1.96                     | 0.63              |
| 1:CM:82:ARG:HH11  | 1:CM:82:ARG:CG    | 2.11                     | 0.63              |
| 1:AQ:13:LYS:HZ3   | 1:BU:43:GLU:HG2   | 1.61                     | 0.63              |
| 1:AR:82:ARG:HH11  | 1:AR:82:ARG:CG    | 2.11                     | 0.63              |
| 1:AV:58:ILE:N     | 1:AV:59:PRO:HD2   | 2.14                     | 0.63              |
| 1:AF:58:ILE:N     | 1:AF:59:PRO:HD2   | 2.14                     | 0.63              |
| 1:A1:58:ILE:N     | 1:A1:59:PRO:HD2   | 2.14                     | 0.63              |
| 1:BB:58:ILE:N     | 1:BB:59:PRO:HD2   | 2.14                     | 0.63              |
| 1:BB:107:ASP:HB2  | 1:BB:152:TRP:HZ3  | 1.62                     | 0.63              |
| 1:BD:7:LEU:HD23   | 1:BJ:40:HIS:CE1   | 2.34                     | 0.63              |
| 1:BG:58:ILE:N     | 1:BG:59:PRO:HD2   | 2.14                     | 0.63              |
| 1:BL:98:GLY:HA2   | 1:BL:102:LEU:HD23 | 1.80                     | 0.63              |
| 1:CB:18:VAL:HG22  | 1:CB:77:LEU:HB2   | 1.80                     | 0.63              |
| 1:CP:34:LEU:HD11  | 1:CP:38:LYS:HD2   | 1.80                     | 0.63              |
| 1:CR:82:ARG:HH11  | 1:CR:82:ARG:CG    | 2.11                     | 0.63              |
| 1:CV:58:ILE:N     | 1:CV:59:PRO:HD2   | 2.14                     | 0.63              |
| 1:AL:98:GLY:HA2   | 1:AL:102:LEU:HD23 | 1.80                     | 0.62              |
| 1:AN:119:THR:HG22 | 1:AN:121:GLU:H    | 1.63                     | 0.62              |
| 1:A1:18:VAL:HG22  | 1:A1:77:LEU:HB2   | 1.80                     | 0.62              |
| 1:BK:34:LEU:HD11  | 1:BK:38:LYS:HD2   | 1.80                     | 0.62              |
| 1:BZ:34:LEU:HD11  | 1:BZ:38:LYS:HD2   | 1.80                     | 0.62              |
| 1:B3:119:THR:HG22 | 1:B3:121:GLU:H    | 1.63                     | 0.62              |
| 1:CH:82:ARG:HH11  | 1:CH:82:ARG:CG    | 2.11                     | 0.62              |
| 1:CU:58:ILE:N     | 1:CU:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:C1:58:ILE:N     | 1:C1:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:AB:98:GLY:HA2   | 1:AB:102:LEU:HD23 | 1.80                     | 0.62              |
| 1:AQ:58:ILE:N     | 1:AQ:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:AW:97:LYS:HG3   | 1:AX:97:LYS:HZ3   | 1.65                     | 0.62              |
| 1:BL:18:VAL:HG22  | 1:BL:77:LEU:HB2   | 1.80                     | 0.62              |
| 1:BL:58:ILE:N     | 1:BL:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:CT:7:LEU:HD23   | 1:C3:40:HIS:CE1   | 2.34                     | 0.62              |
| 1:BG:18:VAL:HG22  | 1:BG:77:LEU:HB2   | 1.80                     | 0.62              |
| 1:BI:124:ILE:O    | 1:BI:129:THR:OG1  | 2.16                     | 0.62              |
| 1:BN:119:THR:HG22 | 1:BN:121:GLU:H    | 1.63                     | 0.62              |
| 1:BX:151:HIS:HB3  | 1:BY:64:LYS:HB3   | 1.82                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CF:34:LEU:HD11  | 1:CF:38:LYS:HD2   | 1.80                     | 0.62              |
| 1:CN:151:HIS:HB3  | 1:CO:64:LYS:HB3   | 1.82                     | 0.62              |
| 1:CS:119:THR:HG22 | 1:CS:121:GLU:H    | 1.63                     | 0.62              |
| 1:AB:58:ILE:N     | 1:AB:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:AK:58:ILE:N     | 1:AK:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:AU:7:LEU:HD11   | 1:AU:140:VAL:HG13 | 1.79                     | 0.62              |
| 1:A3:124:ILE:O    | 1:A3:129:THR:OG1  | 2.16                     | 0.62              |
| 1:BK:58:ILE:N     | 1:BK:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:BP:58:ILE:N     | 1:BP:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:CB:58:ILE:N     | 1:CB:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:CD:120:ILE:CD1  | 1:CR:129:THR:HG21 | 2.30                     | 0.62              |
| 1:CD:151:HIS:HB3  | 1:CE:64:LYS:HB3   | 1.82                     | 0.62              |
| 1:CF:58:ILE:N     | 1:CF:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:C2:82:ARG:HH11  | 1:C2:82:ARG:CG    | 2.11                     | 0.62              |
| 1:AG:58:ILE:N     | 1:AG:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:AP:58:ILE:N     | 1:AP:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:AS:151:HIS:HB3  | 1:AT:64:LYS:HB3   | 1.81                     | 0.62              |
| 1:AT:152:TRP:HE3  | 1:AT:153:ALA:H    | 1.48                     | 0.62              |
| 1:BH:82:ARG:HH11  | 1:BH:82:ARG:CG    | 2.11                     | 0.62              |
| 1:B4:152:TRP:HE3  | 1:B4:153:ALA:H    | 1.48                     | 0.62              |
| 1:CK:58:ILE:N     | 1:CK:59:PRO:HD2   | 2.15                     | 0.62              |
| 1:CX:22:ASN:HA    | 1:C2:128:GLY:O    | 2.00                     | 0.62              |
| 1:C4:152:TRP:HE3  | 1:C4:153:ALA:H    | 1.47                     | 0.62              |
| 1:AD:119:THR:HG22 | 1:AD:121:GLU:H    | 1.63                     | 0.62              |
| 1:AK:34:LEU:HD11  | 1:AK:38:LYS:HD2   | 1.80                     | 0.62              |
| 1:A3:151:HIS:HB3  | 1:A4:64:LYS:HB3   | 1.82                     | 0.62              |
| 1:BN:151:HIS:HB3  | 1:BO:64:LYS:HB3   | 1.82                     | 0.62              |
| 1:BU:34:LEU:HD11  | 1:BU:38:LYS:HD2   | 1.80                     | 0.62              |
| 1:B2:82:ARG:HH11  | 1:B2:82:ARG:CG    | 2.11                     | 0.62              |
| 1:CG:98:GLY:O     | 1:CG:102:LEU:HB3  | 1.98                     | 0.62              |
| 1:CK:34:LEU:HD11  | 1:CK:38:LYS:HD2   | 1.80                     | 0.62              |
| 1:CQ:58:ILE:N     | 1:CQ:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:CS:151:HIS:HB3  | 1:CT:64:LYS:HB3   | 1.82                     | 0.62              |
| 1:CV:18:VAL:HG22  | 1:CV:77:LEU:HB2   | 1.80                     | 0.62              |
| 1:AH:82:ARG:HH11  | 1:AH:82:ARG:CG    | 2.11                     | 0.62              |
| 1:AI:151:HIS:HB3  | 1:AJ:64:LYS:HB3   | 1.82                     | 0.62              |
| 1:CB:98:GLY:HA2   | 1:CB:102:LEU:HD23 | 1.80                     | 0.62              |
| 1:CC:8:VAL:HG13   | 1:CR:8:VAL:HG21   | 1.81                     | 0.62              |
| 1:CC:97:LYS:HG3   | 1:CD:97:LYS:HZ3   | 1.64                     | 0.62              |
| 1:CE:152:TRP:HE3  | 1:CE:153:ALA:H    | 1.48                     | 0.62              |
| 1:CG:58:ILE:N     | 1:CG:59:PRO:HD2   | 2.14                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C1:107:ASP:HB2  | 1:C1:152:TRP:HZ3  | 1.62                     | 0.62              |
| 1:AV:98:GLY:HA2   | 1:AV:102:LEU:HD23 | 1.80                     | 0.62              |
| 1:A4:58:ILE:N     | 1:A4:59:PRO:HD2   | 2.15                     | 0.62              |
| 1:BN:124:ILE:O    | 1:BN:129:THR:OG1  | 2.16                     | 0.62              |
| 1:CT:58:ILE:N     | 1:CT:59:PRO:HD2   | 2.15                     | 0.62              |
| 1:AX:124:ILE:O    | 1:AX:129:THR:OG1  | 2.16                     | 0.62              |
| 1:BD:151:HIS:HB3  | 1:BE:64:LYS:HB3   | 1.82                     | 0.62              |
| 1:BJ:152:TRP:HE3  | 1:BJ:153:ALA:H    | 1.47                     | 0.62              |
| 1:BQ:58:ILE:N     | 1:BQ:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:CP:58:ILE:N     | 1:CP:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:BS:124:ILE:O    | 1:BS:129:THR:OG1  | 2.16                     | 0.62              |
| 1:BT:152:TRP:HE3  | 1:BT:153:ALA:H    | 1.48                     | 0.62              |
| 1:BU:58:ILE:N     | 1:BU:59:PRO:HD2   | 2.14                     | 0.62              |
| 1:B4:58:ILE:N     | 1:B4:59:PRO:HD2   | 2.15                     | 0.62              |
| 1:CC:129:THR:O    | 1:CC:132:GLY:N    | 2.25                     | 0.62              |
| 1:AU:58:ILE:N     | 1:AU:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:AY:58:ILE:N     | 1:AY:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:AZ:58:ILE:N     | 1:AZ:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:BI:151:HIS:HB3  | 1:BJ:64:LYS:HB3   | 1.82                     | 0.61              |
| 1:BO:152:TRP:HE3  | 1:BO:153:ALA:H    | 1.48                     | 0.61              |
| 1:CZ:58:ILE:N     | 1:CZ:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:AA:34:LEU:HD11  | 1:AA:38:LYS:HD2   | 1.80                     | 0.61              |
| 1:AA:58:ILE:N     | 1:AA:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:AD:151:HIS:HB3  | 1:AE:64:LYS:HB3   | 1.82                     | 0.61              |
| 1:AE:58:ILE:N     | 1:AE:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:BF:58:ILE:N     | 1:BF:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:CI:151:HIS:HB3  | 1:CJ:64:LYS:HB3   | 1.81                     | 0.61              |
| 1:CP:39:ARG:HH22  | 1:CV:144:GLU:CD   | 2.08                     | 0.61              |
| 1:CR:129:THR:O    | 1:CR:132:GLY:N    | 2.25                     | 0.61              |
| 1:AC:97:LYS:HG3   | 1:AD:97:LYS:HZ3   | 1.65                     | 0.61              |
| 1:BT:58:ILE:N     | 1:BT:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:B2:6:HIS:HE1    | 1:B2:8:VAL:HB     | 1.66                     | 0.61              |
| 1:AA:34:LEU:HD12  | 1:AA:38:LYS:HB2   | 1.83                     | 0.61              |
| 1:AE:152:TRP:HE3  | 1:AE:153:ALA:H    | 1.48                     | 0.61              |
| 1:AX:151:HIS:HB3  | 1:AY:64:LYS:HB3   | 1.82                     | 0.61              |
| 1:A1:148:LEU:HD13 | 1:A2:61:ILE:HD11  | 1.83                     | 0.61              |
| 1:BA:58:ILE:N     | 1:BA:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:CE:58:ILE:N     | 1:CE:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:CJ:58:ILE:N     | 1:CJ:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:CV:97:LYS:HE3   | 1:CW:97:LYS:HZ3   | 1.65                     | 0.61              |
| 1:CW:100:ALA:HB2  | 1:CX:56:PHE:CZ    | 2.36                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C4:58:ILE:N     | 1:C4:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:AJ:58:ILE:N     | 1:AJ:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:AR:6:HIS:HE1    | 1:AR:8:VAL:HB     | 1.66                     | 0.61              |
| 1:AS:119:THR:HG22 | 1:AS:121:GLU:H    | 1.63                     | 0.61              |
| 1:BJ:58:ILE:N     | 1:BJ:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:BS:151:HIS:HB3  | 1:BT:64:LYS:HB3   | 1.82                     | 0.61              |
| 1:B1:58:ILE:N     | 1:B1:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:B2:100:ALA:HB2  | 1:B3:56:PHE:CZ    | 2.36                     | 0.61              |
| 1:CC:6:HIS:HE1    | 1:CC:8:VAL:HB     | 1.66                     | 0.61              |
| 1:CL:58:ILE:N     | 1:CL:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:CT:152:TRP:HE3  | 1:CT:153:ALA:H    | 1.47                     | 0.61              |
| 1:CZ:34:LEU:HD12  | 1:CZ:38:LYS:HB2   | 1.83                     | 0.61              |
| 1:AQ:148:LEU:HD13 | 1:AR:61:ILE:HD11  | 1.83                     | 0.61              |
| 1:AR:100:ALA:HB2  | 1:AS:56:PHE:CZ    | 2.36                     | 0.61              |
| 1:AW:6:HIS:HE1    | 1:AW:8:VAL:HB     | 1.66                     | 0.61              |
| 1:AW:129:THR:O    | 1:AW:132:GLY:N    | 2.25                     | 0.61              |
| 1:BA:34:LEU:HD12  | 1:BA:38:LYS:HB2   | 1.83                     | 0.61              |
| 1:BF:34:LEU:HD12  | 1:BF:38:LYS:HB2   | 1.83                     | 0.61              |
| 1:BM:100:ALA:HB2  | 1:BN:56:PHE:CZ    | 2.36                     | 0.61              |
| 1:BP:34:LEU:HD12  | 1:BP:38:LYS:HB2   | 1.83                     | 0.61              |
| 1:BQ:148:LEU:HD13 | 1:BR:61:ILE:HD11  | 1.83                     | 0.61              |
| 1:BU:34:LEU:HD12  | 1:BU:38:LYS:HB2   | 1.83                     | 0.61              |
| 1:BV:58:ILE:N     | 1:BV:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:BW:100:ALA:HB2  | 1:BX:56:PHE:CZ    | 2.36                     | 0.61              |
| 1:B3:151:HIS:HB3  | 1:B4:64:LYS:HB3   | 1.82                     | 0.61              |
| 1:CA:58:ILE:N     | 1:CA:59:PRO:HD2   | 2.14                     | 0.61              |
| 1:CM:6:HIS:HE1    | 1:CM:8:VAL:HB     | 1.66                     | 0.61              |
| 1:CO:53:PRO:CD    | 1:CO:57:GLU:HG3   | 2.29                     | 0.61              |
| 1:CQ:148:LEU:HD13 | 1:CR:61:ILE:HD11  | 1.83                     | 0.61              |
| 1:AP:34:LEU:HD11  | 1:AP:38:LYS:HD2   | 1.80                     | 0.61              |
| 1:AT:58:ILE:N     | 1:AT:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:AU:34:LEU:HD12  | 1:AU:38:LYS:HB2   | 1.83                     | 0.61              |
| 1:AW:100:ALA:HB2  | 1:AX:56:PHE:CZ    | 2.36                     | 0.61              |
| 1:A2:100:ALA:HB2  | 1:A3:56:PHE:CZ    | 2.36                     | 0.61              |
| 1:BO:58:ILE:N     | 1:BO:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:BV:148:LEU:HD13 | 1:BW:61:ILE:HD11  | 1.83                     | 0.61              |
| 1:CG:24:PHE:CE2   | 1:CQ:124:ILE:HD11 | 2.35                     | 0.61              |
| 1:CH:100:ALA:HB2  | 1:CI:56:PHE:CZ    | 2.36                     | 0.61              |
| 1:CO:58:ILE:N     | 1:CO:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:AO:58:ILE:N     | 1:AO:59:PRO:HD2   | 2.15                     | 0.61              |
| 1:AP:34:LEU:HD12  | 1:AP:38:LYS:HB2   | 1.83                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AQ:97:LYS:HE3   | 1:AR:97:LYS:HZ3  | 1.64                     | 0.61              |
| 1:AY:53:PRO:CD    | 1:AY:57:GLU:HG3  | 2.29                     | 0.61              |
| 1:BH:129:THR:O    | 1:BH:132:GLY:N   | 2.25                     | 0.61              |
| 1:BR:63:LYS:O     | 1:BR:67:ASN:HB2  | 2.01                     | 0.61              |
| 1:BW:82:ARG:HH11  | 1:BW:82:ARG:CG   | 2.11                     | 0.61              |
| 1:B2:63:LYS:O     | 1:B2:67:ASN:HB2  | 2.01                     | 0.61              |
| 1:CH:6:HIS:HE1    | 1:CH:8:VAL:HB    | 1.66                     | 0.61              |
| 1:C1:148:LEU:HD13 | 1:C2:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:AB:148:LEU:HD13 | 1:AC:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:AC:100:ALA:HB2  | 1:AD:56:PHE:CZ   | 2.36                     | 0.61              |
| 1:AG:148:LEU:HD13 | 1:AH:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:AM:6:HIS:HE1    | 1:AM:8:VAL:HB    | 1.66                     | 0.61              |
| 1:AV:148:LEU:HD13 | 1:AW:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:AW:63:LYS:O     | 1:AW:67:ASN:HB2  | 2.01                     | 0.61              |
| 1:BC:6:HIS:HE1    | 1:BC:8:VAL:HB    | 1.66                     | 0.61              |
| 1:BE:58:ILE:N     | 1:BE:59:PRO:HD2  | 2.15                     | 0.61              |
| 1:BM:63:LYS:O     | 1:BM:67:ASN:HB2  | 2.01                     | 0.61              |
| 1:BZ:34:LEU:HD12  | 1:BZ:38:LYS:HB2  | 1.83                     | 0.61              |
| 1:B1:148:LEU:HD13 | 1:B2:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:B2:97:LYS:HG3   | 1:B3:97:LYS:HZ3  | 1.65                     | 0.61              |
| 1:B4:53:PRO:CD    | 1:B4:57:GLU:HG3  | 2.29                     | 0.61              |
| 1:CH:63:LYS:O     | 1:CH:67:ASN:HB2  | 2.01                     | 0.61              |
| 1:CH:129:THR:O    | 1:CH:132:GLY:N   | 2.25                     | 0.61              |
| 1:CI:124:ILE:O    | 1:CI:129:THR:OG1 | 2.16                     | 0.61              |
| 1:CM:63:LYS:O     | 1:CM:67:ASN:HB2  | 2.01                     | 0.61              |
| 1:CV:148:LEU:HD13 | 1:CW:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:CY:152:TRP:HE3  | 1:CY:153:ALA:H   | 1.48                     | 0.61              |
| 1:AD:124:ILE:O    | 1:AD:129:THR:OG1 | 2.16                     | 0.61              |
| 1:AF:39:ARG:O     | 1:AQ:7:LEU:HB3   | 2.01                     | 0.61              |
| 1:AH:100:ALA:HB2  | 1:AI:56:PHE:CZ   | 2.36                     | 0.61              |
| 1:AJ:152:TRP:HE3  | 1:AJ:153:ALA:H   | 1.48                     | 0.61              |
| 1:AL:58:ILE:N     | 1:AL:59:PRO:HD2  | 2.14                     | 0.61              |
| 1:AN:151:HIS:HB3  | 1:AO:64:LYS:HB3  | 1.82                     | 0.61              |
| 1:AZ:34:LEU:HD12  | 1:AZ:38:LYS:HB2  | 1.83                     | 0.61              |
| 1:BG:148:LEU:HD13 | 1:BH:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:BH:100:ALA:HB2  | 1:BI:56:PHE:CZ   | 2.36                     | 0.61              |
| 1:BW:6:HIS:HE1    | 1:BW:8:VAL:HB    | 1.66                     | 0.61              |
| 1:BZ:58:ILE:N     | 1:BZ:59:PRO:HD2  | 2.14                     | 0.61              |
| 1:CB:148:LEU:HD13 | 1:CC:61:ILE:HD11 | 1.83                     | 0.61              |
| 1:CK:34:LEU:HD12  | 1:CK:38:LYS:HB2  | 1.83                     | 0.61              |
| 1:CY:58:ILE:N     | 1:CY:59:PRO:HD2  | 2.15                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C2:6:HIS:HE1   | 1:C2:8:VAL:HB    | 1.66                     | 0.61              |
| 1:C3:151:HIS:HB3 | 1:C4:64:LYS:HB3  | 1.82                     | 0.61              |
| 1:AK:34:LEU:HD12 | 1:AK:38:LYS:HB2  | 1.83                     | 0.60              |
| 1:A2:6:HIS:HE1   | 1:A2:8:VAL:HB    | 1.66                     | 0.60              |
| 1:BM:82:ARG:HH11 | 1:BM:82:ARG:CG   | 2.11                     | 0.60              |
| 1:CM:100:ALA:HB2 | 1:CN:56:PHE:CZ   | 2.36                     | 0.60              |
| 1:AR:63:LYS:O    | 1:AR:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:BR:20:ARG:HG3  | 1:BR:52:VAL:O    | 2.01                     | 0.60              |
| 1:BY:58:ILE:N    | 1:BY:59:PRO:HD2  | 2.15                     | 0.60              |
| 1:CA:34:LEU:HD12 | 1:CA:38:LYS:HB2  | 1.83                     | 0.60              |
| 1:CD:124:ILE:O   | 1:CD:129:THR:OG1 | 2.16                     | 0.60              |
| 1:CP:34:LEU:HD12 | 1:CP:38:LYS:HB2  | 1.83                     | 0.60              |
| 1:C2:63:LYS:O    | 1:C2:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:C2:100:ALA:HB2 | 1:C3:56:PHE:CZ   | 2.36                     | 0.60              |
| 1:AF:34:LEU:HD12 | 1:AF:38:LYS:HB2  | 1.83                     | 0.60              |
| 1:AM:100:ALA:HB2 | 1:AN:56:PHE:CZ   | 2.36                     | 0.60              |
| 1:BC:20:ARG:HG3  | 1:BC:52:VAL:O    | 2.01                     | 0.60              |
| 1:BC:63:LYS:O    | 1:BC:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:BH:6:HIS:HE1   | 1:BH:8:VAL:HB    | 1.66                     | 0.60              |
| 1:CP:28:LYS:HD2  | 1:CW:24:PHE:CD1  | 2.36                     | 0.60              |
| 1:CQ:97:LYS:HE3  | 1:CR:97:LYS:HZ3  | 1.66                     | 0.60              |
| 1:CW:129:THR:O   | 1:CW:132:GLY:N   | 2.25                     | 0.60              |
| 1:CX:151:HIS:HB3 | 1:CY:64:LYS:HB3  | 1.82                     | 0.60              |
| 1:BR:6:HIS:HE1   | 1:BR:8:VAL:HB    | 1.66                     | 0.60              |
| 1:CC:20:ARG:HG3  | 1:CC:52:VAL:O    | 2.01                     | 0.60              |
| 1:CO:152:TRP:HE3 | 1:CO:153:ALA:H   | 1.47                     | 0.60              |
| 1:CR:20:ARG:HG3  | 1:CR:52:VAL:O    | 2.02                     | 0.60              |
| 1:CW:63:LYS:O    | 1:CW:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:AH:63:LYS:O    | 1:AH:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:AL:97:LYS:HE3  | 1:AM:97:LYS:HZ3  | 1.65                     | 0.60              |
| 1:BE:152:TRP:HE3 | 1:BE:153:ALA:H   | 1.48                     | 0.60              |
| 1:BL:97:LYS:HE3  | 1:BM:97:LYS:HZ3  | 1.65                     | 0.60              |
| 1:BM:6:HIS:HE1   | 1:BM:8:VAL:HB    | 1.66                     | 0.60              |
| 1:CC:100:ALA:HB2 | 1:CD:56:PHE:CZ   | 2.36                     | 0.60              |
| 1:CJ:152:TRP:HE3 | 1:CJ:153:ALA:H   | 1.47                     | 0.60              |
| 1:CR:100:ALA:HB2 | 1:CS:56:PHE:CZ   | 2.36                     | 0.60              |
| 1:CY:53:PRO:CD   | 1:CY:57:GLU:HG3  | 2.29                     | 0.60              |
| 1:AC:63:LYS:O    | 1:AC:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:AM:63:LYS:O    | 1:AM:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:BC:100:ALA:HB2 | 1:BD:56:PHE:CZ   | 2.36                     | 0.60              |
| 1:CW:6:HIS:HE1   | 1:CW:8:VAL:HB    | 1.66                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AH:20:ARG:HG3   | 1:AH:52:VAL:O    | 2.02                     | 0.60              |
| 1:AP:95:VAL:HG12  | 1:AP:112:PHE:HE1 | 1.67                     | 0.60              |
| 1:AW:20:ARG:HG3   | 1:AW:52:VAL:O    | 2.01                     | 0.60              |
| 1:BD:124:ILE:O    | 1:BD:129:THR:OG1 | 2.16                     | 0.60              |
| 1:BH:63:LYS:O     | 1:BH:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:BK:34:LEU:HD12  | 1:BK:38:LYS:HB2  | 1.83                     | 0.60              |
| 1:CK:95:VAL:HG12  | 1:CK:112:PHE:HE1 | 1.67                     | 0.60              |
| 1:C2:20:ARG:HG3   | 1:C2:52:VAL:O    | 2.01                     | 0.60              |
| 1:AH:6:HIS:HE1    | 1:AH:8:VAL:HB    | 1.66                     | 0.60              |
| 1:AN:124:ILE:O    | 1:AN:129:THR:OG1 | 2.16                     | 0.60              |
| 1:A2:63:LYS:O     | 1:A2:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:A4:152:TRP:HE3  | 1:A4:153:ALA:H   | 1.48                     | 0.60              |
| 1:BA:95:VAL:HG12  | 1:BA:112:PHE:HE1 | 1.67                     | 0.60              |
| 1:BH:20:ARG:HG3   | 1:BH:52:VAL:O    | 2.01                     | 0.60              |
| 1:BQ:97:LYS:HE3   | 1:BR:97:LYS:HZ3  | 1.65                     | 0.60              |
| 1:BZ:95:VAL:HG12  | 1:BZ:112:PHE:HE1 | 1.67                     | 0.60              |
| 1:B1:97:LYS:HE3   | 1:B2:97:LYS:HZ3  | 1.67                     | 0.60              |
| 1:CW:20:ARG:HG3   | 1:CW:52:VAL:O    | 2.01                     | 0.60              |
| 1:CC:63:LYS:O     | 1:CC:67:ASN:HB2  | 2.01                     | 0.60              |
| 1:AC:6:HIS:HE1    | 1:AC:8:VAL:HB    | 1.66                     | 0.60              |
| 1:AL:148:LEU:HD13 | 1:AM:61:ILE:HD11 | 1.83                     | 0.60              |
| 1:AM:20:ARG:HG3   | 1:AM:52:VAL:O    | 2.02                     | 0.60              |
| 1:AR:20:ARG:HG3   | 1:AR:52:VAL:O    | 2.01                     | 0.60              |
| 1:BK:95:VAL:HG12  | 1:BK:112:PHE:HE1 | 1.67                     | 0.60              |
| 1:BR:100:ALA:HB2  | 1:BS:56:PHE:CZ   | 2.36                     | 0.60              |
| 1:BW:20:ARG:HG3   | 1:BW:52:VAL:O    | 2.01                     | 0.60              |
| 1:CA:95:VAL:HG12  | 1:CA:112:PHE:HE1 | 1.67                     | 0.60              |
| 1:AE:58:ILE:O     | 1:AE:58:ILE:CG2  | 2.50                     | 0.59              |
| 1:AG:97:LYS:HE3   | 1:AH:97:LYS:NZ   | 2.17                     | 0.59              |
| 1:AG:97:LYS:HE3   | 1:AH:97:LYS:HZ3  | 1.65                     | 0.59              |
| 1:AT:53:PRO:CD    | 1:AT:57:GLU:HG3  | 2.29                     | 0.59              |
| 1:BQ:97:LYS:HE3   | 1:BR:97:LYS:NZ   | 2.17                     | 0.59              |
| 1:BW:63:LYS:O     | 1:BW:67:ASN:HB2  | 2.01                     | 0.59              |
| 1:BY:152:TRP:HE3  | 1:BY:153:ALA:H   | 1.48                     | 0.59              |
| 1:B3:124:ILE:O    | 1:B3:129:THR:OG1 | 2.16                     | 0.59              |
| 1:CF:95:VAL:HG12  | 1:CF:112:PHE:HE1 | 1.67                     | 0.59              |
| 1:CG:148:LEU:HD13 | 1:CH:61:ILE:HD11 | 1.83                     | 0.59              |
| 1:CL:97:LYS:HE3   | 1:CM:97:LYS:HZ3  | 1.67                     | 0.59              |
| 1:CR:63:LYS:O     | 1:CR:67:ASN:HB2  | 2.01                     | 0.59              |
| 1:CZ:95:VAL:HG12  | 1:CZ:112:PHE:HE1 | 1.67                     | 0.59              |
| 1:AA:95:VAL:HG12  | 1:AA:112:PHE:HE1 | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AF:83:GLY:HA3  | 2:AF:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:AL:97:LYS:HE3  | 1:AM:97:LYS:NZ    | 2.17                     | 0.59              |
| 1:AO:58:ILE:O    | 1:AO:58:ILE:CG2   | 2.51                     | 0.59              |
| 1:AP:83:GLY:HA3  | 2:AP:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:AQ:97:LYS:HE3  | 1:AR:97:LYS:NZ    | 2.17                     | 0.59              |
| 1:AS:33:ALA:O    | 1:AS:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:AU:83:GLY:HA3  | 2:AU:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:AZ:83:GLY:HA3  | 2:AZ:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:A1:97:LYS:HE3  | 1:A2:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:BD:33:ALA:O    | 1:BD:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:BM:20:ARG:HG3  | 1:BM:52:VAL:O     | 2.02                     | 0.59              |
| 1:B2:20:ARG:HG3  | 1:B2:52:VAL:O     | 2.01                     | 0.59              |
| 1:CP:83:GLY:HA3  | 2:CP:201:PO4:O2   | 2.03                     | 0.59              |
| 1:CU:83:GLY:HA3  | 2:CU:201:PO4:O2   | 2.02                     | 0.59              |
| 1:CW:39:ARG:O    | 1:C2:7:LEU:HB3    | 2.02                     | 0.59              |
| 1:AB:97:LYS:HE3  | 1:AC:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:AB:107:ASP:CB  | 1:AB:152:TRP:CZ3  | 2.86                     | 0.59              |
| 1:AF:95:VAL:HG12 | 1:AF:112:PHE:HE1  | 1.67                     | 0.59              |
| 1:AN:33:ALA:O    | 1:AN:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:AO:152:TRP:HE3 | 1:AO:153:ALA:H    | 1.48                     | 0.59              |
| 1:AV:107:ASP:CB  | 1:AV:152:TRP:CZ3  | 2.86                     | 0.59              |
| 1:AY:152:TRP:HE3 | 1:AY:153:ALA:H    | 1.48                     | 0.59              |
| 1:BV:97:LYS:HE3  | 1:BW:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:BZ:83:GLY:HA3  | 2:BZ:1001:PO4:O2  | 2.02                     | 0.59              |
| 1:B1:6:HIS:HE1   | 1:B1:8:VAL:HB     | 1.68                     | 0.59              |
| 1:C1:97:LYS:HE3  | 1:C2:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:AI:33:ALA:O    | 1:AI:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:AL:6:HIS:HE1   | 1:AL:8:VAL:HB     | 1.68                     | 0.59              |
| 1:AL:107:ASP:CB  | 1:AL:152:TRP:CZ3  | 2.86                     | 0.59              |
| 1:AQ:107:ASP:CB  | 1:AQ:152:TRP:CZ3  | 2.86                     | 0.59              |
| 1:AU:148:LEU:O   | 1:AU:148:LEU:HD23 | 2.03                     | 0.59              |
| 1:AZ:148:LEU:O   | 1:AZ:148:LEU:HD23 | 2.03                     | 0.59              |
| 1:BK:148:LEU:O   | 1:BK:148:LEU:HD23 | 2.03                     | 0.59              |
| 1:BP:148:LEU:O   | 1:BP:148:LEU:HD23 | 2.03                     | 0.59              |
| 1:CA:83:GLY:HA3  | 2:CA:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:CH:20:ARG:HG3  | 1:CH:52:VAL:O     | 2.02                     | 0.59              |
| 1:CK:58:ILE:O    | 1:CK:58:ILE:CG2   | 2.50                     | 0.59              |
| 1:CN:33:ALA:O    | 1:CN:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:CV:97:LYS:HE3  | 1:CW:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:AG:107:ASP:CB  | 1:AG:152:TRP:CZ3  | 2.86                     | 0.59              |
| 1:AK:95:VAL:HG12 | 1:AK:112:PHE:HE1  | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:148:LEU:HD23 | 1:AK:148:LEU:O    | 2.03                     | 0.59              |
| 1:A2:20:ARG:HG3   | 1:A2:52:VAL:O     | 2.01                     | 0.59              |
| 1:BB:148:LEU:HD13 | 1:BC:61:ILE:HD11  | 1.83                     | 0.59              |
| 1:BG:97:LYS:HE3   | 1:BH:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:BG:107:ASP:HB2  | 1:BG:152:TRP:HZ3  | 1.62                     | 0.59              |
| 1:BP:83:GLY:HA3   | 2:BP:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:BX:33:ALA:O     | 1:BX:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:CA:148:LEU:O    | 1:CA:148:LEU:HD23 | 2.03                     | 0.59              |
| 1:CG:97:LYS:HE3   | 1:CH:97:LYS:HZ3   | 1.67                     | 0.59              |
| 1:CK:148:LEU:HD23 | 1:CK:148:LEU:O    | 2.03                     | 0.59              |
| 1:CM:20:ARG:HG3   | 1:CM:52:VAL:O     | 2.01                     | 0.59              |
| 1:CO:58:ILE:O     | 1:CO:58:ILE:CG2   | 2.51                     | 0.59              |
| 1:AC:20:ARG:HG3   | 1:AC:52:VAL:O     | 2.01                     | 0.59              |
| 1:AH:97:LYS:HG3   | 1:AI:97:LYS:HZ3   | 1.67                     | 0.59              |
| 1:AO:53:PRO:CD    | 1:AO:57:GLU:HG3   | 2.29                     | 0.59              |
| 1:AZ:95:VAL:HG12  | 1:AZ:112:PHE:HE1  | 1.67                     | 0.59              |
| 1:BJ:53:PRO:CD    | 1:BJ:57:GLU:HG3   | 2.29                     | 0.59              |
| 1:BU:83:GLY:HA3   | 2:BU:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:BU:148:LEU:HD23 | 1:BU:148:LEU:O    | 2.03                     | 0.59              |
| 1:B1:97:LYS:HE3   | 1:B2:97:LYS:NZ    | 2.17                     | 0.59              |
| 1:CD:33:ALA:O     | 1:CD:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:CR:6:HIS:HE1    | 1:CR:8:VAL:HB     | 1.66                     | 0.59              |
| 1:C1:97:LYS:HE3   | 1:C2:97:LYS:HZ3   | 1.67                     | 0.59              |
| 1:AA:58:ILE:O     | 1:AA:58:ILE:CG2   | 2.50                     | 0.59              |
| 1:AB:6:HIS:HE1    | 1:AB:8:VAL:HB     | 1.68                     | 0.59              |
| 1:AK:83:GLY:HA3   | 2:AK:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:AP:148:LEU:HD23 | 1:AP:148:LEU:O    | 2.03                     | 0.59              |
| 1:A1:107:ASP:CB   | 1:A1:152:TRP:CZ3  | 2.86                     | 0.59              |
| 1:BF:83:GLY:HA3   | 2:BF:1001:PO4:O2  | 2.03                     | 0.59              |
| 1:CB:6:HIS:HE1    | 1:CB:8:VAL:HB     | 1.68                     | 0.59              |
| 1:CL:148:LEU:HD13 | 1:CM:61:ILE:HD11  | 1.83                     | 0.59              |
| 1:AM:129:THR:O    | 1:AM:132:GLY:N    | 2.25                     | 0.59              |
| 1:AW:116:THR:O    | 1:AX:85:THR:HB    | 2.03                     | 0.59              |
| 1:AX:33:ALA:O     | 1:AX:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:BI:33:ALA:O     | 1:BI:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:BL:148:LEU:HD13 | 1:BM:61:ILE:HD11  | 1.83                     | 0.59              |
| 1:BR:129:THR:O    | 1:BR:132:GLY:N    | 2.25                     | 0.59              |
| 1:BY:58:ILE:O     | 1:BY:58:ILE:CG2   | 2.51                     | 0.59              |
| 1:B3:33:ALA:O     | 1:B3:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:CB:97:LYS:HE3   | 1:CC:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:CX:33:ALA:O     | 1:CX:37:LEU:HB2   | 2.03                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AQ:6:HIS:HE1    | 1:AQ:8:VAL:HB     | 1.68                     | 0.59              |
| 1:A1:97:LYS:HE3   | 1:A2:97:LYS:HZ3   | 1.68                     | 0.59              |
| 1:A3:33:ALA:O     | 1:A3:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:BH:116:THR:O    | 1:BI:85:THR:HB    | 2.03                     | 0.59              |
| 1:BP:95:VAL:HG12  | 1:BP:112:PHE:HE1  | 1.67                     | 0.59              |
| 1:BU:95:VAL:HG12  | 1:BU:112:PHE:HE1  | 1.67                     | 0.59              |
| 1:BV:6:HIS:HE1    | 1:BV:8:VAL:HB     | 1.68                     | 0.59              |
| 1:BZ:148:LEU:HD23 | 1:BZ:148:LEU:O    | 2.03                     | 0.59              |
| 1:B2:129:THR:O    | 1:B2:132:GLY:N    | 2.25                     | 0.59              |
| 1:CF:34:LEU:HD12  | 1:CF:38:LYS:HB2   | 1.83                     | 0.59              |
| 1:CH:116:THR:O    | 1:CI:85:THR:HB    | 2.03                     | 0.59              |
| 1:CK:83:GLY:HA3   | 2:CK:201:PO4:O2   | 2.03                     | 0.59              |
| 1:CQ:6:HIS:HE1    | 1:CQ:8:VAL:HB     | 1.68                     | 0.59              |
| 1:CQ:97:LYS:HE3   | 1:CR:97:LYS:NZ    | 2.18                     | 0.59              |
| 1:CZ:148:LEU:HD23 | 1:CZ:148:LEU:O    | 2.03                     | 0.59              |
| 1:BA:148:LEU:HD23 | 1:BA:148:LEU:O    | 2.03                     | 0.59              |
| 1:BF:148:LEU:O    | 1:BF:148:LEU:HD23 | 2.03                     | 0.59              |
| 1:BG:6:HIS:HE1    | 1:BG:8:VAL:HB     | 1.68                     | 0.59              |
| 1:BW:97:LYS:HG3   | 1:BX:97:LYS:HZ1   | 1.68                     | 0.59              |
| 1:BW:116:THR:O    | 1:BX:85:THR:HB    | 2.03                     | 0.59              |
| 1:B2:116:THR:O    | 1:B3:85:THR:HB    | 2.03                     | 0.59              |
| 1:CC:116:THR:O    | 1:CD:85:THR:HB    | 2.03                     | 0.59              |
| 1:CF:148:LEU:HD23 | 1:CF:148:LEU:O    | 2.03                     | 0.59              |
| 1:CL:6:HIS:HE1    | 1:CL:8:VAL:HB     | 1.68                     | 0.59              |
| 1:CU:34:LEU:HD12  | 1:CU:38:LYS:HB2   | 1.83                     | 0.59              |
| 1:C3:33:ALA:O     | 1:C3:37:LEU:HB2   | 2.03                     | 0.59              |
| 1:AH:116:THR:O    | 1:AI:85:THR:HB    | 2.03                     | 0.58              |
| 1:AI:124:ILE:O    | 1:AI:129:THR:OG1  | 2.16                     | 0.58              |
| 1:AM:116:THR:O    | 1:AN:85:THR:HB    | 2.03                     | 0.58              |
| 1:AU:95:VAL:HG12  | 1:AU:112:PHE:HE1  | 1.67                     | 0.58              |
| 1:BL:97:LYS:HE3   | 1:BM:97:LYS:NZ    | 2.17                     | 0.58              |
| 1:BM:116:THR:O    | 1:BN:85:THR:HB    | 2.03                     | 0.58              |
| 1:BN:33:ALA:O     | 1:BN:37:LEU:HB2   | 2.03                     | 0.58              |
| 1:CG:97:LYS:HE3   | 1:CH:97:LYS:NZ    | 2.18                     | 0.58              |
| 1:CP:148:LEU:O    | 1:CP:148:LEU:HD23 | 2.03                     | 0.58              |
| 1:CS:33:ALA:O     | 1:CS:37:LEU:HB2   | 2.02                     | 0.58              |
| 1:CV:6:HIS:HE1    | 1:CV:8:VAL:HB     | 1.68                     | 0.58              |
| 1:CY:58:ILE:O     | 1:CY:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:C2:116:THR:O    | 1:C3:85:THR:HB    | 2.03                     | 0.58              |
| 1:AD:33:ALA:O     | 1:AD:37:LEU:HB2   | 2.03                     | 0.58              |
| 1:AF:148:LEU:O    | 1:AF:148:LEU:HD23 | 2.03                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BD:39:ARG:O     | 1:BJ:7:LEU:HB3    | 2.02                     | 0.58              |
| 1:BF:95:VAL:HG12  | 1:BF:112:PHE:HE1  | 1.67                     | 0.58              |
| 1:BU:58:ILE:CG2   | 1:BU:58:ILE:O     | 2.50                     | 0.58              |
| 1:AE:53:PRO:CD    | 1:AE:57:GLU:HG3   | 2.29                     | 0.58              |
| 1:AV:97:LYS:HE3   | 1:AW:97:LYS:NZ    | 2.18                     | 0.58              |
| 1:A1:6:HIS:HE1    | 1:A1:8:VAL:HB     | 1.68                     | 0.58              |
| 1:BA:83:GLY:HA3   | 2:BA:1001:PO4:O2  | 2.03                     | 0.58              |
| 1:BB:97:LYS:HE3   | 1:BC:97:LYS:NZ    | 2.17                     | 0.58              |
| 1:BR:116:THR:O    | 1:BS:85:THR:HB    | 2.03                     | 0.58              |
| 1:CF:83:GLY:HA3   | 2:CF:201:PO4:O2   | 2.03                     | 0.58              |
| 1:CJ:53:PRO:CD    | 1:CJ:57:GLU:HG3   | 2.29                     | 0.58              |
| 1:CT:58:ILE:O     | 1:CT:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:AZ:58:ILE:O     | 1:AZ:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:A2:116:THR:O    | 1:A3:85:THR:HB    | 2.03                     | 0.58              |
| 1:BC:97:LYS:HG3   | 1:BD:97:LYS:HZ3   | 1.68                     | 0.58              |
| 1:BK:83:GLY:HA3   | 2:BK:1001:PO4:O2  | 2.03                     | 0.58              |
| 1:CI:33:ALA:O     | 1:CI:37:LEU:HB2   | 2.03                     | 0.58              |
| 1:CM:116:THR:O    | 1:CN:85:THR:HB    | 2.03                     | 0.58              |
| 1:CP:95:VAL:HG12  | 1:CP:112:PHE:HE1  | 1.67                     | 0.58              |
| 1:C1:6:HIS:HE1    | 1:C1:8:VAL:HB     | 1.68                     | 0.58              |
| 1:C3:124:ILE:O    | 1:C3:129:THR:OG1  | 2.16                     | 0.58              |
| 1:BQ:6:HIS:HE1    | 1:BQ:8:VAL:HB     | 1.68                     | 0.58              |
| 1:B4:58:ILE:O     | 1:B4:58:ILE:CG2   | 2.51                     | 0.58              |
| 1:CM:129:THR:O    | 1:CM:132:GLY:N    | 2.25                     | 0.58              |
| 1:CZ:83:GLY:HA3   | 2:CZ:201:PO4:O2   | 2.03                     | 0.58              |
| 1:A4:53:PRO:CD    | 1:A4:57:GLU:HG3   | 2.29                     | 0.58              |
| 1:BB:6:HIS:HE1    | 1:BB:8:VAL:HB     | 1.68                     | 0.58              |
| 1:BC:116:THR:O    | 1:BD:85:THR:HB    | 2.03                     | 0.58              |
| 1:BO:58:ILE:O     | 1:BO:58:ILE:CG2   | 2.51                     | 0.58              |
| 1:CB:97:LYS:HE3   | 1:CC:97:LYS:HZ3   | 1.68                     | 0.58              |
| 1:CC:129:THR:HG21 | 1:CS:120:ILE:HG12 | 1.85                     | 0.58              |
| 1:CE:58:ILE:O     | 1:CE:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:CE:65:MET:HE3   | 1:CE:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:CL:97:LYS:HE3   | 1:CM:97:LYS:NZ    | 2.17                     | 0.58              |
| 1:CU:95:VAL:HG12  | 1:CU:112:PHE:HE1  | 1.67                     | 0.58              |
| 1:C4:58:ILE:O     | 1:C4:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:AJ:58:ILE:O     | 1:AJ:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:AT:58:ILE:O     | 1:AT:58:ILE:CG2   | 2.51                     | 0.58              |
| 1:BJ:58:ILE:O     | 1:BJ:58:ILE:CG2   | 2.51                     | 0.58              |
| 1:BL:107:ASP:HB2  | 1:BL:152:TRP:HZ3  | 1.62                     | 0.58              |
| 1:CD:20:ARG:CZ    | 1:CR:39:ARG:CZ    | 2.81                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CG:6:HIS:HE1    | 1:CG:8:VAL:HB     | 1.68                     | 0.58              |
| 1:CG:107:ASP:HB2  | 1:CG:152:TRP:HZ3  | 1.62                     | 0.58              |
| 1:CL:107:ASP:HB2  | 1:CL:152:TRP:HZ3  | 1.62                     | 0.58              |
| 1:CU:148:LEU:O    | 1:CU:148:LEU:HD23 | 2.03                     | 0.58              |
| 1:CW:116:THR:O    | 1:CX:85:THR:HB    | 2.03                     | 0.58              |
| 1:AA:125:GLU:O    | 1:AA:131:ALA:HB3  | 2.04                     | 0.58              |
| 1:AF:58:ILE:O     | 1:AF:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:AF:125:GLU:O    | 1:AF:131:ALA:HB3  | 2.04                     | 0.58              |
| 1:BO:53:PRO:CD    | 1:BO:57:GLU:HG3   | 2.29                     | 0.58              |
| 1:BT:65:MET:HE3   | 1:BT:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:CJ:58:ILE:O     | 1:CJ:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:CL:121:GLU:O    | 1:CL:124:ILE:HG22 | 2.04                     | 0.58              |
| 1:CW:40:HIS:CE1   | 1:C2:7:LEU:HD23   | 2.39                     | 0.58              |
| 1:C4:65:MET:HE3   | 1:C4:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:AA:83:GLY:HA3   | 2:AA:1001:PO4:O2  | 2.03                     | 0.58              |
| 1:AA:148:LEU:O    | 1:AA:148:LEU:HD23 | 2.03                     | 0.58              |
| 1:AU:125:GLU:O    | 1:AU:131:ALA:HB3  | 2.04                     | 0.58              |
| 1:AY:58:ILE:O     | 1:AY:58:ILE:CG2   | 2.50                     | 0.58              |
| 1:BS:33:ALA:O     | 1:BS:37:LEU:HB2   | 2.03                     | 0.58              |
| 1:BT:53:PRO:HG2   | 1:BT:57:GLU:HG3   | 0.65                     | 0.58              |
| 1:BZ:125:GLU:O    | 1:BZ:131:ALA:HB3  | 2.04                     | 0.58              |
| 1:CF:28:LYS:HZ1   | 1:CR:28:LYS:HZ3   | 1.52                     | 0.58              |
| 1:CJ:65:MET:HE3   | 1:CJ:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:CO:65:MET:HE3   | 1:CO:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:AC:116:THR:O    | 1:AD:85:THR:HB    | 2.03                     | 0.58              |
| 1:AR:116:THR:O    | 1:AS:85:THR:HB    | 2.03                     | 0.58              |
| 1:AY:65:MET:HE3   | 1:AY:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:A1:121:GLU:O    | 1:A1:124:ILE:HG22 | 2.04                     | 0.58              |
| 1:BE:65:MET:HE3   | 1:BE:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:BG:121:GLU:O    | 1:BG:124:ILE:HG22 | 2.04                     | 0.58              |
| 1:BO:65:MET:HE3   | 1:BO:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:BQ:121:GLU:O    | 1:BQ:124:ILE:HG22 | 2.04                     | 0.58              |
| 1:BY:65:MET:HE3   | 1:BY:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:B1:121:GLU:O    | 1:B1:124:ILE:HG22 | 2.04                     | 0.58              |
| 1:CA:125:GLU:O    | 1:CA:131:ALA:HB3  | 2.04                     | 0.58              |
| 1:CP:125:GLU:O    | 1:CP:131:ALA:HB3  | 2.04                     | 0.58              |
| 1:CT:53:PRO:CD    | 1:CT:57:GLU:HG3   | 2.29                     | 0.58              |
| 1:CT:65:MET:HE3   | 1:CT:71:TYR:CZ    | 2.39                     | 0.58              |
| 1:CU:102:LEU:HD22 | 1:CY:104:LEU:HD13 | 1.86                     | 0.58              |
| 1:CU:125:GLU:O    | 1:CU:131:ALA:HB3  | 2.04                     | 0.58              |
| 1:AG:121:GLU:O    | 1:AG:124:ILE:HG22 | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:125:GLU:O    | 1:AK:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:AV:6:HIS:HE1    | 1:AV:8:VAL:HB     | 1.68                     | 0.57              |
| 1:AZ:125:GLU:O    | 1:AZ:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:BA:102:LEU:HD22 | 1:BE:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:BH:97:LYS:HG3   | 1:BI:97:LYS:HZ3   | 1.68                     | 0.57              |
| 1:BU:125:GLU:O    | 1:BU:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:CF:125:GLU:O    | 1:CF:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:CK:125:GLU:O    | 1:CK:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:CP:58:ILE:CG2   | 1:CP:58:ILE:O     | 2.50                     | 0.57              |
| 1:CQ:107:ASP:HB2  | 1:CQ:152:TRP:HZ3  | 1.62                     | 0.57              |
| 1:CY:65:MET:HE3   | 1:CY:71:TYR:CZ    | 2.39                     | 0.57              |
| 1:AG:6:HIS:HE1    | 1:AG:8:VAL:HB     | 1.68                     | 0.57              |
| 1:AJ:65:MET:HE3   | 1:AJ:71:TYR:CZ    | 2.39                     | 0.57              |
| 1:BJ:65:MET:HE3   | 1:BJ:71:TYR:CZ    | 2.39                     | 0.57              |
| 1:BS:7:LEU:HB3    | 1:BY:39:ARG:O     | 2.04                     | 0.57              |
| 1:CP:28:LYS:HZ1   | 1:CW:28:LYS:HZ3   | 1.52                     | 0.57              |
| 1:C4:53:PRO:HG2   | 1:C4:57:GLU:HG3   | 0.65                     | 0.57              |
| 1:AF:102:LEU:HD22 | 1:AJ:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:A4:58:ILE:O     | 1:A4:58:ILE:CG2   | 2.50                     | 0.57              |
| 1:BF:125:GLU:O    | 1:BF:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:BK:125:GLU:O    | 1:BK:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:BL:6:HIS:HE1    | 1:BL:8:VAL:HB     | 1.68                     | 0.57              |
| 1:BZ:102:LEU:HD22 | 1:B4:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:CP:102:LEU:HD22 | 1:CT:104:LEU:HD13 | 1.87                     | 0.57              |
| 1:CR:116:THR:O    | 1:CS:85:THR:HB    | 2.03                     | 0.57              |
| 1:AE:65:MET:HE3   | 1:AE:71:TYR:CZ    | 2.39                     | 0.57              |
| 1:AF:73:ALA:HB2   | 1:AF:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:AI:48:ASP:HB2   | 1:AI:71:TYR:HE1   | 1.70                     | 0.57              |
| 1:CB:121:GLU:O    | 1:CB:124:ILE:HG22 | 2.04                     | 0.57              |
| 1:CK:102:LEU:HD22 | 1:CO:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:CQ:121:GLU:O    | 1:CQ:124:ILE:HG22 | 2.04                     | 0.57              |
| 1:CZ:102:LEU:HD22 | 1:C4:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:AC:24:PHE:CE1   | 1:AU:28:LYS:HD2   | 2.40                     | 0.57              |
| 1:AP:73:ALA:HB2   | 1:AP:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:BB:121:GLU:O    | 1:BB:124:ILE:HG22 | 2.04                     | 0.57              |
| 1:BK:58:ILE:O     | 1:BK:58:ILE:CG2   | 2.50                     | 0.57              |
| 1:BP:102:LEU:HD22 | 1:BT:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:CD:48:ASP:HB2   | 1:CD:71:TYR:HE1   | 1.70                     | 0.57              |
| 1:CD:63:LYS:O     | 1:CD:67:ASN:HB2   | 2.05                     | 0.57              |
| 1:CG:121:GLU:O    | 1:CG:124:ILE:HG22 | 2.04                     | 0.57              |
| 1:CV:121:GLU:O    | 1:CV:124:ILE:HG22 | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:102:LEU:HD22 | 1:AE:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:AN:63:LYS:O     | 1:AN:67:ASN:HB2   | 2.05                     | 0.57              |
| 1:AO:65:MET:HE3   | 1:AO:71:TYR:CZ    | 2.39                     | 0.57              |
| 1:AP:125:GLU:O    | 1:AP:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:BT:58:ILE:O     | 1:BT:58:ILE:CG2   | 2.50                     | 0.57              |
| 1:CA:102:LEU:HD22 | 1:CE:104:LEU:HD13 | 1.87                     | 0.57              |
| 1:CP:73:ALA:HB2   | 1:CP:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:CW:58:ILE:N     | 1:CW:59:PRO:HD2   | 2.20                     | 0.57              |
| 1:CZ:125:GLU:O    | 1:CZ:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:AU:102:LEU:HD22 | 1:AY:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:BA:125:GLU:O    | 1:BA:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:BL:121:GLU:O    | 1:BL:124:ILE:HG22 | 2.04                     | 0.57              |
| 1:BM:58:ILE:N     | 1:BM:59:PRO:HD2   | 2.20                     | 0.57              |
| 1:BR:58:ILE:N     | 1:BR:59:PRO:HD2   | 2.20                     | 0.57              |
| 1:BU:73:ALA:HB2   | 1:BU:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:BW:129:THR:O    | 1:BW:132:GLY:N    | 2.25                     | 0.57              |
| 1:CA:73:ALA:HB2   | 1:CA:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:CC:8:VAL:HG21   | 1:CR:8:VAL:HG13   | 1.86                     | 0.57              |
| 1:CS:48:ASP:HB2   | 1:CS:71:TYR:HE1   | 1.70                     | 0.57              |
| 1:CU:73:ALA:HB2   | 1:CU:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:CY:53:PRO:HG2   | 1:CY:57:GLU:HG3   | 0.65                     | 0.57              |
| 1:CZ:73:ALA:HB2   | 1:CZ:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:C4:53:PRO:CD    | 1:C4:57:GLU:HG3   | 2.29                     | 0.57              |
| 1:AV:121:GLU:O    | 1:AV:124:ILE:HG22 | 2.04                     | 0.57              |
| 1:A2:58:ILE:N     | 1:A2:59:PRO:HD2   | 2.20                     | 0.57              |
| 1:A4:65:MET:HE3   | 1:A4:71:TYR:CZ    | 2.39                     | 0.57              |
| 1:BG:97:LYS:HE3   | 1:BH:97:LYS:HZ3   | 1.69                     | 0.57              |
| 1:BH:58:ILE:N     | 1:BH:59:PRO:HD2   | 2.20                     | 0.57              |
| 1:BI:63:LYS:O     | 1:BI:67:ASN:HB2   | 2.05                     | 0.57              |
| 1:BP:125:GLU:O    | 1:BP:131:ALA:HB3  | 2.04                     | 0.57              |
| 1:BV:97:LYS:HE3   | 1:BW:97:LYS:HZ3   | 1.69                     | 0.57              |
| 1:CF:102:LEU:HD22 | 1:CJ:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:CN:48:ASP:HB2   | 1:CN:71:TYR:HE1   | 1.70                     | 0.57              |
| 1:CX:63:LYS:O     | 1:CX:67:ASN:HB2   | 2.05                     | 0.57              |
| 1:C2:129:THR:O    | 1:C2:132:GLY:N    | 2.25                     | 0.57              |
| 1:AJ:53:PRO:CD    | 1:AJ:57:GLU:HG3   | 2.29                     | 0.57              |
| 1:AK:58:ILE:O     | 1:AK:58:ILE:CG2   | 2.50                     | 0.57              |
| 1:AK:73:ALA:HB2   | 1:AK:146:ALA:HB2  | 1.87                     | 0.57              |
| 1:AM:58:ILE:N     | 1:AM:59:PRO:HD2   | 2.20                     | 0.57              |
| 1:AP:102:LEU:HD22 | 1:AT:104:LEU:HD13 | 1.86                     | 0.57              |
| 1:AX:63:LYS:O     | 1:AX:67:ASN:HB2   | 2.05                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BE:58:ILE:O    | 1:BE:58:ILE:CG2   | 2.50                     | 0.57              |
| 1:BF:39:ARG:O    | 1:BQ:7:LEU:HB3    | 2.04                     | 0.57              |
| 1:BM:37:LEU:HD12 | 1:BM:47:ILE:HD13  | 1.87                     | 0.57              |
| 1:BN:48:ASP:HB2  | 1:BN:71:TYR:HE1   | 1.70                     | 0.57              |
| 1:BS:63:LYS:O    | 1:BS:67:ASN:HB2   | 2.05                     | 0.57              |
| 1:B3:63:LYS:O    | 1:B3:67:ASN:HB2   | 2.05                     | 0.57              |
| 1:CF:58:ILE:O    | 1:CF:58:ILE:CG2   | 2.50                     | 0.57              |
| 1:CX:7:LEU:HD11  | 1:CX:140:VAL:HG22 | 1.87                     | 0.57              |
| 1:BC:58:ILE:N    | 1:BC:59:PRO:HD2   | 2.20                     | 0.57              |
| 1:BR:6:HIS:CE1   | 1:BR:8:VAL:HB     | 2.40                     | 0.57              |
| 1:BX:48:ASP:HB2  | 1:BX:71:TYR:HE1   | 1.70                     | 0.57              |
| 1:CC:8:VAL:HG13  | 1:CR:8:VAL:CG2    | 2.34                     | 0.57              |
| 1:CK:152:TRP:CD1 | 1:CK:153:ALA:H    | 2.23                     | 0.57              |
| 1:CS:63:LYS:O    | 1:CS:67:ASN:HB2   | 2.05                     | 0.57              |
| 1:AB:121:GLU:O   | 1:AB:124:ILE:HG22 | 2.04                     | 0.56              |
| 1:AC:58:ILE:N    | 1:AC:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:AL:121:GLU:O   | 1:AL:124:ILE:HG22 | 2.04                     | 0.56              |
| 1:AM:37:LEU:HD12 | 1:AM:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:AP:82:ARG:HG3  | 1:AP:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:AQ:121:GLU:O   | 1:AQ:124:ILE:HG22 | 2.04                     | 0.56              |
| 1:AR:58:ILE:N    | 1:AR:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:AS:124:ILE:O   | 1:AS:129:THR:OG1  | 2.16                     | 0.56              |
| 1:AZ:152:TRP:CD1 | 1:AZ:153:ALA:H    | 2.23                     | 0.56              |
| 1:BF:58:ILE:CG2  | 1:BF:58:ILE:O     | 2.50                     | 0.56              |
| 1:BF:73:ALA:HB2  | 1:BF:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:BF:152:TRP:CD1 | 1:BF:153:ALA:H    | 2.23                     | 0.56              |
| 1:BK:73:ALA:HB2  | 1:BK:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:BP:73:ALA:HB2  | 1:BP:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:BW:6:HIS:CE1   | 1:BW:8:VAL:HB     | 2.40                     | 0.56              |
| 1:B4:53:PRO:HG2  | 1:B4:57:GLU:HG3   | 0.65                     | 0.56              |
| 1:B4:65:MET:HE3  | 1:B4:71:TYR:CZ    | 2.39                     | 0.56              |
| 1:CA:58:ILE:O    | 1:CA:58:ILE:CG2   | 2.50                     | 0.56              |
| 1:CC:37:LEU:HD12 | 1:CC:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:CK:73:ALA:HB2  | 1:CK:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:CT:52:VAL:CB   | 1:CT:53:PRO:HD2   | 2.34                     | 0.56              |
| 1:CU:152:TRP:CD1 | 1:CU:153:ALA:H    | 2.23                     | 0.56              |
| 1:AD:48:ASP:HB2  | 1:AD:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:BB:144:GLU:CD  | 1:BU:39:ARG:NH2   | 2.61                     | 0.56              |
| 1:BC:6:HIS:CE1   | 1:BC:8:VAL:HB     | 2.41                     | 0.56              |
| 1:BC:37:LEU:HD12 | 1:BC:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:BQ:107:ASP:HB2 | 1:BQ:152:TRP:HZ3  | 1.62                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BS:48:ASP:HB2   | 1:BS:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:BU:102:LEU:HD22 | 1:BY:104:LEU:HD13 | 1.86                     | 0.56              |
| 1:BW:58:ILE:N     | 1:BW:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:BZ:73:ALA:HB2   | 1:BZ:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:BZ:82:ARG:HG3   | 1:BZ:118:GLU:OE2  | 2.05                     | 0.56              |
| 1:B2:58:ILE:N     | 1:B2:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:CA:82:ARG:HG3   | 1:CA:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:CF:82:ARG:HG3   | 1:CF:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:CF:152:TRP:CD1  | 1:CF:153:ALA:H    | 2.23                     | 0.56              |
| 1:CH:6:HIS:CE1    | 1:CH:8:VAL:HB     | 2.40                     | 0.56              |
| 1:CP:152:TRP:CD1  | 1:CP:153:ALA:H    | 2.23                     | 0.56              |
| 1:AA:73:ALA:HB2   | 1:AA:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:AA:82:ARG:HG3   | 1:AA:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:AH:58:ILE:N     | 1:AH:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:AK:82:ARG:HG3   | 1:AK:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:AN:7:LEU:HD11   | 1:AN:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:AR:37:LEU:HD12  | 1:AR:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:AS:48:ASP:HB2   | 1:AS:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:AT:65:MET:HE3   | 1:AT:71:TYR:CZ    | 2.39                     | 0.56              |
| 1:AU:100:ALA:HB2  | 1:AV:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:AW:6:HIS:CE1    | 1:AW:8:VAL:HB     | 2.41                     | 0.56              |
| 1:AX:48:ASP:HB2   | 1:AX:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:AY:53:PRO:CG    | 1:AY:57:GLU:CG    | 2.46                     | 0.56              |
| 1:BA:82:ARG:HG3   | 1:BA:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:BD:48:ASP:HB2   | 1:BD:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:BE:83:GLY:HA3   | 2:BE:1001:PO4:P   | 2.46                     | 0.56              |
| 1:BK:100:ALA:HB2  | 1:BL:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:BP:152:TRP:CD1  | 1:BP:153:ALA:H    | 2.23                     | 0.56              |
| 1:CC:58:ILE:N     | 1:CC:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:CE:83:GLY:HA3   | 2:CE:1001:PO4:P   | 2.46                     | 0.56              |
| 1:CG:144:GLU:CD   | 1:CU:39:ARG:NH2   | 2.63                     | 0.56              |
| 1:CH:58:ILE:N     | 1:CH:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:CI:48:ASP:HB2   | 1:CI:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:CM:58:ILE:N     | 1:CM:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:CM:97:LYS:HG3   | 1:CN:97:LYS:HZ1   | 1.68                     | 0.56              |
| 1:CZ:82:ARG:HG3   | 1:CZ:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:C2:6:HIS:CE1    | 1:C2:8:VAL:HB     | 2.41                     | 0.56              |
| 1:C2:58:ILE:N     | 1:C2:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:C3:48:ASP:HB2   | 1:C3:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:AE:53:PRO:HG2   | 1:AE:57:GLU:HG3   | 0.65                     | 0.56              |
| 1:AU:82:ARG:HG3   | 1:AU:118:GLU:OE2  | 2.05                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AU:152:TRP:CD1 | 1:AU:153:ALA:H    | 2.23                     | 0.56              |
| 1:AZ:100:ALA:HB2 | 1:A1:56:PHE:CZ    | 2.40                     | 0.56              |
| 1:A3:63:LYS:O    | 1:A3:67:ASN:HB2   | 2.05                     | 0.56              |
| 1:BI:48:ASP:HB2  | 1:BI:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:BN:7:LEU:HD11  | 1:BN:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:BU:152:TRP:CD1 | 1:BU:153:ALA:H    | 2.23                     | 0.56              |
| 1:BV:121:GLU:O   | 1:BV:124:ILE:HG22 | 2.04                     | 0.56              |
| 1:CG:96:ALA:O    | 1:CG:100:ALA:HB2  | 2.06                     | 0.56              |
| 1:CM:6:HIS:CE1   | 1:CM:8:VAL:HB     | 2.40                     | 0.56              |
| 1:CU:100:ALA:HB2 | 1:CV:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:CW:37:LEU:HD12 | 1:CW:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:CX:48:ASP:HB2  | 1:CX:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:CZ:100:ALA:HB2 | 1:C1:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:AB:144:GLU:CD  | 1:AU:39:ARG:HH22  | 2.13                     | 0.56              |
| 1:AE:83:GLY:HA3  | 2:AE:1001:PO4:P   | 2.46                     | 0.56              |
| 1:AS:63:LYS:O    | 1:AS:67:ASN:HB2   | 2.05                     | 0.56              |
| 1:AV:96:ALA:O    | 1:AV:100:ALA:HB2  | 2.06                     | 0.56              |
| 1:BC:39:ARG:O    | 1:BR:7:LEU:HB3    | 2.06                     | 0.56              |
| 1:BJ:53:PRO:HG2  | 1:BJ:57:GLU:HG3   | 0.65                     | 0.56              |
| 1:BJ:83:GLY:HA3  | 2:BJ:1001:PO4:P   | 2.46                     | 0.56              |
| 1:BM:6:HIS:CE1   | 1:BM:8:VAL:HB     | 2.40                     | 0.56              |
| 1:BN:63:LYS:O    | 1:BN:67:ASN:HB2   | 2.05                     | 0.56              |
| 1:CI:63:LYS:O    | 1:CI:67:ASN:HB2   | 2.05                     | 0.56              |
| 1:CJ:53:PRO:CG   | 1:CJ:57:GLU:CG    | 2.46                     | 0.56              |
| 1:CS:7:LEU:HD11  | 1:CS:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:CS:124:ILE:O   | 1:CS:129:THR:OG1  | 2.16                     | 0.56              |
| 1:AD:63:LYS:O    | 1:AD:67:ASN:HB2   | 2.05                     | 0.56              |
| 1:AF:100:ALA:HB2 | 1:AG:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:AH:6:HIS:CE1   | 1:AH:8:VAL:HB     | 2.41                     | 0.56              |
| 1:AK:100:ALA:HB2 | 1:AL:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:AQ:70:LYS:HE3  | 1:BU:43:GLU:OE2   | 2.05                     | 0.56              |
| 1:AU:73:ALA:HB2  | 1:AU:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:AV:97:LYS:HE3  | 1:AW:97:LYS:HZ3   | 1.70                     | 0.56              |
| 1:AX:7:LEU:HD11  | 1:AX:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:AZ:73:ALA:HB2  | 1:AZ:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:A3:7:LEU:HD11  | 1:A3:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:A3:48:ASP:HB2  | 1:A3:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:BK:82:ARG:HG3  | 1:BK:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:BU:100:ALA:HB2 | 1:BV:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:CA:100:ALA:HB2 | 1:CB:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:CA:152:TRP:CD1 | 1:CA:153:ALA:H    | 2.23                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CP:100:ALA:HB2  | 1:CQ:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:CY:83:GLY:HA3   | 2:CY:4201:PO4:P   | 2.46                     | 0.56              |
| 1:C1:121:GLU:O    | 1:C1:124:ILE:HG22 | 2.04                     | 0.56              |
| 1:AA:152:TRP:CD1  | 1:AA:153:ALA:H    | 2.23                     | 0.56              |
| 1:AO:83:GLY:HA3   | 2:AO:1001:PO4:P   | 2.46                     | 0.56              |
| 1:AY:83:GLY:HA3   | 2:AY:1001:PO4:P   | 2.46                     | 0.56              |
| 1:BH:37:LEU:HD12  | 1:BH:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:BM:129:THR:O    | 1:BM:132:GLY:N    | 2.25                     | 0.56              |
| 1:CU:58:ILE:O     | 1:CU:58:ILE:CG2   | 2.50                     | 0.56              |
| 1:CZ:152:TRP:CD1  | 1:CZ:153:ALA:H    | 2.23                     | 0.56              |
| 1:C3:7:LEU:HD11   | 1:C3:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:C3:63:LYS:O     | 1:C3:67:ASN:HB2   | 2.05                     | 0.56              |
| 1:C4:83:GLY:HA3   | 2:C4:4201:PO4:P   | 2.46                     | 0.56              |
| 1:AA:100:ALA:HB2  | 1:AB:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:AD:7:LEU:HD11   | 1:AD:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:AI:7:LEU:HD11   | 1:AI:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:AI:63:LYS:O     | 1:AI:67:ASN:HB2   | 2.05                     | 0.56              |
| 1:AJ:53:PRO:HG2   | 1:AJ:57:GLU:HG3   | 0.65                     | 0.56              |
| 1:AK:102:LEU:HD22 | 1:AO:104:LEU:HD13 | 1.86                     | 0.56              |
| 1:AK:152:TRP:CD1  | 1:AK:153:ALA:H    | 2.23                     | 0.56              |
| 1:BI:7:LEU:HD11   | 1:BI:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:BO:83:GLY:HA3   | 2:BO:1001:PO4:P   | 2.46                     | 0.56              |
| 1:CJ:52:VAL:CB    | 1:CJ:53:PRO:HD2   | 2.34                     | 0.56              |
| 1:CO:83:GLY:HA3   | 2:CO:4201:PO4:P   | 2.46                     | 0.56              |
| 1:CR:6:HIS:CE1    | 1:CR:8:VAL:HB     | 2.40                     | 0.56              |
| 1:CR:58:ILE:N     | 1:CR:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:CW:6:HIS:CE1    | 1:CW:8:VAL:HB     | 2.41                     | 0.56              |
| 1:C2:37:LEU:HD12  | 1:C2:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:AF:82:ARG:HG3   | 1:AF:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:AF:152:TRP:CD1  | 1:AF:153:ALA:H    | 2.23                     | 0.56              |
| 1:AU:58:ILE:CG2   | 1:AU:58:ILE:O     | 2.50                     | 0.56              |
| 1:A3:95:VAL:HG12  | 1:A3:112:PHE:HE1  | 1.71                     | 0.56              |
| 1:BF:102:LEU:HD22 | 1:BJ:104:LEU:HD13 | 1.86                     | 0.56              |
| 1:BK:152:TRP:CD1  | 1:BK:153:ALA:H    | 2.23                     | 0.56              |
| 1:BP:58:ILE:O     | 1:BP:58:ILE:CG2   | 2.50                     | 0.56              |
| 1:BY:83:GLY:HA3   | 2:BY:1001:PO4:P   | 2.46                     | 0.56              |
| 1:BZ:100:ALA:HB2  | 1:B1:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:B2:37:LEU:HD12  | 1:B2:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:B3:48:ASP:HB2   | 1:B3:71:TYR:HE1   | 1.70                     | 0.56              |
| 1:CK:82:ARG:HG3   | 1:CK:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:CV:96:ALA:O     | 1:CV:100:ALA:HB2  | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AD:151:HIS:HB2  | 1:AE:64:LYS:HB3   | 1.88                     | 0.56              |
| 1:AJ:53:PRO:CG    | 1:AJ:57:GLU:CG    | 2.46                     | 0.56              |
| 1:AO:107:ASP:O    | 1:AO:107:ASP:OD1  | 2.24                     | 0.56              |
| 1:AP:100:ALA:HB2  | 1:AQ:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:AW:58:ILE:N     | 1:AW:59:PRO:HD2   | 2.20                     | 0.56              |
| 1:AZ:102:LEU:HD22 | 1:A4:104:LEU:HD13 | 1.87                     | 0.56              |
| 1:BA:73:ALA:HB2   | 1:BA:146:ALA:HB2  | 1.87                     | 0.56              |
| 1:BA:100:ALA:HB2  | 1:BB:56:PHE:CZ    | 2.41                     | 0.56              |
| 1:BD:151:HIS:HB2  | 1:BE:64:LYS:HB3   | 1.88                     | 0.56              |
| 1:BJ:52:VAL:CB    | 1:BJ:53:PRO:HD2   | 2.34                     | 0.56              |
| 1:B2:6:HIS:CE1    | 1:B2:8:VAL:HB     | 2.41                     | 0.56              |
| 1:CD:7:LEU:HD11   | 1:CD:140:VAL:HG22 | 1.87                     | 0.56              |
| 1:CJ:83:GLY:HA3   | 2:CJ:4201:PO4:P   | 2.46                     | 0.56              |
| 1:CP:82:ARG:HG3   | 1:CP:118:GLU:OE2  | 2.06                     | 0.56              |
| 1:CR:37:LEU:HD12  | 1:CR:47:ILE:HD13  | 1.87                     | 0.56              |
| 1:CS:151:HIS:HB2  | 1:CT:64:LYS:HB3   | 1.88                     | 0.56              |
| 1:AE:53:PRO:CG    | 1:AE:57:GLU:CG    | 2.46                     | 0.55              |
| 1:AI:151:HIS:HB2  | 1:AJ:64:LYS:HB3   | 1.88                     | 0.55              |
| 1:AN:48:ASP:HB2   | 1:AN:71:TYR:HE1   | 1.70                     | 0.55              |
| 1:AS:151:HIS:HB2  | 1:AT:64:LYS:HB3   | 1.89                     | 0.55              |
| 1:AV:95:VAL:HG12  | 1:AV:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:A4:83:GLY:HA3   | 2:A4:1001:PO4:P   | 2.46                     | 0.55              |
| 1:BD:63:LYS:O     | 1:BD:67:ASN:HB2   | 2.05                     | 0.55              |
| 1:BF:85:THR:HB    | 1:BJ:116:THR:O    | 2.07                     | 0.55              |
| 1:BF:100:ALA:HB2  | 1:BG:56:PHE:CZ    | 2.40                     | 0.55              |
| 1:BH:65:MET:HE3   | 1:BH:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:BW:65:MET:HE3   | 1:BW:71:TYR:CE1   | 2.41                     | 0.55              |
| 1:BX:124:ILE:O    | 1:BX:129:THR:OG1  | 2.16                     | 0.55              |
| 1:CH:37:LEU:HD12  | 1:CH:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:CK:100:ALA:HB2  | 1:CL:56:PHE:CZ    | 2.41                     | 0.55              |
| 1:CM:37:LEU:HD12  | 1:CM:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:CT:107:ASP:O    | 1:CT:107:ASP:OD1  | 2.24                     | 0.55              |
| 1:CU:82:ARG:HG3   | 1:CU:118:GLU:OE2  | 2.06                     | 0.55              |
| 1:CY:53:PRO:CG    | 1:CY:57:GLU:CG    | 2.46                     | 0.55              |
| 1:CZ:58:ILE:O     | 1:CZ:58:ILE:CG2   | 2.50                     | 0.55              |
| 1:C4:107:ASP:O    | 1:C4:107:ASP:OD1  | 2.24                     | 0.55              |
| 1:AK:85:THR:HB    | 1:AO:116:THR:O    | 2.07                     | 0.55              |
| 1:AR:129:THR:O    | 1:AR:132:GLY:N    | 2.25                     | 0.55              |
| 1:A2:65:MET:HE3   | 1:A2:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:BA:58:ILE:O     | 1:BA:58:ILE:CG2   | 2.50                     | 0.55              |
| 1:BA:85:THR:HB    | 1:BE:116:THR:O    | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BB:95:VAL:HG12  | 1:BB:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:BF:82:ARG:HG3   | 1:BF:118:GLU:OE2  | 2.06                     | 0.55              |
| 1:BK:102:LEU:HD22 | 1:BO:104:LEU:HD13 | 1.86                     | 0.55              |
| 1:BP:82:ARG:HG3   | 1:BP:118:GLU:OE2  | 2.05                     | 0.55              |
| 1:BR:65:MET:HE3   | 1:BR:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:BS:7:LEU:HD11   | 1:BS:140:VAL:HG22 | 1.87                     | 0.55              |
| 1:BW:37:LEU:HD12  | 1:BW:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:CB:96:ALA:O     | 1:CB:100:ALA:HB2  | 2.06                     | 0.55              |
| 1:CF:39:ARG:NH2   | 1:CQ:144:GLU:CD   | 2.63                     | 0.55              |
| 1:CF:73:ALA:HB2   | 1:CF:146:ALA:HB2  | 1.87                     | 0.55              |
| 1:CF:85:THR:HB    | 1:CJ:116:THR:O    | 2.07                     | 0.55              |
| 1:CN:124:ILE:O    | 1:CN:129:THR:OG1  | 2.16                     | 0.55              |
| 1:CT:83:GLY:HA3   | 2:CT:4201:PO4:P   | 2.46                     | 0.55              |
| 1:AE:107:ASP:C    | 1:AE:107:ASP:OD1  | 2.50                     | 0.55              |
| 1:AM:6:HIS:CE1    | 1:AM:8:VAL:HB     | 2.41                     | 0.55              |
| 1:AM:65:MET:HE3   | 1:AM:71:TYR:CE1   | 2.41                     | 0.55              |
| 1:AP:85:THR:HB    | 1:AT:116:THR:O    | 2.07                     | 0.55              |
| 1:AR:6:HIS:CE1    | 1:AR:8:VAL:HB     | 2.40                     | 0.55              |
| 1:AX:151:HIS:HB2  | 1:AY:64:LYS:HB3   | 1.88                     | 0.55              |
| 1:AZ:85:THR:HB    | 1:A4:116:THR:O    | 2.07                     | 0.55              |
| 1:A2:6:HIS:CE1    | 1:A2:8:VAL:HB     | 2.40                     | 0.55              |
| 1:A4:71:TYR:C     | 1:A4:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:BE:107:ASP:O    | 1:BE:107:ASP:OD1  | 2.24                     | 0.55              |
| 1:BN:151:HIS:HB2  | 1:BO:64:LYS:HB3   | 1.88                     | 0.55              |
| 1:BU:85:THR:HB    | 1:BY:116:THR:O    | 2.07                     | 0.55              |
| 1:BY:71:TYR:C     | 1:BY:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:BZ:152:TRP:CD1  | 1:BZ:153:ALA:H    | 2.23                     | 0.55              |
| 1:B4:71:TYR:C     | 1:B4:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:CC:6:HIS:CE1    | 1:CC:8:VAL:HB     | 2.41                     | 0.55              |
| 1:CF:100:ALA:HB2  | 1:CG:56:PHE:CZ    | 2.41                     | 0.55              |
| 1:CH:152:TRP:HD1  | 1:CI:68:SER:HB2   | 1.72                     | 0.55              |
| 1:CQ:100:ALA:HA   | 1:CR:56:PHE:CZ    | 2.42                     | 0.55              |
| 1:CV:95:VAL:HG12  | 1:CV:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:CV:97:LYS:O     | 1:CV:102:LEU:HB2  | 2.07                     | 0.55              |
| 1:C2:65:MET:HE3   | 1:C2:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:AC:6:HIS:CE1    | 1:AC:8:VAL:HB     | 2.40                     | 0.55              |
| 1:AC:152:TRP:HD1  | 1:AD:68:SER:HB2   | 1.72                     | 0.55              |
| 1:AQ:100:ALA:HA   | 1:AR:56:PHE:CZ    | 2.42                     | 0.55              |
| 1:AZ:3:PHE:CD2    | 1:AZ:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:BJ:71:TYR:C     | 1:BJ:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:BM:65:MET:HE3   | 1:BM:71:TYR:CE1   | 2.42                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BR:37:LEU:HD12 | 1:BR:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:BV:96:ALA:O    | 1:BV:100:ALA:HB2  | 2.06                     | 0.55              |
| 1:BV:97:LYS:O    | 1:BV:102:LEU:HB2  | 2.07                     | 0.55              |
| 1:BX:63:LYS:O    | 1:BX:67:ASN:HB2   | 2.05                     | 0.55              |
| 1:B3:95:VAL:HG12 | 1:B3:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:CF:3:PHE:CD2   | 1:CF:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:CI:7:LEU:HD11  | 1:CI:140:VAL:HG22 | 1.87                     | 0.55              |
| 1:CK:3:PHE:CD2   | 1:CK:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:CO:53:PRO:HG2  | 1:CO:57:GLU:HG3   | 0.65                     | 0.55              |
| 1:CR:152:TRP:HD1 | 1:CS:68:SER:HB2   | 1.72                     | 0.55              |
| 1:CU:3:PHE:CD2   | 1:CU:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:CV:107:ASP:HB2 | 1:CV:152:TRP:HZ3  | 1.62                     | 0.55              |
| 1:CY:107:ASP:O   | 1:CY:107:ASP:OD1  | 2.24                     | 0.55              |
| 1:CZ:85:THR:HB   | 1:C4:116:THR:O    | 2.07                     | 0.55              |
| 1:AA:3:PHE:CD2   | 1:AA:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:AA:85:THR:HB   | 1:AE:116:THR:O    | 2.07                     | 0.55              |
| 1:AE:71:TYR:C    | 1:AE:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:AJ:83:GLY:HA3  | 2:AJ:1001:PO4:P   | 2.46                     | 0.55              |
| 1:AL:97:LYS:O    | 1:AL:102:LEU:HB2  | 2.07                     | 0.55              |
| 1:AT:83:GLY:HA3  | 2:AT:1001:PO4:P   | 2.46                     | 0.55              |
| 1:AY:53:PRO:HG2  | 1:AY:57:GLU:HG3   | 0.65                     | 0.55              |
| 1:BH:6:HIS:CE1   | 1:BH:8:VAL:HB     | 2.41                     | 0.55              |
| 1:BK:85:THR:HB   | 1:BO:116:THR:O    | 2.07                     | 0.55              |
| 1:BP:100:ALA:HB2 | 1:BQ:56:PHE:CZ    | 2.41                     | 0.55              |
| 1:BU:3:PHE:CD2   | 1:BU:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:BY:53:PRO:CD   | 1:BY:57:GLU:HG3   | 2.29                     | 0.55              |
| 1:B1:100:ALA:HA  | 1:B2:56:PHE:CZ    | 2.42                     | 0.55              |
| 1:CG:97:LYS:O    | 1:CG:102:LEU:HB2  | 2.07                     | 0.55              |
| 1:CH:65:MET:HE3  | 1:CH:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:CM:152:TRP:HD1 | 1:CN:68:SER:HB2   | 1.72                     | 0.55              |
| 1:CN:63:LYS:O    | 1:CN:67:ASN:HB2   | 2.05                     | 0.55              |
| 1:CT:71:TYR:C    | 1:CT:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:CW:152:TRP:HD1 | 1:CX:68:SER:HB2   | 1.72                     | 0.55              |
| 1:CX:124:ILE:O   | 1:CX:129:THR:OG1  | 2.16                     | 0.55              |
| 1:AD:95:VAL:HG12 | 1:AD:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:AH:37:LEU:HD12 | 1:AH:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:AK:3:PHE:CD2   | 1:AK:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:AX:95:VAL:HG12 | 1:AX:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:AY:107:ASP:C   | 1:AY:107:ASP:OD1  | 2.50                     | 0.55              |
| 1:AZ:82:ARG:HG3  | 1:AZ:118:GLU:OE2  | 2.06                     | 0.55              |
| 1:A1:97:LYS:O    | 1:A1:102:LEU:HB2  | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BC:65:MET:HE3   | 1:BC:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:BH:152:TRP:HD1  | 1:BI:68:SER:HB2   | 1.72                     | 0.55              |
| 1:BK:3:PHE:CD2    | 1:BK:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:BP:3:PHE:CD2    | 1:BP:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:BP:85:THR:HB    | 1:BT:116:THR:O    | 2.07                     | 0.55              |
| 1:BZ:85:THR:HB    | 1:B4:116:THR:O    | 2.07                     | 0.55              |
| 1:B1:95:VAL:HG12  | 1:B1:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:B4:83:GLY:HA3   | 2:B4:1001:PO4:P   | 2.46                     | 0.55              |
| 1:CD:28:LYS:HZ1   | 1:CF:28:LYS:HZ2   | 1.55                     | 0.55              |
| 1:CG:95:VAL:HG12  | 1:CG:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:CI:95:VAL:HG12  | 1:CI:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:CN:95:VAL:HG12  | 1:CN:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:CO:107:ASP:O    | 1:CO:107:ASP:OD1  | 2.25                     | 0.55              |
| 1:CP:3:PHE:CD2    | 1:CP:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:CZ:3:PHE:CD2    | 1:CZ:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:C1:95:VAL:HG12  | 1:C1:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:AC:37:LEU:HD12  | 1:AC:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:AE:107:ASP:O    | 1:AE:107:ASP:OD1  | 2.24                     | 0.55              |
| 1:AG:129:THR:HG22 | 1:AG:130:LYS:H    | 1.72                     | 0.55              |
| 1:AJ:107:ASP:C    | 1:AJ:107:ASP:OD1  | 2.50                     | 0.55              |
| 1:AN:151:HIS:HB2  | 1:AO:64:LYS:HB3   | 1.88                     | 0.55              |
| 1:AS:95:VAL:HG12  | 1:AS:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:BA:152:TRP:CD1  | 1:BA:153:ALA:H    | 2.23                     | 0.55              |
| 1:BJ:107:ASP:C    | 1:BJ:107:ASP:OD1  | 2.50                     | 0.55              |
| 1:BM:152:TRP:HD1  | 1:BN:68:SER:HB2   | 1.72                     | 0.55              |
| 1:BQ:97:LYS:O     | 1:BQ:102:LEU:HB2  | 2.07                     | 0.55              |
| 1:CC:65:MET:HE3   | 1:CC:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:CJ:107:ASP:C    | 1:CJ:107:ASP:OD1  | 2.50                     | 0.55              |
| 1:CN:7:LEU:HD11   | 1:CN:140:VAL:HG22 | 1.87                     | 0.55              |
| 1:CQ:95:VAL:HG12  | 1:CQ:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:CW:39:ARG:CZ    | 1:C3:20:ARG:NH1   | 2.69                     | 0.55              |
| 1:C2:97:LYS:HG3   | 1:C3:97:LYS:HZ3   | 1.72                     | 0.55              |
| 1:AQ:96:ALA:O     | 1:AQ:100:ALA:HB2  | 2.06                     | 0.55              |
| 1:AW:37:LEU:HD12  | 1:AW:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:A4:107:ASP:OD1  | 1:A4:107:ASP:C    | 2.50                     | 0.55              |
| 1:BB:152:TRP:C    | 1:BB:152:TRP:CD1  | 2.85                     | 0.55              |
| 1:BC:152:TRP:HD1  | 1:BD:68:SER:HB2   | 1.72                     | 0.55              |
| 1:BD:95:VAL:HG12  | 1:BD:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:BE:107:ASP:OD1  | 1:BE:107:ASP:C    | 2.50                     | 0.55              |
| 1:BJ:107:ASP:O    | 1:BJ:107:ASP:OD1  | 2.24                     | 0.55              |
| 1:BY:107:ASP:O    | 1:BY:107:ASP:OD1  | 2.24                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B1:152:TRP:C    | 1:B1:152:TRP:CD1  | 2.85                     | 0.55              |
| 1:B2:65:MET:HE3   | 1:B2:71:TYR:CE1   | 2.41                     | 0.55              |
| 1:CA:3:PHE:CD2    | 1:CA:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:CB:97:LYS:O     | 1:CB:102:LEU:HB2  | 2.07                     | 0.55              |
| 1:CE:53:PRO:HG2   | 1:CE:57:GLU:HG3   | 0.65                     | 0.55              |
| 1:CL:95:VAL:HG12  | 1:CL:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:CR:97:LYS:HG3   | 1:CS:97:LYS:HZ1   | 1.72                     | 0.55              |
| 1:CS:95:VAL:HG12  | 1:CS:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:CV:100:ALA:HA   | 1:CW:56:PHE:CZ    | 2.42                     | 0.55              |
| 1:CV:129:THR:HG22 | 1:CV:130:LYS:H    | 1.72                     | 0.55              |
| 1:AO:107:ASP:OD1  | 1:AO:107:ASP:C    | 2.50                     | 0.55              |
| 1:AP:58:ILE:O     | 1:AP:58:ILE:CG2   | 2.50                     | 0.55              |
| 1:AR:65:MET:HE3   | 1:AR:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:AS:7:LEU:HD11   | 1:AS:140:VAL:HG22 | 1.87                     | 0.55              |
| 1:AT:71:TYR:C     | 1:AT:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:AT:107:ASP:O    | 1:AT:107:ASP:OD1  | 2.25                     | 0.55              |
| 1:AU:3:PHE:CD2    | 1:AU:150:LYS:HE2  | 2.42                     | 0.55              |
| 1:AW:152:TRP:HD1  | 1:AX:68:SER:HB2   | 1.72                     | 0.55              |
| 1:A2:37:LEU:HD12  | 1:A2:47:ILE:HD13  | 1.87                     | 0.55              |
| 1:BE:18:VAL:HG12  | 1:BE:77:LEU:CB    | 2.37                     | 0.55              |
| 1:BG:100:ALA:HA   | 1:BH:56:PHE:CZ    | 2.42                     | 0.55              |
| 1:BL:97:LYS:O     | 1:BL:102:LEU:HB2  | 2.07                     | 0.55              |
| 1:BL:129:THR:HG22 | 1:BL:130:LYS:H    | 1.72                     | 0.55              |
| 1:BM:97:LYS:HG3   | 1:BN:97:LYS:HZ3   | 1.71                     | 0.55              |
| 1:BU:82:ARG:HG3   | 1:BU:118:GLU:OE2  | 2.06                     | 0.55              |
| 1:B3:7:LEU:HD11   | 1:B3:140:VAL:HG22 | 1.87                     | 0.55              |
| 1:CB:129:THR:HG22 | 1:CB:130:LYS:H    | 1.72                     | 0.55              |
| 1:CR:65:MET:HE3   | 1:CR:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:CT:53:PRO:HG2   | 1:CT:57:GLU:HG3   | 0.65                     | 0.55              |
| 1:CW:65:MET:HE3   | 1:CW:71:TYR:CE1   | 2.42                     | 0.55              |
| 1:C3:95:VAL:HG12  | 1:C3:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:AG:95:VAL:HG12  | 1:AG:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:AQ:95:VAL:HG12  | 1:AQ:112:PHE:HE1  | 1.72                     | 0.55              |
| 1:AV:129:THR:HG22 | 1:AV:130:LYS:H    | 1.72                     | 0.55              |
| 1:AY:18:VAL:HG12  | 1:AY:77:LEU:CB    | 2.37                     | 0.55              |
| 1:A1:152:TRP:CD1  | 1:A1:152:TRP:C    | 2.85                     | 0.55              |
| 1:A2:129:THR:O    | 1:A2:132:GLY:N    | 2.25                     | 0.55              |
| 1:BC:18:VAL:HG21  | 1:BC:30:LEU:HD13  | 1.89                     | 0.55              |
| 1:BD:7:LEU:HD11   | 1:BD:140:VAL:HG22 | 1.87                     | 0.55              |
| 1:BE:53:PRO:HG2   | 1:BE:57:GLU:HG3   | 0.65                     | 0.55              |
| 1:BG:95:VAL:HG12  | 1:BG:112:PHE:HE1  | 1.72                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BI:95:VAL:HG12  | 1:BI:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:BI:151:HIS:HB2  | 1:BJ:64:LYS:HB3   | 1.88                     | 0.55              |
| 1:BO:107:ASP:O    | 1:BO:107:ASP:OD1  | 2.24                     | 0.55              |
| 1:BX:7:LEU:HD11   | 1:BX:140:VAL:HG22 | 1.87                     | 0.55              |
| 1:BZ:75:ILE:HG22  | 1:BZ:77:LEU:HD13  | 1.90                     | 0.55              |
| 1:CB:152:TRP:CD1  | 1:CB:152:TRP:C    | 2.85                     | 0.55              |
| 1:CM:65:MET:HE3   | 1:CM:71:TYR:CE1   | 2.41                     | 0.55              |
| 1:CQ:129:THR:HG22 | 1:CQ:130:LYS:H    | 1.72                     | 0.55              |
| 1:CT:52:VAL:HB    | 1:CT:53:PRO:CD    | 2.35                     | 0.55              |
| 1:CX:95:VAL:HG12  | 1:CX:112:PHE:HE1  | 1.71                     | 0.55              |
| 1:C4:71:TYR:C     | 1:C4:150:LYS:HZ3  | 2.15                     | 0.55              |
| 1:AE:39:ARG:O     | 1:AN:7:LEU:HB3    | 2.05                     | 0.54              |
| 1:AO:52:VAL:CB    | 1:AO:53:PRO:HD2   | 2.34                     | 0.54              |
| 1:AW:65:MET:HE3   | 1:AW:71:TYR:CE1   | 2.41                     | 0.54              |
| 1:BB:97:LYS:O     | 1:BB:102:LEU:HB2  | 2.07                     | 0.54              |
| 1:BF:28:LYS:CE    | 1:BR:28:LYS:HZ3   | 2.20                     | 0.54              |
| 1:BQ:95:VAL:HG12  | 1:BQ:112:PHE:HE1  | 1.72                     | 0.54              |
| 1:BX:95:VAL:HG12  | 1:BX:112:PHE:HE1  | 1.71                     | 0.54              |
| 1:BX:151:HIS:HB2  | 1:BY:64:LYS:HB3   | 1.88                     | 0.54              |
| 1:BZ:3:PHE:CD2    | 1:BZ:150:LYS:HE2  | 2.42                     | 0.54              |
| 1:B4:107:ASP:C    | 1:B4:107:ASP:OD1  | 2.50                     | 0.54              |
| 1:CB:95:VAL:HG12  | 1:CB:112:PHE:HE1  | 1.72                     | 0.54              |
| 1:CG:152:TRP:CD1  | 1:CG:152:TRP:C    | 2.85                     | 0.54              |
| 1:CI:151:HIS:HB2  | 1:CJ:64:LYS:HB3   | 1.88                     | 0.54              |
| 1:CK:85:THR:HB    | 1:CO:116:THR:O    | 2.07                     | 0.54              |
| 1:CP:85:THR:HB    | 1:CT:116:THR:O    | 2.07                     | 0.54              |
| 1:CT:128:GLY:O    | 1:C4:22:ASN:HA    | 2.07                     | 0.54              |
| 1:CY:107:ASP:OD1  | 1:CY:107:ASP:C    | 2.50                     | 0.54              |
| 1:C4:18:VAL:HG12  | 1:C4:77:LEU:CB    | 2.37                     | 0.54              |
| 1:AF:85:THR:HB    | 1:AJ:116:THR:O    | 2.07                     | 0.54              |
| 1:AG:97:LYS:O     | 1:AG:102:LEU:HB2  | 2.07                     | 0.54              |
| 1:AH:38:LYS:HZ2   | 1:AH:44:GLU:HA    | 1.72                     | 0.54              |
| 1:AI:95:VAL:HG12  | 1:AI:112:PHE:HE1  | 1.71                     | 0.54              |
| 1:AP:152:TRP:CD1  | 1:AP:153:ALA:H    | 2.23                     | 0.54              |
| 1:AV:152:TRP:CD1  | 1:AV:152:TRP:C    | 2.85                     | 0.54              |
| 1:BG:129:THR:HG22 | 1:BG:130:LYS:H    | 1.72                     | 0.54              |
| 1:BG:152:TRP:CD1  | 1:BG:152:TRP:C    | 2.85                     | 0.54              |
| 1:BH:18:VAL:HG21  | 1:BH:30:LEU:HD13  | 1.89                     | 0.54              |
| 1:BR:18:VAL:HG21  | 1:BR:30:LEU:HD13  | 1.89                     | 0.54              |
| 1:BR:152:TRP:HD1  | 1:BS:68:SER:HB2   | 1.72                     | 0.54              |
| 1:BS:151:HIS:HB2  | 1:BT:64:LYS:HB3   | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BT:83:GLY:HA3   | 2:BT:1001:PO4:P  | 2.46                     | 0.54              |
| 1:BV:152:TRP:CD1  | 1:BV:152:TRP:C   | 2.85                     | 0.54              |
| 1:BW:18:VAL:HG21  | 1:BW:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:BZ:58:ILE:CG2   | 1:BZ:58:ILE:O    | 2.50                     | 0.54              |
| 1:CM:18:VAL:HG21  | 1:CM:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:CW:7:LEU:HD23   | 1:C2:40:HIS:CE1  | 2.42                     | 0.54              |
| 1:AA:75:ILE:HG22  | 1:AA:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:AB:97:LYS:O     | 1:AB:102:LEU:HB2 | 2.07                     | 0.54              |
| 1:AC:65:MET:HE3   | 1:AC:71:TYR:CE1  | 2.41                     | 0.54              |
| 1:AH:65:MET:HE3   | 1:AH:71:TYR:CE1  | 2.42                     | 0.54              |
| 1:AJ:18:VAL:HG12  | 1:AJ:77:LEU:CB   | 2.37                     | 0.54              |
| 1:AL:152:TRP:CD1  | 1:AL:152:TRP:C   | 2.85                     | 0.54              |
| 1:AU:85:THR:HB    | 1:AY:116:THR:O   | 2.07                     | 0.54              |
| 1:A1:129:THR:HG22 | 1:A1:130:LYS:H   | 1.72                     | 0.54              |
| 1:A4:53:PRO:HG2   | 1:A4:57:GLU:HG3  | 0.65                     | 0.54              |
| 1:A4:107:ASP:O    | 1:A4:107:ASP:OD1 | 2.24                     | 0.54              |
| 1:BB:129:THR:HG22 | 1:BB:130:LYS:H   | 1.72                     | 0.54              |
| 1:BE:71:TYR:C     | 1:BE:150:LYS:HZ3 | 2.15                     | 0.54              |
| 1:BG:97:LYS:O     | 1:BG:102:LEU:HB2 | 2.07                     | 0.54              |
| 1:BP:75:ILE:HG22  | 1:BP:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:BV:95:VAL:HG12  | 1:BV:112:PHE:HE1 | 1.72                     | 0.54              |
| 1:B1:107:ASP:HB2  | 1:B1:152:TRP:HZ3 | 1.62                     | 0.54              |
| 1:CC:152:TRP:HD1  | 1:CD:68:SER:HB2  | 1.72                     | 0.54              |
| 1:CE:107:ASP:C    | 1:CE:107:ASP:OD1 | 2.50                     | 0.54              |
| 1:CH:97:LYS:HG3   | 1:CI:97:LYS:HZ3  | 1.71                     | 0.54              |
| 1:CL:152:TRP:C    | 1:CL:152:TRP:CD1 | 2.85                     | 0.54              |
| 1:CQ:152:TRP:CD1  | 1:CQ:152:TRP:C   | 2.85                     | 0.54              |
| 1:C2:18:VAL:HG21  | 1:C2:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:AC:18:VAL:HG21  | 1:AC:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:AC:129:THR:O    | 1:AC:132:GLY:N   | 2.25                     | 0.54              |
| 1:AF:3:PHE:CD2    | 1:AF:150:LYS:HE2 | 2.42                     | 0.54              |
| 1:AP:75:ILE:HG22  | 1:AP:77:LEU:HD13 | 1.89                     | 0.54              |
| 1:AR:18:VAL:HG21  | 1:AR:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:AT:52:VAL:HB    | 1:AT:53:PRO:CD   | 2.35                     | 0.54              |
| 1:AW:18:VAL:HG21  | 1:AW:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:AZ:75:ILE:HG22  | 1:AZ:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:BJ:52:VAL:HB    | 1:BJ:53:PRO:CD   | 2.35                     | 0.54              |
| 1:B2:18:VAL:HG21  | 1:B2:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:CJ:52:VAL:HB    | 1:CJ:53:PRO:CD   | 2.35                     | 0.54              |
| 1:CL:100:ALA:HA   | 1:CM:56:PHE:CZ   | 2.42                     | 0.54              |
| 1:CP:75:ILE:HG22  | 1:CP:77:LEU:HD13 | 1.90                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C1:75:ILE:HG22  | 1:C1:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:C3:151:HIS:HB2  | 1:C4:64:LYS:HB3  | 1.88                     | 0.54              |
| 1:AM:18:VAL:HG21  | 1:AM:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:AP:3:PHE:CD2    | 1:AP:150:LYS:HE2 | 2.42                     | 0.54              |
| 1:AU:75:ILE:HG22  | 1:AU:77:LEU:HD13 | 1.89                     | 0.54              |
| 1:A4:52:VAL:CB    | 1:A4:53:PRO:HD2  | 2.33                     | 0.54              |
| 1:BF:3:PHE:CD2    | 1:BF:150:LYS:HE2 | 2.42                     | 0.54              |
| 1:BN:18:VAL:HG12  | 1:BN:77:LEU:CB   | 2.37                     | 0.54              |
| 1:BY:107:ASP:OD1  | 1:BY:107:ASP:C   | 2.50                     | 0.54              |
| 1:B3:151:HIS:HB2  | 1:B4:64:LYS:HB3  | 1.88                     | 0.54              |
| 1:CD:151:HIS:HB2  | 1:CE:64:LYS:HB3  | 1.88                     | 0.54              |
| 1:CE:107:ASP:O    | 1:CE:107:ASP:OD1 | 2.25                     | 0.54              |
| 1:CJ:53:PRO:HG2   | 1:CJ:57:GLU:HG3  | 0.65                     | 0.54              |
| 1:CJ:107:ASP:O    | 1:CJ:107:ASP:OD1 | 2.25                     | 0.54              |
| 1:CL:75:ILE:HG22  | 1:CL:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:C1:152:TRP:CD1  | 1:C1:152:TRP:C   | 2.85                     | 0.54              |
| 1:C4:107:ASP:OD1  | 1:C4:107:ASP:C   | 2.50                     | 0.54              |
| 1:AH:152:TRP:HD1  | 1:AI:68:SER:HB2  | 1.72                     | 0.54              |
| 1:AO:18:VAL:HG12  | 1:AO:77:LEU:CB   | 2.37                     | 0.54              |
| 1:AQ:129:THR:HG22 | 1:AQ:130:LYS:H   | 1.72                     | 0.54              |
| 1:A3:151:HIS:HB2  | 1:A4:64:LYS:HB3  | 1.88                     | 0.54              |
| 1:BO:107:ASP:OD1  | 1:BO:107:ASP:C   | 2.50                     | 0.54              |
| 1:BQ:100:ALA:HA   | 1:BR:56:PHE:CZ   | 2.42                     | 0.54              |
| 1:BS:39:ARG:O     | 1:BY:7:LEU:HB3   | 2.07                     | 0.54              |
| 1:BT:107:ASP:C    | 1:BT:107:ASP:OD1 | 2.50                     | 0.54              |
| 1:B3:18:VAL:HG12  | 1:B3:77:LEU:CB   | 2.37                     | 0.54              |
| 1:CD:95:VAL:HG12  | 1:CD:112:PHE:HE1 | 1.71                     | 0.54              |
| 1:CL:97:LYS:O     | 1:CL:102:LEU:HB2 | 2.07                     | 0.54              |
| 1:CW:18:VAL:HG21  | 1:CW:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:CY:71:TYR:C     | 1:CY:150:LYS:HZ3 | 2.15                     | 0.54              |
| 1:CZ:75:ILE:HG22  | 1:CZ:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:C4:53:PRO:CG    | 1:C4:57:GLU:CG   | 2.46                     | 0.54              |
| 1:AL:100:ALA:HA   | 1:AM:56:PHE:CZ   | 2.42                     | 0.54              |
| 1:AM:152:TRP:HD1  | 1:AN:68:SER:HB2  | 1.72                     | 0.54              |
| 1:AQ:152:TRP:C    | 1:AQ:152:TRP:CD1 | 2.85                     | 0.54              |
| 1:BL:95:VAL:HG12  | 1:BL:112:PHE:HE1 | 1.72                     | 0.54              |
| 1:BN:95:VAL:HG12  | 1:BN:112:PHE:HE1 | 1.71                     | 0.54              |
| 1:BT:107:ASP:O    | 1:BT:107:ASP:OD1 | 2.24                     | 0.54              |
| 1:B1:97:LYS:O     | 1:B1:102:LEU:HB2 | 2.07                     | 0.54              |
| 1:CA:75:ILE:HG22  | 1:CA:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:CD:22:ASN:HA    | 1:CR:128:GLY:O   | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CE:71:TYR:C     | 1:CE:150:LYS:HZ3  | 2.15                     | 0.54              |
| 1:CI:39:ARG:O     | 1:CO:7:LEU:HB3    | 2.08                     | 0.54              |
| 1:AB:129:THR:HG22 | 1:AB:130:LYS:H    | 1.72                     | 0.54              |
| 1:AB:152:TRP:CD1  | 1:AB:152:TRP:C    | 2.85                     | 0.54              |
| 1:AC:129:THR:HG21 | 1:AS:120:ILE:HD11 | 1.89                     | 0.54              |
| 1:AI:18:VAL:HG12  | 1:AI:77:LEU:CB    | 2.37                     | 0.54              |
| 1:AL:129:THR:HG22 | 1:AL:130:LYS:H    | 1.72                     | 0.54              |
| 1:AV:97:LYS:O     | 1:AV:102:LEU:HB2  | 2.07                     | 0.54              |
| 1:BA:3:PHE:CD2    | 1:BA:150:LYS:HE2  | 2.42                     | 0.54              |
| 1:BE:53:PRO:CD    | 1:BE:57:GLU:HG3   | 2.29                     | 0.54              |
| 1:BF:75:ILE:HG22  | 1:BF:77:LEU:HD13  | 1.90                     | 0.54              |
| 1:BS:95:VAL:HG12  | 1:BS:112:PHE:HE1  | 1.71                     | 0.54              |
| 1:BV:75:ILE:HG22  | 1:BV:77:LEU:HD13  | 1.90                     | 0.54              |
| 1:CG:100:ALA:HA   | 1:CH:56:PHE:CZ    | 2.42                     | 0.54              |
| 1:CN:151:HIS:HB2  | 1:CO:64:LYS:HB3   | 1.88                     | 0.54              |
| 1:CQ:97:LYS:O     | 1:CQ:102:LEU:HB2  | 2.07                     | 0.54              |
| 1:C2:152:TRP:HD1  | 1:C3:68:SER:HB2   | 1.72                     | 0.54              |
| 1:AJ:107:ASP:O    | 1:AJ:107:ASP:OD1  | 2.25                     | 0.54              |
| 1:AN:95:VAL:HG12  | 1:AN:112:PHE:HE1  | 1.71                     | 0.54              |
| 1:AY:107:ASP:O    | 1:AY:107:ASP:OD1  | 2.24                     | 0.54              |
| 1:A1:100:ALA:HA   | 1:A2:56:PHE:CZ    | 2.42                     | 0.54              |
| 1:A2:97:LYS:HG3   | 1:A3:97:LYS:HZ1   | 1.73                     | 0.54              |
| 1:BA:75:ILE:HG22  | 1:BA:77:LEU:HD13  | 1.90                     | 0.54              |
| 1:BE:52:VAL:HB    | 1:BE:53:PRO:CD    | 2.35                     | 0.54              |
| 1:BK:75:ILE:HG22  | 1:BK:77:LEU:HD13  | 1.90                     | 0.54              |
| 1:BO:71:TYR:C     | 1:BO:150:LYS:HZ3  | 2.16                     | 0.54              |
| 1:BV:129:THR:HG22 | 1:BV:130:LYS:H    | 1.72                     | 0.54              |
| 1:BW:70:LYS:HB2   | 1:BW:71:TYR:CE1   | 2.43                     | 0.54              |
| 1:CJ:71:TYR:C     | 1:CJ:150:LYS:HZ3  | 2.15                     | 0.54              |
| 1:CR:18:VAL:HG21  | 1:CR:30:LEU:HD13  | 1.89                     | 0.54              |
| 1:CT:107:ASP:OD1  | 1:CT:107:ASP:C    | 2.50                     | 0.54              |
| 1:CX:151:HIS:HB2  | 1:CY:64:LYS:HB3   | 1.88                     | 0.54              |
| 1:C1:100:ALA:HA   | 1:C2:56:PHE:CZ    | 2.42                     | 0.54              |
| 1:AQ:75:ILE:HG22  | 1:AQ:77:LEU:HD13  | 1.90                     | 0.54              |
| 1:AQ:97:LYS:O     | 1:AQ:102:LEU:HB2  | 2.07                     | 0.54              |
| 1:AT:107:ASP:OD1  | 1:AT:107:ASP:C    | 2.50                     | 0.54              |
| 1:AY:71:TYR:C     | 1:AY:150:LYS:HZ3  | 2.15                     | 0.54              |
| 1:A2:70:LYS:HB2   | 1:A2:71:TYR:CE1   | 2.43                     | 0.54              |
| 1:BE:53:PRO:CG    | 1:BE:57:GLU:CG    | 2.46                     | 0.54              |
| 1:BG:75:ILE:HG22  | 1:BG:77:LEU:HD13  | 1.90                     | 0.54              |
| 1:BM:18:VAL:HG21  | 1:BM:30:LEU:HD13  | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BQ:152:TRP:CD1  | 1:BQ:152:TRP:C   | 2.85                     | 0.54              |
| 1:CH:18:VAL:HG21  | 1:CH:30:LEU:HD13 | 1.89                     | 0.54              |
| 1:CI:7:LEU:HB3    | 1:CO:39:ARG:O    | 2.08                     | 0.54              |
| 1:CK:75:ILE:HG22  | 1:CK:77:LEU:HD13 | 1.90                     | 0.54              |
| 1:CP:22:ASN:HA    | 1:C3:128:GLY:O   | 2.08                     | 0.54              |
| 1:AB:100:ALA:HA   | 1:AC:56:PHE:CZ   | 2.42                     | 0.53              |
| 1:AH:18:VAL:HG21  | 1:AH:30:LEU:HD13 | 1.89                     | 0.53              |
| 1:A2:152:TRP:HD1  | 1:A3:68:SER:HB2  | 1.72                     | 0.53              |
| 1:BW:152:TRP:HD1  | 1:BX:68:SER:HB2  | 1.72                     | 0.53              |
| 1:CD:28:LYS:HZ1   | 1:CF:28:LYS:NZ   | 2.06                     | 0.53              |
| 1:CH:70:LYS:HB2   | 1:CH:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:CO:107:ASP:OD1  | 1:CO:107:ASP:C   | 2.50                     | 0.53              |
| 1:CU:85:THR:HB    | 1:CY:116:THR:O   | 2.07                     | 0.53              |
| 1:CV:152:TRP:CD1  | 1:CV:152:TRP:C   | 2.85                     | 0.53              |
| 1:CZ:143:ILE:O    | 1:CZ:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:C1:97:LYS:O     | 1:C1:102:LEU:HB2 | 2.07                     | 0.53              |
| 1:AA:6:HIS:HB2    | 1:AA:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:AB:95:VAL:HG12  | 1:AB:112:PHE:HE1 | 1.72                     | 0.53              |
| 1:AI:7:LEU:HD23   | 1:AO:40:HIS:CE1  | 2.43                     | 0.53              |
| 1:AL:95:VAL:HG12  | 1:AL:112:PHE:HE1 | 1.72                     | 0.53              |
| 1:AY:52:VAL:HB    | 1:AY:53:PRO:CD   | 2.35                     | 0.53              |
| 1:BF:6:HIS:HB2    | 1:BF:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:BQ:75:ILE:HG22  | 1:BQ:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:BQ:129:THR:HG22 | 1:BQ:130:LYS:H   | 1.72                     | 0.53              |
| 1:BT:52:VAL:HB    | 1:BT:53:PRO:CD   | 2.35                     | 0.53              |
| 1:BU:6:HIS:HB2    | 1:BU:147:HIS:ND1 | 2.23                     | 0.53              |
| 1:BY:53:PRO:CG    | 1:BY:57:GLU:CG   | 2.46                     | 0.53              |
| 1:BY:53:PRO:HG2   | 1:BY:57:GLU:HG3  | 0.65                     | 0.53              |
| 1:B1:129:THR:HG22 | 1:B1:130:LYS:H   | 1.72                     | 0.53              |
| 1:B2:152:TRP:HD1  | 1:B3:68:SER:HB2  | 1.72                     | 0.53              |
| 1:CF:75:ILE:HG22  | 1:CF:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:CJ:152:TRP:HE3  | 1:CJ:153:ALA:N   | 2.07                     | 0.53              |
| 1:CM:70:LYS:HB2   | 1:CM:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:CO:152:TRP:HE3  | 1:CO:153:ALA:N   | 2.07                     | 0.53              |
| 1:CR:70:LYS:HB2   | 1:CR:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:AJ:52:VAL:CB    | 1:AJ:53:PRO:HD2  | 2.34                     | 0.53              |
| 1:AK:6:HIS:HB2    | 1:AK:147:HIS:ND1 | 2.23                     | 0.53              |
| 1:AK:75:ILE:HG22  | 1:AK:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:AW:70:LYS:HB2   | 1:AW:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:AY:152:TRP:HE3  | 1:AY:153:ALA:N   | 2.07                     | 0.53              |
| 1:BG:121:GLU:O    | 1:BG:125:GLU:HG3 | 2.09                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BL:152:TRP:CD1  | 1:BL:152:TRP:C   | 2.85                     | 0.53              |
| 1:BP:3:PHE:HD2    | 1:BP:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:BV:121:GLU:O    | 1:BV:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:B4:18:VAL:HG12  | 1:B4:77:LEU:CB   | 2.37                     | 0.53              |
| 1:CA:143:ILE:O    | 1:CA:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:CN:104:LEU:HD13 | 1:CO:102:LEU:HG  | 1.91                     | 0.53              |
| 1:CP:6:HIS:HB2    | 1:CP:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:CU:75:ILE:HG22  | 1:CU:77:LEU:HD13 | 1.89                     | 0.53              |
| 1:CY:52:VAL:HB    | 1:CY:53:PRO:CD   | 2.35                     | 0.53              |
| 1:C3:104:LEU:HD13 | 1:C4:102:LEU:HG  | 1.91                     | 0.53              |
| 1:AF:143:ILE:O    | 1:AF:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:AJ:152:TRP:HE3  | 1:AJ:153:ALA:N   | 2.07                     | 0.53              |
| 1:AO:52:VAL:HB    | 1:AO:53:PRO:CD   | 2.35                     | 0.53              |
| 1:AR:70:LYS:HB2   | 1:AR:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:AR:97:LYS:HE3   | 1:AS:97:LYS:HZ3  | 1.74                     | 0.53              |
| 1:BK:143:ILE:O    | 1:BK:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:CI:104:LEU:HD13 | 1:CJ:102:LEU:HG  | 1.91                     | 0.53              |
| 1:CK:3:PHE:HD2    | 1:CK:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:CK:6:HIS:HB2    | 1:CK:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:AB:124:ILE:HD11 | 1:AV:24:PHE:CE2  | 2.43                     | 0.53              |
| 1:AG:152:TRP:CD1  | 1:AG:152:TRP:C   | 2.85                     | 0.53              |
| 1:AL:121:GLU:O    | 1:AL:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:AO:71:TYR:C     | 1:AO:150:LYS:HZ3 | 2.15                     | 0.53              |
| 1:AU:6:HIS:HB2    | 1:AU:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:BA:6:HIS:HB2    | 1:BA:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:BD:128:GLY:O    | 1:BF:22:ASN:HA   | 2.09                     | 0.53              |
| 1:BL:75:ILE:HG22  | 1:BL:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:BT:18:VAL:HG12  | 1:BT:77:LEU:CB   | 2.37                     | 0.53              |
| 1:BV:100:ALA:HA   | 1:BW:56:PHE:CZ   | 2.42                     | 0.53              |
| 1:B1:75:ILE:HG22  | 1:B1:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:B2:38:LYS:HZ2   | 1:B2:44:GLU:HA   | 1.74                     | 0.53              |
| 1:B4:107:ASP:O    | 1:B4:107:ASP:OD1 | 2.24                     | 0.53              |
| 1:CA:3:PHE:HD2    | 1:CA:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:CF:3:PHE:HD2    | 1:CF:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:CL:121:GLU:O    | 1:CL:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:CT:18:VAL:HG12  | 1:CT:77:LEU:CB   | 2.37                     | 0.53              |
| 1:CV:75:ILE:HG22  | 1:CV:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:C2:70:LYS:HB2   | 1:C2:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:C4:152:TRP:HE3  | 1:C4:153:ALA:N   | 2.07                     | 0.53              |
| 1:AG:75:ILE:HG22  | 1:AG:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:AR:152:TRP:HD1  | 1:AS:68:SER:HB2  | 1.72                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AU:3:PHE:HD2    | 1:AU:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:A1:95:VAL:HG12  | 1:A1:112:PHE:HE1 | 1.72                     | 0.53              |
| 1:A4:18:VAL:HG12  | 1:A4:77:LEU:CB   | 2.37                     | 0.53              |
| 1:BA:3:PHE:HD2    | 1:BA:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:BA:143:ILE:O    | 1:BA:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:BL:100:ALA:HA   | 1:BM:56:PHE:CZ   | 2.42                     | 0.53              |
| 1:BR:97:LYS:HG3   | 1:BS:97:LYS:HZ3  | 1.74                     | 0.53              |
| 1:B1:121:GLU:O    | 1:B1:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:CC:70:LYS:HB2   | 1:CC:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:CD:104:LEU:HD13 | 1:CE:102:LEU:HG  | 1.91                     | 0.53              |
| 1:CG:129:THR:HG22 | 1:CG:130:LYS:H   | 1.72                     | 0.53              |
| 1:CW:97:LYS:HG3   | 1:CX:97:LYS:HZ1  | 1.72                     | 0.53              |
| 1:CZ:3:PHE:HD2    | 1:CZ:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:C1:129:THR:HG22 | 1:C1:130:LYS:H   | 1.72                     | 0.53              |
| 1:AF:75:ILE:HG22  | 1:AF:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:AG:121:GLU:O    | 1:AG:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:AZ:6:HIS:HB2    | 1:AZ:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:A1:75:ILE:HG22  | 1:A1:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:A2:18:VAL:HG21  | 1:A2:30:LEU:HD13 | 1.89                     | 0.53              |
| 1:BE:152:TRP:HE3  | 1:BE:153:ALA:N   | 2.07                     | 0.53              |
| 1:BP:143:ILE:O    | 1:BP:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:BR:70:LYS:HB2   | 1:BR:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:BT:71:TYR:C     | 1:BT:150:LYS:HZ3 | 2.15                     | 0.53              |
| 1:CD:20:ARG:NH1   | 1:CR:39:ARG:CZ   | 2.72                     | 0.53              |
| 1:AD:104:LEU:HD13 | 1:AE:102:LEU:HG  | 1.91                     | 0.53              |
| 1:AE:52:VAL:HB    | 1:AE:53:PRO:CD   | 2.35                     | 0.53              |
| 1:AG:100:ALA:HA   | 1:AH:56:PHE:CZ   | 2.42                     | 0.53              |
| 1:AM:70:LYS:HB2   | 1:AM:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:AU:143:ILE:O    | 1:AU:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:AV:75:ILE:HG22  | 1:AV:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:A1:121:GLU:O    | 1:A1:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:BB:75:ILE:HG22  | 1:BB:77:LEU:HD13 | 1.90                     | 0.53              |
| 1:BE:37:LEU:HD12  | 1:BE:47:ILE:HD11 | 1.91                     | 0.53              |
| 1:BK:6:HIS:HB2    | 1:BK:147:HIS:ND1 | 2.23                     | 0.53              |
| 1:BO:18:VAL:HG12  | 1:BO:77:LEU:CB   | 2.37                     | 0.53              |
| 1:BZ:3:PHE:HD2    | 1:BZ:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:CA:6:HIS:HB2    | 1:CA:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:CB:121:GLU:O    | 1:CB:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:CS:18:VAL:HG12  | 1:CS:77:LEU:CB   | 2.37                     | 0.53              |
| 1:CT:152:TRP:HE3  | 1:CT:153:ALA:N   | 2.07                     | 0.53              |
| 1:CU:3:PHE:HD2    | 1:CU:150:LYS:HE2 | 1.74                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:CU:6:HIS:HB2    | 1:CU:147:HIS:ND1 | 2.24                     | 0.53              |
| 1:CX:104:LEU:HD13 | 1:CY:102:LEU:HG  | 1.91                     | 0.53              |
| 1:AB:40:HIS:CE1   | 1:AU:7:LEU:HD23  | 2.44                     | 0.53              |
| 1:AK:3:PHE:HD2    | 1:AK:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:AT:53:PRO:HG2   | 1:AT:57:GLU:HG3  | 0.65                     | 0.53              |
| 1:AV:100:ALA:HA   | 1:AW:56:PHE:CZ   | 2.42                     | 0.53              |
| 1:AX:104:LEU:HD13 | 1:AY:102:LEU:HG  | 1.91                     | 0.53              |
| 1:BB:100:ALA:HA   | 1:BC:56:PHE:CZ   | 2.42                     | 0.53              |
| 1:BD:13:LYS:HZ1   | 1:CM:13:LYS:HD3  | 1.73                     | 0.53              |
| 1:BV:6:HIS:CE1    | 1:BV:8:VAL:HB    | 2.44                     | 0.53              |
| 1:B2:70:LYS:HB2   | 1:B2:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:B4:52:VAL:HB    | 1:B4:53:PRO:CD   | 2.35                     | 0.53              |
| 1:CA:85:THR:HB    | 1:CE:116:THR:O   | 2.07                     | 0.53              |
| 1:CO:71:TYR:C     | 1:CO:150:LYS:HZ3 | 2.15                     | 0.53              |
| 1:CQ:121:GLU:O    | 1:CQ:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:CU:143:ILE:O    | 1:CU:147:HIS:HB2 | 2.09                     | 0.53              |
| 1:C1:121:GLU:O    | 1:C1:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:C4:52:VAL:CB    | 1:C4:53:PRO:HD2  | 2.34                     | 0.53              |
| 1:AC:70:LYS:HB2   | 1:AC:71:TYR:CE1  | 2.43                     | 0.53              |
| 1:AN:104:LEU:HD13 | 1:AO:102:LEU:HG  | 1.91                     | 0.53              |
| 1:A2:38:LYS:HZ2   | 1:A2:44:GLU:HA   | 1.74                     | 0.53              |
| 1:BL:121:GLU:O    | 1:BL:125:GLU:HG3 | 2.09                     | 0.53              |
| 1:BR:38:LYS:HZ2   | 1:BR:44:GLU:HA   | 1.74                     | 0.53              |
| 1:CP:3:PHE:HD2    | 1:CP:150:LYS:HE2 | 1.74                     | 0.53              |
| 1:C2:97:LYS:HG3   | 1:C3:97:LYS:NZ   | 2.24                     | 0.53              |
| 1:AJ:71:TYR:C     | 1:AJ:150:LYS:HZ3 | 2.15                     | 0.52              |
| 1:AK:143:ILE:O    | 1:AK:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:AM:97:LYS:HG3   | 1:AN:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:AO:37:LEU:HD12  | 1:AO:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:AQ:121:GLU:O    | 1:AQ:125:GLU:HG3 | 2.09                     | 0.52              |
| 1:AR:152:TRP:HE1  | 1:AS:64:LYS:C    | 2.17                     | 0.52              |
| 1:AT:52:VAL:CB    | 1:AT:53:PRO:HD2  | 2.34                     | 0.52              |
| 1:AT:152:TRP:HE3  | 1:AT:153:ALA:N   | 2.07                     | 0.52              |
| 1:A4:37:LEU:HD12  | 1:A4:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:BC:152:TRP:HE1  | 1:BD:64:LYS:C    | 2.18                     | 0.52              |
| 1:BF:143:ILE:O    | 1:BF:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:BM:70:LYS:HB2   | 1:BM:71:TYR:CE1  | 2.43                     | 0.52              |
| 1:BR:6:HIS:HB3    | 1:BR:147:HIS:CG  | 2.45                     | 0.52              |
| 1:BT:53:PRO:CD    | 1:BT:57:GLU:HG3  | 2.29                     | 0.52              |
| 1:BT:152:TRP:HE3  | 1:BT:153:ALA:N   | 2.07                     | 0.52              |
| 1:BU:75:ILE:HG22  | 1:BU:77:LEU:HD13 | 1.90                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BY:18:VAL:HG12  | 1:BY:77:LEU:CB   | 2.37                     | 0.52              |
| 1:BZ:6:HIS:HB2    | 1:BZ:147:HIS:ND1 | 2.24                     | 0.52              |
| 1:CP:143:ILE:O    | 1:CP:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:AA:3:PHE:HD2    | 1:AA:150:LYS:HE2 | 1.74                     | 0.52              |
| 1:AB:75:ILE:HG22  | 1:AB:77:LEU:HD13 | 1.90                     | 0.52              |
| 1:AB:121:GLU:O    | 1:AB:125:GLU:HG3 | 2.09                     | 0.52              |
| 1:AK:125:GLU:CA   | 1:AK:129:THR:OG1 | 2.57                     | 0.52              |
| 1:AL:75:ILE:HG22  | 1:AL:77:LEU:HD13 | 1.90                     | 0.52              |
| 1:AP:143:ILE:O    | 1:AP:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:AY:37:LEU:HD12  | 1:AY:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:A2:97:LYS:HG3   | 1:A3:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:A3:104:LEU:HD13 | 1:A4:102:LEU:HG  | 1.91                     | 0.52              |
| 1:BJ:18:VAL:HG12  | 1:BJ:77:LEU:CB   | 2.37                     | 0.52              |
| 1:BJ:37:LEU:HD12  | 1:BJ:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:BK:125:GLU:CA   | 1:BK:129:THR:OG1 | 2.57                     | 0.52              |
| 1:BM:6:HIS:HB3    | 1:BM:147:HIS:CG  | 2.45                     | 0.52              |
| 1:BU:143:ILE:O    | 1:BU:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:BW:97:LYS:HG3   | 1:BX:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:BY:37:LEU:HD12  | 1:BY:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:CC:18:VAL:HG21  | 1:CC:30:LEU:HD13 | 1.89                     | 0.52              |
| 1:CF:143:ILE:O    | 1:CF:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:CG:121:GLU:O    | 1:CG:125:GLU:HG3 | 2.09                     | 0.52              |
| 1:CQ:75:ILE:HG22  | 1:CQ:77:LEU:HD13 | 1.90                     | 0.52              |
| 1:CS:104:LEU:HD13 | 1:CT:102:LEU:HG  | 1.91                     | 0.52              |
| 1:CU:109:PRO:HB3  | 1:CU:145:MET:HB3 | 1.91                     | 0.52              |
| 1:CU:125:GLU:CA   | 1:CU:129:THR:OG1 | 2.57                     | 0.52              |
| 1:CW:70:LYS:HB2   | 1:CW:71:TYR:CE1  | 2.43                     | 0.52              |
| 1:CW:152:TRP:HE1  | 1:CX:64:LYS:C    | 2.18                     | 0.52              |
| 1:AC:6:HIS:HB3    | 1:AC:147:HIS:CG  | 2.45                     | 0.52              |
| 1:AC:97:LYS:HG3   | 1:AD:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:AH:70:LYS:HB2   | 1:AH:71:TYR:CE1  | 2.43                     | 0.52              |
| 1:AH:97:LYS:HG3   | 1:AI:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:AM:6:HIS:HB3    | 1:AM:147:HIS:CG  | 2.45                     | 0.52              |
| 1:AQ:6:HIS:CE1    | 1:AQ:8:VAL:HB    | 2.45                     | 0.52              |
| 1:AR:97:LYS:HG3   | 1:AS:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:AW:152:TRP:HE1  | 1:AX:64:LYS:C    | 2.18                     | 0.52              |
| 1:AX:35:ASP:O     | 1:AX:39:ARG:HG3  | 2.10                     | 0.52              |
| 1:AZ:143:ILE:O    | 1:AZ:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:BB:121:GLU:O    | 1:BB:125:GLU:HG3 | 2.09                     | 0.52              |
| 1:BC:7:LEU:HB3    | 1:BR:39:ARG:O    | 2.09                     | 0.52              |
| 1:BC:70:LYS:HB2   | 1:BC:71:TYR:CE1  | 2.43                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BC:129:THR:O    | 1:BC:132:GLY:N   | 2.25                     | 0.52              |
| 1:BG:6:HIS:CE1    | 1:BG:8:VAL:HB    | 2.45                     | 0.52              |
| 1:BK:3:PHE:HD2    | 1:BK:150:LYS:HE2 | 1.74                     | 0.52              |
| 1:BQ:121:GLU:O    | 1:BQ:125:GLU:HG3 | 2.09                     | 0.52              |
| 1:BR:97:LYS:HG3   | 1:BS:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:BS:18:VAL:HG12  | 1:BS:77:LEU:CB   | 2.37                     | 0.52              |
| 1:BU:3:PHE:HD2    | 1:BU:150:LYS:HE2 | 1.74                     | 0.52              |
| 1:CC:6:HIS:HB3    | 1:CC:147:HIS:CG  | 2.45                     | 0.52              |
| 1:CC:152:TRP:HE1  | 1:CD:64:LYS:C    | 2.18                     | 0.52              |
| 1:CE:53:PRO:CD    | 1:CE:57:GLU:HG3  | 2.29                     | 0.52              |
| 1:CF:6:HIS:HB2    | 1:CF:147:HIS:ND1 | 2.24                     | 0.52              |
| 1:CH:97:LYS:HG3   | 1:CI:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:CK:109:PRO:HB3  | 1:CK:145:MET:HB3 | 1.91                     | 0.52              |
| 1:AA:143:ILE:O    | 1:AA:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:AD:18:VAL:HG12  | 1:AD:77:LEU:CB   | 2.37                     | 0.52              |
| 1:AE:18:VAL:HG12  | 1:AE:77:LEU:CB   | 2.37                     | 0.52              |
| 1:AW:6:HIS:HB3    | 1:AW:147:HIS:CG  | 2.45                     | 0.52              |
| 1:BD:104:LEU:HD13 | 1:BE:102:LEU:HG  | 1.91                     | 0.52              |
| 1:BM:152:TRP:HE1  | 1:BN:64:LYS:C    | 2.17                     | 0.52              |
| 1:BP:125:GLU:CA   | 1:BP:129:THR:OG1 | 2.57                     | 0.52              |
| 1:BS:35:ASP:O     | 1:BS:39:ARG:HG3  | 2.10                     | 0.52              |
| 1:BW:6:HIS:HB3    | 1:BW:147:HIS:CG  | 2.45                     | 0.52              |
| 1:BW:152:TRP:HE1  | 1:BX:64:LYS:C    | 2.18                     | 0.52              |
| 1:BZ:109:PRO:HB3  | 1:BZ:145:MET:HB3 | 1.91                     | 0.52              |
| 1:CJ:18:VAL:HG12  | 1:CJ:77:LEU:CB   | 2.37                     | 0.52              |
| 1:CM:97:LYS:HG3   | 1:CN:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:CM:152:TRP:HE1  | 1:CN:64:LYS:C    | 2.17                     | 0.52              |
| 1:CT:53:PRO:CG    | 1:CT:57:GLU:CG   | 2.46                     | 0.52              |
| 1:CY:152:TRP:HE3  | 1:CY:153:ALA:N   | 2.07                     | 0.52              |
| 1:CZ:6:HIS:HB2    | 1:CZ:147:HIS:ND1 | 2.24                     | 0.52              |
| 1:CZ:109:PRO:HB3  | 1:CZ:145:MET:HB3 | 1.91                     | 0.52              |
| 1:AA:125:GLU:CA   | 1:AA:129:THR:OG1 | 2.57                     | 0.52              |
| 1:AG:6:HIS:CE1    | 1:AG:8:VAL:HB    | 2.44                     | 0.52              |
| 1:AI:104:LEU:HD13 | 1:AJ:102:LEU:HG  | 1.91                     | 0.52              |
| 1:AS:6:HIS:HE1    | 1:AS:8:VAL:HB    | 1.75                     | 0.52              |
| 1:AT:18:VAL:HG12  | 1:AT:77:LEU:CB   | 2.37                     | 0.52              |
| 1:AV:121:GLU:O    | 1:AV:125:GLU:HG3 | 2.09                     | 0.52              |
| 1:BC:6:HIS:HB3    | 1:BC:147:HIS:CG  | 2.45                     | 0.52              |
| 1:BO:152:TRP:HE3  | 1:BO:153:ALA:N   | 2.07                     | 0.52              |
| 1:BX:35:ASP:O     | 1:BX:39:ARG:HG3  | 2.10                     | 0.52              |
| 1:BY:152:TRP:HE3  | 1:BY:153:ALA:N   | 2.07                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B2:6:HIS:HB3    | 1:B2:147:HIS:CG  | 2.45                     | 0.52              |
| 1:B2:152:TRP:HE1  | 1:B3:64:LYS:C    | 2.17                     | 0.52              |
| 1:B4:152:TRP:HE3  | 1:B4:153:ALA:N   | 2.07                     | 0.52              |
| 1:CB:75:ILE:HG22  | 1:CB:77:LEU:HD13 | 1.90                     | 0.52              |
| 1:CE:18:VAL:HG12  | 1:CE:77:LEU:CB   | 2.37                     | 0.52              |
| 1:CO:18:VAL:HG12  | 1:CO:77:LEU:CB   | 2.37                     | 0.52              |
| 1:CY:37:LEU:HD12  | 1:CY:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:CY:52:VAL:CB    | 1:CY:53:PRO:HD2  | 2.34                     | 0.52              |
| 1:AF:6:HIS:HB2    | 1:AF:147:HIS:ND1 | 2.24                     | 0.52              |
| 1:AP:6:HIS:HB2    | 1:AP:147:HIS:ND1 | 2.24                     | 0.52              |
| 1:AR:6:HIS:HB3    | 1:AR:147:HIS:CG  | 2.45                     | 0.52              |
| 1:A1:96:ALA:O     | 1:A1:100:ALA:HB2 | 2.06                     | 0.52              |
| 1:BD:11:GLY:HA3   | 1:CM:11:GLY:N    | 2.25                     | 0.52              |
| 1:BG:120:ILE:HD11 | 1:BQ:130:LYS:HG3 | 1.91                     | 0.52              |
| 1:BJ:53:PRO:CG    | 1:BJ:57:GLU:CG   | 2.46                     | 0.52              |
| 1:BP:6:HIS:HB2    | 1:BP:147:HIS:ND1 | 2.24                     | 0.52              |
| 1:BQ:96:ALA:O     | 1:BQ:100:ALA:HB2 | 2.06                     | 0.52              |
| 1:BR:152:TRP:HE1  | 1:BS:64:LYS:C    | 2.18                     | 0.52              |
| 1:BV:82:ARG:HG3   | 1:BV:118:GLU:OE2 | 2.10                     | 0.52              |
| 1:B1:6:HIS:CE1    | 1:B1:8:VAL:HB    | 2.44                     | 0.52              |
| 1:CD:35:ASP:O     | 1:CD:39:ARG:HG3  | 2.10                     | 0.52              |
| 1:CE:37:LEU:HD12  | 1:CE:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:CK:143:ILE:O    | 1:CK:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:CW:6:HIS:HB3    | 1:CW:147:HIS:CG  | 2.45                     | 0.52              |
| 1:C2:6:HIS:HB3    | 1:C2:147:HIS:CG  | 2.45                     | 0.52              |
| 1:C2:152:TRP:HE1  | 1:C3:64:LYS:C    | 2.18                     | 0.52              |
| 1:AD:97:LYS:HG3   | 1:AE:97:LYS:NZ   | 2.25                     | 0.52              |
| 1:AI:28:LYS:HG3   | 1:AK:24:PHE:CD1  | 2.44                     | 0.52              |
| 1:AM:97:LYS:HE3   | 1:AN:97:LYS:HZ1  | 1.75                     | 0.52              |
| 1:AM:152:TRP:HE1  | 1:AN:64:LYS:C    | 2.18                     | 0.52              |
| 1:AV:6:HIS:CE1    | 1:AV:8:VAL:HB    | 2.45                     | 0.52              |
| 1:AZ:3:PHE:HD2    | 1:AZ:150:LYS:HE2 | 1.74                     | 0.52              |
| 1:BO:52:VAL:HB    | 1:BO:53:PRO:CD   | 2.35                     | 0.52              |
| 1:BY:52:VAL:CB    | 1:BY:53:PRO:HD2  | 2.34                     | 0.52              |
| 1:B3:6:HIS:HE1    | 1:B3:8:VAL:HB    | 1.75                     | 0.52              |
| 1:CE:52:VAL:CB    | 1:CE:53:PRO:HD2  | 2.34                     | 0.52              |
| 1:CH:6:HIS:HB3    | 1:CH:147:HIS:CG  | 2.45                     | 0.52              |
| 1:CN:97:LYS:HG3   | 1:CO:97:LYS:NZ   | 2.25                     | 0.52              |
| 1:AE:152:TRP:HE3  | 1:AE:153:ALA:N   | 2.07                     | 0.52              |
| 1:AF:3:PHE:HD2    | 1:AF:150:LYS:HE2 | 1.74                     | 0.52              |
| 1:AF:109:PRO:HB3  | 1:AF:145:MET:HB3 | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AH:63:LYS:C     | 1:AH:65:MET:H    | 2.18                     | 0.52              |
| 1:AP:109:PRO:HB3  | 1:AP:145:MET:HB3 | 1.91                     | 0.52              |
| 1:AT:37:LEU:HD12  | 1:AT:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:AX:97:LYS:HG3   | 1:AY:97:LYS:NZ   | 2.25                     | 0.52              |
| 1:A4:152:TRP:HE3  | 1:A4:153:ALA:N   | 2.07                     | 0.52              |
| 1:BD:97:LYS:HG3   | 1:BE:97:LYS:NZ   | 2.25                     | 0.52              |
| 1:BH:70:LYS:HB2   | 1:BH:71:TYR:CE1  | 2.43                     | 0.52              |
| 1:BO:37:LEU:HD12  | 1:BO:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:B4:37:LEU:HD12  | 1:B4:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:CB:100:ALA:HA   | 1:CC:56:PHE:CZ   | 2.42                     | 0.52              |
| 1:CC:38:LYS:HZ2   | 1:CC:44:GLU:HA   | 1.75                     | 0.52              |
| 1:CC:97:LYS:HG3   | 1:CD:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:CH:63:LYS:C     | 1:CH:65:MET:H    | 2.18                     | 0.52              |
| 1:CI:35:ASP:O     | 1:CI:39:ARG:HG3  | 2.10                     | 0.52              |
| 1:CL:82:ARG:HG3   | 1:CL:118:GLU:OE2 | 2.10                     | 0.52              |
| 1:CL:129:THR:HG22 | 1:CL:130:LYS:H   | 1.72                     | 0.52              |
| 1:CW:97:LYS:HG3   | 1:CX:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:C1:82:ARG:HG3   | 1:C1:118:GLU:OE2 | 2.10                     | 0.52              |
| 1:AC:152:TRP:HE1  | 1:AD:64:LYS:C    | 2.17                     | 0.52              |
| 1:AH:129:THR:O    | 1:AH:132:GLY:N   | 2.25                     | 0.52              |
| 1:AK:109:PRO:HB3  | 1:AK:145:MET:HB3 | 1.92                     | 0.52              |
| 1:AN:6:HIS:HE1    | 1:AN:8:VAL:HB    | 1.75                     | 0.52              |
| 1:AN:35:ASP:O     | 1:AN:39:ARG:HG3  | 2.10                     | 0.52              |
| 1:AO:152:TRP:HE3  | 1:AO:153:ALA:N   | 2.07                     | 0.52              |
| 1:AP:3:PHE:HD2    | 1:AP:150:LYS:HE2 | 1.74                     | 0.52              |
| 1:AQ:13:LYS:CE    | 1:BU:43:GLU:HG2  | 2.40                     | 0.52              |
| 1:AR:97:LYS:HG3   | 1:AS:97:LYS:HZ3  | 1.75                     | 0.52              |
| 1:A1:6:HIS:CE1    | 1:A1:8:VAL:HB    | 2.45                     | 0.52              |
| 1:BC:97:LYS:HG3   | 1:BD:97:LYS:NZ   | 2.24                     | 0.52              |
| 1:BG:82:ARG:HG3   | 1:BG:118:GLU:OE2 | 2.10                     | 0.52              |
| 1:BI:104:LEU:HD13 | 1:BJ:102:LEU:HG  | 1.91                     | 0.52              |
| 1:BL:82:ARG:HG3   | 1:BL:118:GLU:OE2 | 2.10                     | 0.52              |
| 1:BO:52:VAL:CB    | 1:BO:53:PRO:HD2  | 2.34                     | 0.52              |
| 1:BR:63:LYS:C     | 1:BR:65:MET:H    | 2.18                     | 0.52              |
| 1:BS:104:LEU:HD13 | 1:BT:102:LEU:HG  | 1.91                     | 0.52              |
| 1:BX:104:LEU:HD13 | 1:BY:102:LEU:HG  | 1.91                     | 0.52              |
| 1:BZ:143:ILE:O    | 1:BZ:147:HIS:HB2 | 2.09                     | 0.52              |
| 1:CE:152:TRP:HE3  | 1:CE:153:ALA:N   | 2.07                     | 0.52              |
| 1:CP:109:PRO:HB3  | 1:CP:145:MET:HB3 | 1.91                     | 0.52              |
| 1:CV:121:GLU:O    | 1:CV:125:GLU:HG3 | 2.09                     | 0.52              |
| 1:CY:18:VAL:HG12  | 1:CY:77:LEU:CB   | 2.37                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C4:37:LEU:HD12  | 1:C4:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:AI:97:LYS:HG3   | 1:AJ:97:LYS:NZ   | 2.25                     | 0.52              |
| 1:AJ:37:LEU:HD12  | 1:AJ:47:ILE:HD11 | 1.91                     | 0.52              |
| 1:AT:109:PRO:HB3  | 1:AT:145:MET:HB3 | 1.92                     | 0.52              |
| 1:A3:35:ASP:O     | 1:A3:39:ARG:HG3  | 2.10                     | 0.52              |
| 1:BA:109:PRO:HB3  | 1:BA:145:MET:HB3 | 1.91                     | 0.52              |
| 1:BD:7:LEU:HB3    | 1:BJ:39:ARG:O    | 2.10                     | 0.52              |
| 1:BS:6:HIS:HE1    | 1:BS:8:VAL:HB    | 1.75                     | 0.52              |
| 1:BW:63:LYS:C     | 1:BW:65:MET:H    | 2.18                     | 0.52              |
| 1:CC:129:THR:CG2  | 1:CS:120:ILE:CD1 | 2.78                     | 0.52              |
| 1:CD:97:LYS:HG3   | 1:CE:97:LYS:NZ   | 2.25                     | 0.52              |
| 1:CR:63:LYS:C     | 1:CR:65:MET:H    | 2.18                     | 0.52              |
| 1:CS:6:HIS:HE1    | 1:CS:8:VAL:HB    | 1.75                     | 0.52              |
| 1:CV:6:HIS:CE1    | 1:CV:8:VAL:HB    | 2.44                     | 0.52              |
| 1:AI:35:ASP:O     | 1:AI:39:ARG:HG3  | 2.10                     | 0.51              |
| 1:AJ:109:PRO:HB3  | 1:AJ:145:MET:HB3 | 1.92                     | 0.51              |
| 1:AL:82:ARG:HG3   | 1:AL:118:GLU:OE2 | 2.10                     | 0.51              |
| 1:AN:97:LYS:HG3   | 1:AO:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:AS:97:LYS:HG3   | 1:AT:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:BD:35:ASP:O     | 1:BD:39:ARG:HG3  | 2.10                     | 0.51              |
| 1:BM:97:LYS:HG3   | 1:BN:97:LYS:NZ   | 2.24                     | 0.51              |
| 1:BN:104:LEU:HD13 | 1:BO:102:LEU:HG  | 1.91                     | 0.51              |
| 1:BR:97:LYS:HE3   | 1:BS:97:LYS:HZ3  | 1.75                     | 0.51              |
| 1:BT:37:LEU:HD12  | 1:BT:47:ILE:HD11 | 1.91                     | 0.51              |
| 1:CF:15:GLY:HA3   | 1:CF:65:MET:HE1  | 1.92                     | 0.51              |
| 1:CG:75:ILE:HG22  | 1:CG:77:LEU:HD13 | 1.90                     | 0.51              |
| 1:CL:6:HIS:CE1    | 1:CL:8:VAL:HB    | 2.45                     | 0.51              |
| 1:CO:37:LEU:HD12  | 1:CO:47:ILE:HD11 | 1.91                     | 0.51              |
| 1:CV:82:ARG:HG3   | 1:CV:118:GLU:OE2 | 2.10                     | 0.51              |
| 1:CW:129:THR:HG21 | 1:C3:120:ILE:CD1 | 2.40                     | 0.51              |
| 1:CX:18:VAL:HG12  | 1:CX:77:LEU:CB   | 2.37                     | 0.51              |
| 1:AL:6:HIS:CE1    | 1:AL:8:VAL:HB    | 2.44                     | 0.51              |
| 1:AR:63:LYS:C     | 1:AR:65:MET:H    | 2.18                     | 0.51              |
| 1:AU:125:GLU:CA   | 1:AU:129:THR:OG1 | 2.57                     | 0.51              |
| 1:AW:38:LYS:HZ2   | 1:AW:44:GLU:HA   | 1.76                     | 0.51              |
| 1:BC:63:LYS:C     | 1:BC:65:MET:H    | 2.18                     | 0.51              |
| 1:BH:152:TRP:HE1  | 1:BI:64:LYS:C    | 2.17                     | 0.51              |
| 1:BI:18:VAL:HG12  | 1:BI:77:LEU:CB   | 2.37                     | 0.51              |
| 1:BI:97:LYS:HG3   | 1:BJ:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:BK:109:PRO:HB3  | 1:BK:145:MET:HB3 | 1.91                     | 0.51              |
| 1:BM:63:LYS:C     | 1:BM:65:MET:H    | 2.18                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BN:35:ASP:O     | 1:BN:39:ARG:HG3  | 2.10                     | 0.51              |
| 1:BQ:82:ARG:HG3   | 1:BQ:118:GLU:OE2 | 2.10                     | 0.51              |
| 1:BU:125:GLU:CA   | 1:BU:129:THR:OG1 | 2.57                     | 0.51              |
| 1:B2:97:LYS:HG3   | 1:B3:97:LYS:NZ   | 2.24                     | 0.51              |
| 1:B3:104:LEU:HD13 | 1:B4:102:LEU:HG  | 1.91                     | 0.51              |
| 1:CE:53:PRO:CG    | 1:CE:57:GLU:CG   | 2.46                     | 0.51              |
| 1:CJ:37:LEU:HD12  | 1:CJ:47:ILE:HD11 | 1.91                     | 0.51              |
| 1:CT:37:LEU:HD12  | 1:CT:47:ILE:HD11 | 1.91                     | 0.51              |
| 1:AE:37:LEU:HD12  | 1:AE:47:ILE:HD11 | 1.91                     | 0.51              |
| 1:AM:63:LYS:C     | 1:AM:65:MET:H    | 2.18                     | 0.51              |
| 1:A1:82:ARG:HG3   | 1:A1:118:GLU:OE2 | 2.10                     | 0.51              |
| 1:A2:6:HIS:HB3    | 1:A2:147:HIS:CG  | 2.45                     | 0.51              |
| 1:A2:152:TRP:HE1  | 1:A3:64:LYS:C    | 2.18                     | 0.51              |
| 1:A3:18:VAL:HG12  | 1:A3:77:LEU:CB   | 2.37                     | 0.51              |
| 1:A3:97:LYS:HG3   | 1:A4:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:BA:125:GLU:CA   | 1:BA:129:THR:OG1 | 2.57                     | 0.51              |
| 1:BH:97:LYS:HG3   | 1:BI:97:LYS:NZ   | 2.24                     | 0.51              |
| 1:BS:97:LYS:HG3   | 1:BT:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:BX:6:HIS:HE1    | 1:BX:8:VAL:HB    | 1.75                     | 0.51              |
| 1:CB:6:HIS:CE1    | 1:CB:8:VAL:HB    | 2.45                     | 0.51              |
| 1:CP:28:LYS:HD2   | 1:CW:24:PHE:CE1  | 2.45                     | 0.51              |
| 1:CZ:15:GLY:HA3   | 1:CZ:65:MET:HE1  | 1.92                     | 0.51              |
| 1:AD:23:GLU:HA    | 1:AD:26:THR:OG1  | 2.11                     | 0.51              |
| 1:AD:35:ASP:O     | 1:AD:39:ARG:HG3  | 2.10                     | 0.51              |
| 1:AH:6:HIS:HB3    | 1:AH:147:HIS:CG  | 2.45                     | 0.51              |
| 1:AT:53:PRO:CG    | 1:AT:57:GLU:CG   | 2.46                     | 0.51              |
| 1:AU:15:GLY:HA3   | 1:AU:65:MET:HE1  | 1.92                     | 0.51              |
| 1:AU:109:PRO:HB3  | 1:AU:145:MET:HB3 | 1.91                     | 0.51              |
| 1:AZ:109:PRO:HB3  | 1:AZ:145:MET:HB3 | 1.92                     | 0.51              |
| 1:A3:23:GLU:HA    | 1:A3:26:THR:OG1  | 2.11                     | 0.51              |
| 1:BI:6:HIS:HE1    | 1:BI:8:VAL:HB    | 1.75                     | 0.51              |
| 1:BL:6:HIS:CE1    | 1:BL:8:VAL:HB    | 2.44                     | 0.51              |
| 1:BQ:6:HIS:CE1    | 1:BQ:8:VAL:HB    | 2.45                     | 0.51              |
| 1:B2:63:LYS:C     | 1:B2:65:MET:H    | 2.18                     | 0.51              |
| 1:B4:109:PRO:HB3  | 1:B4:145:MET:HB3 | 1.92                     | 0.51              |
| 1:CD:18:VAL:HG12  | 1:CD:77:LEU:CB   | 2.37                     | 0.51              |
| 1:CM:6:HIS:HB3    | 1:CM:147:HIS:CG  | 2.45                     | 0.51              |
| 1:CR:97:LYS:HG3   | 1:CS:97:LYS:NZ   | 2.24                     | 0.51              |
| 1:CS:23:GLU:HA    | 1:CS:26:THR:OG1  | 2.11                     | 0.51              |
| 1:CU:15:GLY:HA3   | 1:CU:65:MET:HE1  | 1.92                     | 0.51              |
| 1:C3:97:LYS:HG3   | 1:C4:97:LYS:NZ   | 2.25                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AA:109:PRO:HB3 | 1:AA:145:MET:HB3 | 1.91                     | 0.51              |
| 1:AM:82:ARG:CG   | 1:AM:82:ARG:NH1  | 2.73                     | 0.51              |
| 1:AR:82:ARG:CG   | 1:AR:82:ARG:NH1  | 2.73                     | 0.51              |
| 1:AW:63:LYS:C    | 1:AW:65:MET:H    | 2.18                     | 0.51              |
| 1:A4:109:PRO:HB3 | 1:A4:145:MET:HB3 | 1.92                     | 0.51              |
| 1:BB:6:HIS:CE1   | 1:BB:8:VAL:HB    | 2.45                     | 0.51              |
| 1:BD:6:HIS:HE1   | 1:BD:8:VAL:HB    | 1.75                     | 0.51              |
| 1:BJ:109:PRO:HB3 | 1:BJ:145:MET:HB3 | 1.92                     | 0.51              |
| 1:BN:97:LYS:HG3  | 1:BO:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:BP:109:PRO:HB3 | 1:BP:145:MET:HB3 | 1.91                     | 0.51              |
| 1:BR:82:ARG:CG   | 1:BR:82:ARG:NH1  | 2.73                     | 0.51              |
| 1:BZ:15:GLY:HA3  | 1:BZ:65:MET:HE1  | 1.93                     | 0.51              |
| 1:B2:82:ARG:CG   | 1:B2:82:ARG:NH1  | 2.73                     | 0.51              |
| 1:B3:35:ASP:O    | 1:B3:39:ARG:HG3  | 2.10                     | 0.51              |
| 1:CA:109:PRO:HB3 | 1:CA:145:MET:HB3 | 1.91                     | 0.51              |
| 1:CD:23:GLU:HA   | 1:CD:26:THR:OG1  | 2.11                     | 0.51              |
| 1:CH:152:TRP:HE1 | 1:CI:64:LYS:C    | 2.18                     | 0.51              |
| 1:CN:6:HIS:HE1   | 1:CN:8:VAL:HB    | 1.75                     | 0.51              |
| 1:CQ:82:ARG:HG3  | 1:CQ:118:GLU:OE2 | 2.10                     | 0.51              |
| 1:CR:152:TRP:HE1 | 1:CS:64:LYS:C    | 2.18                     | 0.51              |
| 1:C2:82:ARG:CG   | 1:C2:82:ARG:NH1  | 2.73                     | 0.51              |
| 1:AC:24:PHE:CD1  | 1:AU:28:LYS:HD2  | 2.46                     | 0.51              |
| 1:AX:6:HIS:HE1   | 1:AX:8:VAL:HB    | 1.75                     | 0.51              |
| 1:BH:6:HIS:HB3   | 1:BH:147:HIS:CG  | 2.45                     | 0.51              |
| 1:BI:35:ASP:O    | 1:BI:39:ARG:HG3  | 2.10                     | 0.51              |
| 1:BM:38:LYS:HZ2  | 1:BM:44:GLU:HA   | 1.75                     | 0.51              |
| 1:BN:23:GLU:HA   | 1:BN:26:THR:OG1  | 2.11                     | 0.51              |
| 1:BT:109:PRO:HB3 | 1:BT:145:MET:HB3 | 1.92                     | 0.51              |
| 1:BX:23:GLU:HA   | 1:BX:26:THR:OG1  | 2.11                     | 0.51              |
| 1:B4:52:VAL:CB   | 1:B4:53:PRO:HD2  | 2.34                     | 0.51              |
| 1:CB:82:ARG:HG3  | 1:CB:118:GLU:OE2 | 2.10                     | 0.51              |
| 1:CI:23:GLU:HA   | 1:CI:26:THR:OG1  | 2.11                     | 0.51              |
| 1:CM:63:LYS:C    | 1:CM:65:MET:H    | 2.18                     | 0.51              |
| 1:CS:97:LYS:HG3  | 1:CT:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:CW:63:LYS:C    | 1:CW:65:MET:H    | 2.18                     | 0.51              |
| 1:CX:97:LYS:HG3  | 1:CY:97:LYS:NZ   | 2.25                     | 0.51              |
| 1:C3:6:HIS:HE1   | 1:C3:8:VAL:HB    | 1.75                     | 0.51              |
| 1:C3:35:ASP:O    | 1:C3:39:ARG:HG3  | 2.10                     | 0.51              |
| 1:AA:15:GLY:HA3  | 1:AA:65:MET:HE1  | 1.92                     | 0.51              |
| 1:AD:6:HIS:HE1   | 1:AD:8:VAL:HB    | 1.75                     | 0.51              |
| 1:AF:15:GLY:HA3  | 1:AF:65:MET:HE1  | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AM:97:LYS:HG3   | 1:AN:97:LYS:HZ1   | 1.74                     | 0.51              |
| 1:AP:15:GLY:HA3   | 1:AP:65:MET:HE1   | 1.92                     | 0.51              |
| 1:AS:35:ASP:O     | 1:AS:39:ARG:HG3   | 2.10                     | 0.51              |
| 1:AY:109:PRO:HB3  | 1:AY:145:MET:HB3  | 1.92                     | 0.51              |
| 1:AZ:15:GLY:HA3   | 1:AZ:65:MET:HE1   | 1.92                     | 0.51              |
| 1:BB:82:ARG:HG3   | 1:BB:118:GLU:OE2  | 2.10                     | 0.51              |
| 1:BO:53:PRO:CG    | 1:BO:57:GLU:CG    | 2.46                     | 0.51              |
| 1:B1:82:ARG:HG3   | 1:B1:118:GLU:OE2  | 2.10                     | 0.51              |
| 1:CC:63:LYS:C     | 1:CC:65:MET:H     | 2.18                     | 0.51              |
| 1:CE:109:PRO:HB3  | 1:CE:145:MET:HB3  | 1.92                     | 0.51              |
| 1:CR:6:HIS:HB3    | 1:CR:147:HIS:CG   | 2.45                     | 0.51              |
| 1:CX:6:HIS:HE1    | 1:CX:8:VAL:HB     | 1.75                     | 0.51              |
| 1:C3:23:GLU:HA    | 1:C3:26:THR:OG1   | 2.11                     | 0.51              |
| 1:AB:82:ARG:HG3   | 1:AB:118:GLU:OE2  | 2.10                     | 0.51              |
| 1:AX:39:ARG:O     | 1:A4:7:LEU:HB3    | 2.11                     | 0.51              |
| 1:A3:6:HIS:HE1    | 1:A3:8:VAL:HB     | 1.75                     | 0.51              |
| 1:BC:129:THR:HG21 | 1:BS:120:ILE:HD13 | 1.89                     | 0.51              |
| 1:BF:3:PHE:HD2    | 1:BF:150:LYS:HE2  | 1.74                     | 0.51              |
| 1:BG:24:PHE:CE2   | 1:BQ:124:ILE:HD11 | 2.46                     | 0.51              |
| 1:B3:97:LYS:HG3   | 1:B4:97:LYS:NZ    | 2.25                     | 0.51              |
| 1:CE:7:LEU:HB3    | 1:CN:39:ARG:O     | 2.10                     | 0.51              |
| 1:CQ:6:HIS:CE1    | 1:CQ:8:VAL:HB     | 2.44                     | 0.51              |
| 1:CX:23:GLU:HA    | 1:CX:26:THR:OG1   | 2.11                     | 0.51              |
| 1:CY:53:PRO:HD2   | 1:CY:57:GLU:HB2   | 1.93                     | 0.51              |
| 1:C4:109:PRO:HB3  | 1:C4:145:MET:HB3  | 1.92                     | 0.51              |
| 1:AH:152:TRP:HE1  | 1:AI:64:LYS:C     | 2.17                     | 0.51              |
| 1:AN:23:GLU:HA    | 1:AN:26:THR:OG1   | 2.11                     | 0.51              |
| 1:AQ:82:ARG:HG3   | 1:AQ:118:GLU:OE2  | 2.10                     | 0.51              |
| 1:AS:104:LEU:HD13 | 1:AT:102:LEU:HG   | 1.91                     | 0.51              |
| 1:AW:97:LYS:HG3   | 1:AX:97:LYS:NZ    | 2.24                     | 0.51              |
| 1:BF:109:PRO:HB3  | 1:BF:145:MET:HB3  | 1.91                     | 0.51              |
| 1:BO:109:PRO:HB3  | 1:BO:145:MET:HB3  | 1.92                     | 0.51              |
| 1:BY:52:VAL:HB    | 1:BY:53:PRO:CD    | 2.35                     | 0.51              |
| 1:CG:82:ARG:HG3   | 1:CG:118:GLU:OE2  | 2.10                     | 0.51              |
| 1:CJ:53:PRO:HD2   | 1:CJ:57:GLU:HB2   | 1.93                     | 0.51              |
| 1:C1:6:HIS:CE1    | 1:C1:8:VAL:HB     | 2.45                     | 0.51              |
| 1:AB:6:HIS:CE1    | 1:AB:8:VAL:HB     | 2.45                     | 0.51              |
| 1:AC:82:ARG:CG    | 1:AC:82:ARG:NH1   | 2.73                     | 0.51              |
| 1:AO:53:PRO:HG2   | 1:AO:57:GLU:HG3   | 0.65                     | 0.51              |
| 1:AY:53:PRO:HD2   | 1:AY:57:GLU:HB2   | 1.93                     | 0.51              |
| 1:A4:52:VAL:HB    | 1:A4:53:PRO:CD    | 2.35                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A4:53:PRO:HD2  | 1:A4:57:GLU:HB2   | 1.93                     | 0.51              |
| 1:BJ:152:TRP:HE3 | 1:BJ:153:ALA:N    | 2.07                     | 0.51              |
| 1:BW:82:ARG:CG   | 1:BW:82:ARG:NH1   | 2.73                     | 0.51              |
| 1:B4:53:PRO:HD2  | 1:B4:57:GLU:HB2   | 1.93                     | 0.51              |
| 1:CF:109:PRO:HB3 | 1:CF:145:MET:HB3  | 1.91                     | 0.51              |
| 1:CI:18:VAL:HG12 | 1:CI:77:LEU:CB    | 2.37                     | 0.51              |
| 1:CI:97:LYS:HG3  | 1:CJ:97:LYS:NZ    | 2.25                     | 0.51              |
| 1:CK:15:GLY:HA3  | 1:CK:65:MET:HE1   | 1.93                     | 0.51              |
| 1:CN:35:ASP:O    | 1:CN:39:ARG:HG3   | 2.10                     | 0.51              |
| 1:CX:35:ASP:O    | 1:CX:39:ARG:HG3   | 2.10                     | 0.51              |
| 1:C2:38:LYS:HZ2  | 1:C2:44:GLU:HA    | 1.75                     | 0.51              |
| 1:AC:39:ARG:O    | 1:AR:7:LEU:HB3    | 2.11                     | 0.50              |
| 1:AG:82:ARG:HG3  | 1:AG:118:GLU:OE2  | 2.10                     | 0.50              |
| 1:AK:15:GLY:HA3  | 1:AK:65:MET:HE1   | 1.92                     | 0.50              |
| 1:AO:53:PRO:CG   | 1:AO:57:GLU:CG    | 2.46                     | 0.50              |
| 1:AW:52:VAL:CG1  | 1:AW:61:ILE:HD12  | 2.35                     | 0.50              |
| 1:BD:23:GLU:HA   | 1:BD:26:THR:OG1   | 2.11                     | 0.50              |
| 1:BW:38:LYS:HZ2  | 1:BW:44:GLU:HA    | 1.76                     | 0.50              |
| 1:BX:97:LYS:HG3  | 1:BY:97:LYS:NZ    | 2.25                     | 0.50              |
| 1:CC:52:VAL:CG1  | 1:CC:61:ILE:HD12  | 2.35                     | 0.50              |
| 1:CS:35:ASP:O    | 1:CS:39:ARG:HG3   | 2.10                     | 0.50              |
| 1:C2:63:LYS:C    | 1:C2:65:MET:H     | 2.18                     | 0.50              |
| 1:AA:102:LEU:CD2 | 1:AE:104:LEU:HD13 | 2.42                     | 0.50              |
| 1:AC:63:LYS:C    | 1:AC:65:MET:H     | 2.18                     | 0.50              |
| 1:AP:102:LEU:CD2 | 1:AT:104:LEU:HD13 | 2.42                     | 0.50              |
| 1:AU:102:LEU:CD2 | 1:AY:104:LEU:HD13 | 2.42                     | 0.50              |
| 1:AV:82:ARG:HG3  | 1:AV:118:GLU:OE2  | 2.10                     | 0.50              |
| 1:A2:63:LYS:C    | 1:A2:65:MET:H     | 2.18                     | 0.50              |
| 1:BB:125:GLU:HG2 | 1:BV:120:ILE:CD1  | 2.41                     | 0.50              |
| 1:BE:109:PRO:HB3 | 1:BE:145:MET:HB3  | 1.92                     | 0.50              |
| 1:CD:6:HIS:HE1   | 1:CD:8:VAL:HB     | 1.75                     | 0.50              |
| 1:CJ:109:PRO:HB3 | 1:CJ:145:MET:HB3  | 1.92                     | 0.50              |
| 1:CO:52:VAL:HB   | 1:CO:53:PRO:CD    | 2.35                     | 0.50              |
| 1:C4:53:PRO:HD2  | 1:C4:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:AI:6:HIS:HE1   | 1:AI:8:VAL:HB     | 1.75                     | 0.50              |
| 1:AS:18:VAL:HG12 | 1:AS:77:LEU:CB    | 2.37                     | 0.50              |
| 1:AT:53:PRO:HD2  | 1:AT:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:AZ:102:LEU:CD2 | 1:A4:104:LEU:HD13 | 2.42                     | 0.50              |
| 1:BF:15:GLY:HA3  | 1:BF:65:MET:HE1   | 1.92                     | 0.50              |
| 1:BJ:53:PRO:HD2  | 1:BJ:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:BZ:102:LEU:CD2 | 1:B4:104:LEU:HD13 | 2.42                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CG:6:HIS:CE1   | 1:CG:8:VAL:HB     | 2.44                     | 0.50              |
| 1:CP:125:GLU:CA  | 1:CP:129:THR:OG1  | 2.57                     | 0.50              |
| 1:CW:82:ARG:CG   | 1:CW:82:ARG:NH1   | 2.73                     | 0.50              |
| 1:C3:18:VAL:HG12 | 1:C3:77:LEU:CB    | 2.37                     | 0.50              |
| 1:AF:39:ARG:NH2  | 1:AQ:144:GLU:CD   | 2.68                     | 0.50              |
| 1:BY:53:PRO:HD2  | 1:BY:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:CN:18:VAL:HG12 | 1:CN:77:LEU:CB    | 2.37                     | 0.50              |
| 1:CO:53:PRO:HD2  | 1:CO:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:AC:38:LYS:HZ2  | 1:AC:44:GLU:HA    | 1.76                     | 0.50              |
| 1:AE:109:PRO:HB3 | 1:AE:145:MET:HB3  | 1.92                     | 0.50              |
| 1:AJ:53:PRO:HD2  | 1:AJ:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:AO:109:PRO:HB3 | 1:AO:145:MET:HB3  | 1.92                     | 0.50              |
| 1:BU:109:PRO:HB3 | 1:BU:145:MET:HB3  | 1.91                     | 0.50              |
| 1:CO:109:PRO:HB3 | 1:CO:145:MET:HB3  | 1.92                     | 0.50              |
| 1:CP:102:LEU:CD2 | 1:CT:104:LEU:HD13 | 2.42                     | 0.50              |
| 1:CX:20:ARG:NH1  | 1:C2:39:ARG:CZ    | 2.74                     | 0.50              |
| 1:CY:109:PRO:HB3 | 1:CY:145:MET:HB3  | 1.92                     | 0.50              |
| 1:AI:23:GLU:HA   | 1:AI:26:THR:OG1   | 2.11                     | 0.50              |
| 1:AS:23:GLU:HA   | 1:AS:26:THR:OG1   | 2.11                     | 0.50              |
| 1:BA:15:GLY:HA3  | 1:BA:65:MET:HE1   | 1.92                     | 0.50              |
| 1:BK:18:VAL:HG21 | 1:BK:30:LEU:HD13  | 1.94                     | 0.50              |
| 1:BO:16:VAL:HG22 | 1:BO:49:VAL:HG22  | 1.94                     | 0.50              |
| 1:CE:16:VAL:HG22 | 1:CE:49:VAL:HG22  | 1.94                     | 0.50              |
| 1:CS:116:THR:O   | 1:CT:85:THR:HB    | 2.12                     | 0.50              |
| 1:CZ:102:LEU:CD2 | 1:C4:104:LEU:HD13 | 2.42                     | 0.50              |
| 1:AE:82:ARG:HG3  | 1:AE:118:GLU:OE2  | 2.12                     | 0.50              |
| 1:AX:23:GLU:HA   | 1:AX:26:THR:OG1   | 2.11                     | 0.50              |
| 1:AZ:125:GLU:CA  | 1:AZ:129:THR:OG1  | 2.57                     | 0.50              |
| 1:BE:52:VAL:CB   | 1:BE:53:PRO:HD2   | 2.34                     | 0.50              |
| 1:BF:125:GLU:CA  | 1:BF:129:THR:OG1  | 2.57                     | 0.50              |
| 1:BI:23:GLU:HA   | 1:BI:26:THR:OG1   | 2.11                     | 0.50              |
| 1:BN:6:HIS:HE1   | 1:BN:8:VAL:HB     | 1.75                     | 0.50              |
| 1:BP:15:GLY:HA3  | 1:BP:65:MET:HE1   | 1.93                     | 0.50              |
| 1:BS:23:GLU:HA   | 1:BS:26:THR:OG1   | 2.11                     | 0.50              |
| 1:BT:53:PRO:HD2  | 1:BT:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:BU:15:GLY:HA3  | 1:BU:65:MET:HE1   | 1.93                     | 0.50              |
| 1:BY:109:PRO:HB3 | 1:BY:145:MET:HB3  | 1.92                     | 0.50              |
| 1:CC:8:VAL:HG22  | 1:CR:8:VAL:HG22   | 1.93                     | 0.50              |
| 1:CO:82:ARG:HG3  | 1:CO:118:GLU:OE2  | 2.12                     | 0.50              |
| 1:CP:39:ARG:NH2  | 1:CV:144:GLU:CD   | 2.68                     | 0.50              |
| 1:AF:102:LEU:CD2 | 1:AJ:104:LEU:HD13 | 2.42                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AF:125:GLU:CA  | 1:AF:129:THR:OG1  | 2.57                     | 0.50              |
| 1:AH:82:ARG:CG   | 1:AH:82:ARG:NH1   | 2.73                     | 0.50              |
| 1:AI:28:LYS:NZ   | 1:AK:28:LYS:NZ    | 2.59                     | 0.50              |
| 1:AO:16:VAL:HG22 | 1:AO:49:VAL:HG22  | 1.94                     | 0.50              |
| 1:AZ:18:VAL:HG21 | 1:AZ:30:LEU:HD13  | 1.94                     | 0.50              |
| 1:A2:97:LYS:HE3  | 1:A3:97:LYS:HZ1   | 1.76                     | 0.50              |
| 1:BD:116:THR:O   | 1:BE:85:THR:HB    | 2.12                     | 0.50              |
| 1:BG:96:ALA:O    | 1:BG:100:ALA:HB2  | 2.06                     | 0.50              |
| 1:BT:82:ARG:HG3  | 1:BT:118:GLU:OE2  | 2.12                     | 0.50              |
| 1:BU:18:VAL:HG21 | 1:BU:30:LEU:HD13  | 1.94                     | 0.50              |
| 1:BX:116:THR:O   | 1:BY:85:THR:HB    | 2.12                     | 0.50              |
| 1:CA:18:VAL:HG21 | 1:CA:30:LEU:HD13  | 1.94                     | 0.50              |
| 1:CN:23:GLU:HA   | 1:CN:26:THR:OG1   | 2.11                     | 0.50              |
| 1:CR:97:LYS:HE3  | 1:CS:97:LYS:HZ1   | 1.77                     | 0.50              |
| 1:CW:97:LYS:HE3  | 1:CX:97:LYS:HZ1   | 1.77                     | 0.50              |
| 1:AD:6:HIS:CE1   | 1:AD:8:VAL:HB     | 2.47                     | 0.50              |
| 1:AE:16:VAL:HG22 | 1:AE:49:VAL:HG22  | 1.94                     | 0.50              |
| 1:AJ:82:ARG:HG3  | 1:AJ:118:GLU:OE2  | 2.12                     | 0.50              |
| 1:AT:16:VAL:HG22 | 1:AT:49:VAL:HG22  | 1.94                     | 0.50              |
| 1:AX:116:THR:O   | 1:AY:85:THR:HB    | 2.12                     | 0.50              |
| 1:BE:53:PRO:HD2  | 1:BE:57:GLU:HB2   | 1.93                     | 0.50              |
| 1:BT:53:PRO:CG   | 1:BT:57:GLU:CG    | 2.46                     | 0.50              |
| 1:CA:125:GLU:CA  | 1:CA:129:THR:OG1  | 2.57                     | 0.50              |
| 1:CP:18:VAL:HG21 | 1:CP:30:LEU:HD13  | 1.94                     | 0.50              |
| 1:CR:82:ARG:CG   | 1:CR:82:ARG:NH1   | 2.73                     | 0.50              |
| 1:CW:38:LYS:HZ2  | 1:CW:44:GLU:HA    | 1.74                     | 0.50              |
| 1:CW:52:VAL:CG1  | 1:CW:61:ILE:HD12  | 2.35                     | 0.50              |
| 1:CX:116:THR:O   | 1:CY:85:THR:HB    | 2.12                     | 0.50              |
| 1:C4:82:ARG:HG3  | 1:C4:118:GLU:OE2  | 2.12                     | 0.50              |
| 1:AE:53:PRO:HD2  | 1:AE:57:GLU:HB2   | 1.93                     | 0.49              |
| 1:AN:116:THR:O   | 1:AO:85:THR:HB    | 2.12                     | 0.49              |
| 1:AO:53:PRO:HD2  | 1:AO:57:GLU:HB2   | 1.93                     | 0.49              |
| 1:AO:82:ARG:HG3  | 1:AO:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:BA:102:LEU:CD2 | 1:BE:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:BJ:16:VAL:HG22 | 1:BJ:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:BU:102:LEU:CD2 | 1:BY:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:BY:16:VAL:HG22 | 1:BY:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:B4:53:PRO:CG   | 1:B4:57:GLU:CG    | 2.46                     | 0.49              |
| 1:CI:6:HIS:HE1   | 1:CI:8:VAL:HB     | 1.75                     | 0.49              |
| 1:CJ:24:PHE:CD1  | 1:CO:28:LYS:HG3   | 2.46                     | 0.49              |
| 1:CZ:18:VAL:HG21 | 1:CZ:30:LEU:HD13  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C3:6:HIS:CE1   | 1:C3:8:VAL:HB     | 2.47                     | 0.49              |
| 1:AA:18:VAL:HG21 | 1:AA:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:AF:18:VAL:HG21 | 1:AF:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:AI:6:HIS:CE1   | 1:AI:8:VAL:HB     | 2.47                     | 0.49              |
| 1:BE:7:LEU:HD23  | 1:BN:40:HIS:CE1   | 2.46                     | 0.49              |
| 1:BK:58:ILE:O    | 1:BK:58:ILE:HG22  | 2.11                     | 0.49              |
| 1:B3:23:GLU:HA   | 1:B3:26:THR:OG1   | 2.11                     | 0.49              |
| 1:CP:15:GLY:HA3  | 1:CP:65:MET:HE1   | 1.92                     | 0.49              |
| 1:CT:82:ARG:HG3  | 1:CT:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:CT:109:PRO:HB3 | 1:CT:145:MET:HB3  | 1.92                     | 0.49              |
| 1:C2:17:VAL:HG21 | 1:C2:62:ALA:HA    | 1.94                     | 0.49              |
| 1:C3:116:THR:O   | 1:C4:85:THR:HB    | 2.12                     | 0.49              |
| 1:AJ:52:VAL:HB   | 1:AJ:53:PRO:CD    | 2.35                     | 0.49              |
| 1:BF:18:VAL:HG21 | 1:BF:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:BH:63:LYS:C    | 1:BH:65:MET:H     | 2.18                     | 0.49              |
| 1:BI:6:HIS:CE1   | 1:BI:8:VAL:HB     | 2.47                     | 0.49              |
| 1:B2:17:VAL:HG21 | 1:B2:62:ALA:HA    | 1.94                     | 0.49              |
| 1:B2:52:VAL:CG1  | 1:B2:61:ILE:HD12  | 2.35                     | 0.49              |
| 1:B4:16:VAL:HG22 | 1:B4:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:CA:15:GLY:HA3  | 1:CA:65:MET:HE1   | 1.93                     | 0.49              |
| 1:CX:6:HIS:CE1   | 1:CX:8:VAL:HB     | 2.47                     | 0.49              |
| 1:C2:18:VAL:HG22 | 1:C2:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:AD:116:THR:O   | 1:AE:85:THR:HB    | 2.12                     | 0.49              |
| 1:AK:18:VAL:HG21 | 1:AK:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:AM:18:VAL:HG22 | 1:AM:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:AN:6:HIS:CE1   | 1:AN:8:VAL:HB     | 2.47                     | 0.49              |
| 1:AP:18:VAL:HG21 | 1:AP:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:AY:82:ARG:HG3  | 1:AY:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:BJ:18:VAL:HG23 | 1:BJ:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:B3:116:THR:O   | 1:B4:85:THR:HB    | 2.12                     | 0.49              |
| 1:CH:18:VAL:HG22 | 1:CH:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:CT:16:VAL:HG22 | 1:CT:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:CW:17:VAL:HG21 | 1:CW:62:ALA:HA    | 1.95                     | 0.49              |
| 1:C2:97:LYS:HE3  | 1:C3:97:LYS:HZ3   | 1.77                     | 0.49              |
| 1:AY:16:VAL:HG22 | 1:AY:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:BB:96:ALA:O    | 1:BB:100:ALA:HB2  | 2.06                     | 0.49              |
| 1:BE:18:VAL:HG23 | 1:BE:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:BE:82:ARG:HG3  | 1:BE:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:BF:102:LEU:CD2 | 1:BJ:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:BI:116:THR:O   | 1:BJ:85:THR:HB    | 2.12                     | 0.49              |
| 1:BT:16:VAL:HG22 | 1:BT:49:VAL:HG22  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CB:12:LEU:HD11 | 1:CB:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:CE:18:VAL:HG23 | 1:CE:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:CR:17:VAL:HG21 | 1:CR:62:ALA:HA    | 1.95                     | 0.49              |
| 1:CY:16:VAL:HG22 | 1:CY:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:AE:18:VAL:HG23 | 1:AE:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:AH:18:VAL:HG22 | 1:AH:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:AI:116:THR:O   | 1:AJ:85:THR:HB    | 2.12                     | 0.49              |
| 1:AK:102:LEU:CD2 | 1:AO:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:A4:16:VAL:HG22 | 1:A4:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:A4:18:VAL:HG23 | 1:A4:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:A4:82:ARG:HG3  | 1:A4:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:BC:28:LYS:HZ3  | 1:BU:28:LYS:CE    | 2.25                     | 0.49              |
| 1:BO:18:VAL:HG23 | 1:BO:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:BQ:12:LEU:HD11 | 1:BQ:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:BX:6:HIS:CE1   | 1:BX:8:VAL:HB     | 2.47                     | 0.49              |
| 1:BZ:18:VAL:HG21 | 1:BZ:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:CA:102:LEU:CD2 | 1:CE:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:CK:125:GLU:CA  | 1:CK:129:THR:OG1  | 2.57                     | 0.49              |
| 1:CV:12:LEU:HD11 | 1:CV:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:AP:58:ILE:O    | 1:AP:58:ILE:HG22  | 2.11                     | 0.49              |
| 1:AV:12:LEU:HD11 | 1:AV:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:A1:12:LEU:HD11 | 1:A1:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:A2:17:VAL:HG21 | 1:A2:62:ALA:HA    | 1.95                     | 0.49              |
| 1:A3:116:THR:O   | 1:A4:85:THR:HB    | 2.12                     | 0.49              |
| 1:A4:88:TYR:C    | 1:A4:88:TYR:CD2   | 2.91                     | 0.49              |
| 1:BK:15:GLY:HA3  | 1:BK:65:MET:HE1   | 1.93                     | 0.49              |
| 1:BK:102:LEU:CD2 | 1:BO:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:BT:18:VAL:HG23 | 1:BT:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:CC:17:VAL:HG21 | 1:CC:62:ALA:HA    | 1.95                     | 0.49              |
| 1:CC:129:THR:CG2 | 1:CS:120:ILE:HD11 | 2.40                     | 0.49              |
| 1:CE:53:PRO:HD2  | 1:CE:57:GLU:HB2   | 1.93                     | 0.49              |
| 1:CF:102:LEU:CD2 | 1:CJ:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:CK:18:VAL:HG21 | 1:CK:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:CM:82:ARG:CG   | 1:CM:82:ARG:NH1   | 2.73                     | 0.49              |
| 1:CT:53:PRO:HD2  | 1:CT:57:GLU:HB2   | 1.93                     | 0.49              |
| 1:CU:18:VAL:HG21 | 1:CU:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:AL:65:MET:O    | 1:AL:68:SER:HB3   | 2.13                     | 0.49              |
| 1:AT:88:TYR:C    | 1:AT:88:TYR:CD2   | 2.91                     | 0.49              |
| 1:AY:18:VAL:HG23 | 1:AY:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:AY:88:TYR:CD2  | 1:AY:88:TYR:C     | 2.91                     | 0.49              |
| 1:BB:12:LEU:HD11 | 1:BB:143:ILE:HG23 | 1.95                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BE:71:TYR:O    | 1:BE:150:LYS:NZ   | 2.44                     | 0.49              |
| 1:BN:6:HIS:CE1   | 1:BN:8:VAL:HB     | 2.47                     | 0.49              |
| 1:BP:102:LEU:CD2 | 1:BT:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:BT:24:PHE:CD1  | 1:BY:28:LYS:HG3   | 2.48                     | 0.49              |
| 1:CD:6:HIS:CE1   | 1:CD:8:VAL:HB     | 2.47                     | 0.49              |
| 1:CD:106:THR:O   | 1:CD:107:ASP:HB3  | 2.13                     | 0.49              |
| 1:CE:82:ARG:HG3  | 1:CE:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:CJ:16:VAL:HG22 | 1:CJ:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:CK:102:LEU:CD2 | 1:CO:104:LEU:HD13 | 2.42                     | 0.49              |
| 1:CM:18:VAL:HG22 | 1:CM:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:CN:106:THR:O   | 1:CN:107:ASP:HB3  | 2.13                     | 0.49              |
| 1:CW:18:VAL:HG22 | 1:CW:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:C4:16:VAL:HG22 | 1:C4:49:VAL:HG22  | 1.94                     | 0.49              |
| 1:AC:18:VAL:HG22 | 1:AC:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:AJ:88:TYR:CD2  | 1:AJ:88:TYR:C     | 2.91                     | 0.49              |
| 1:AL:12:LEU:HD11 | 1:AL:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:AS:6:HIS:CE1   | 1:AS:8:VAL:HB     | 2.47                     | 0.49              |
| 1:AU:18:VAL:HG21 | 1:AU:30:LEU:HD13  | 1.94                     | 0.49              |
| 1:AY:52:VAL:CB   | 1:AY:53:PRO:HD2   | 2.33                     | 0.49              |
| 1:BC:18:VAL:HG22 | 1:BC:77:LEU:HB2   | 1.95                     | 0.49              |
| 1:BO:53:PRO:HG2  | 1:BO:57:GLU:HG3   | 0.65                     | 0.49              |
| 1:BY:82:ARG:HG3  | 1:BY:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:B1:65:MET:O    | 1:B1:68:SER:HB3   | 2.13                     | 0.49              |
| 1:CH:17:VAL:HG21 | 1:CH:62:ALA:HA    | 1.95                     | 0.49              |
| 1:CN:98:GLY:O    | 1:CN:102:LEU:HB2  | 2.13                     | 0.49              |
| 1:CO:18:VAL:HG23 | 1:CO:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:CS:6:HIS:CE1   | 1:CS:8:VAL:HB     | 2.47                     | 0.49              |
| 1:CY:18:VAL:HG23 | 1:CY:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:CY:82:ARG:HG3  | 1:CY:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:AO:45:ASN:C    | 1:AO:47:ILE:H     | 2.21                     | 0.49              |
| 1:AO:88:TYR:CD2  | 1:AO:88:TYR:C     | 2.91                     | 0.49              |
| 1:AQ:65:MET:O    | 1:AQ:68:SER:HB3   | 2.13                     | 0.49              |
| 1:AR:17:VAL:HG21 | 1:AR:62:ALA:HA    | 1.95                     | 0.49              |
| 1:AR:38:LYS:HZ2  | 1:AR:44:GLU:HA    | 1.78                     | 0.49              |
| 1:AS:98:GLY:O    | 1:AS:102:LEU:HB2  | 2.13                     | 0.49              |
| 1:AT:82:ARG:HG3  | 1:AT:118:GLU:OE2  | 2.12                     | 0.49              |
| 1:AW:18:VAL:HG22 | 1:AW:77:LEU:HB2   | 1.94                     | 0.49              |
| 1:AX:106:THR:O   | 1:AX:107:ASP:HB3  | 2.13                     | 0.49              |
| 1:A4:53:PRO:CG   | 1:A4:57:GLU:CG    | 2.46                     | 0.49              |
| 1:BG:12:LEU:HD11 | 1:BG:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:BI:106:THR:O   | 1:BI:107:ASP:HB3  | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BR:17:VAL:HG21 | 1:BR:62:ALA:HA    | 1.95                     | 0.49              |
| 1:BS:6:HIS:CE1   | 1:BS:8:VAL:HB     | 2.47                     | 0.49              |
| 1:BT:52:VAL:CB   | 1:BT:53:PRO:HD2   | 2.33                     | 0.49              |
| 1:BV:12:LEU:HD11 | 1:BV:143:ILE:HG23 | 1.95                     | 0.49              |
| 1:BY:45:ASN:C    | 1:BY:47:ILE:H     | 2.21                     | 0.49              |
| 1:B3:106:THR:O   | 1:B3:107:ASP:HB3  | 2.13                     | 0.49              |
| 1:CD:116:THR:O   | 1:CE:85:THR:HB    | 2.12                     | 0.49              |
| 1:CI:116:THR:O   | 1:CJ:85:THR:HB    | 2.12                     | 0.49              |
| 1:CT:18:VAL:HG23 | 1:CT:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:CY:45:ASN:C    | 1:CY:47:ILE:H     | 2.21                     | 0.49              |
| 1:C4:18:VAL:HG23 | 1:C4:51:TRP:CE3   | 2.48                     | 0.49              |
| 1:AG:12:LEU:HD11 | 1:AG:143:ILE:HG23 | 1.95                     | 0.48              |
| 1:AN:106:THR:O   | 1:AN:107:ASP:HB3  | 2.13                     | 0.48              |
| 1:AT:18:VAL:HG23 | 1:AT:51:TRP:CE3   | 2.48                     | 0.48              |
| 1:AY:45:ASN:C    | 1:AY:47:ILE:H     | 2.21                     | 0.48              |
| 1:A1:65:MET:O    | 1:A1:68:SER:HB3   | 2.13                     | 0.48              |
| 1:BH:82:ARG:CG   | 1:BH:82:ARG:NH1   | 2.73                     | 0.48              |
| 1:BM:18:VAL:HG22 | 1:BM:77:LEU:HB2   | 1.94                     | 0.48              |
| 1:BN:106:THR:O   | 1:BN:107:ASP:HB3  | 2.13                     | 0.48              |
| 1:BY:88:TYR:C    | 1:BY:88:TYR:CD2   | 2.91                     | 0.48              |
| 1:B3:6:HIS:CE1   | 1:B3:8:VAL:HB     | 2.47                     | 0.48              |
| 1:CI:6:HIS:CE1   | 1:CI:8:VAL:HB     | 2.47                     | 0.48              |
| 1:CI:106:THR:O   | 1:CI:107:ASP:HB3  | 2.13                     | 0.48              |
| 1:CJ:88:TYR:C    | 1:CJ:88:TYR:CD2   | 2.91                     | 0.48              |
| 1:CN:6:HIS:CE1   | 1:CN:8:VAL:HB     | 2.47                     | 0.48              |
| 1:CN:116:THR:O   | 1:CO:85:THR:HB    | 2.12                     | 0.48              |
| 1:CT:39:ARG:O    | 1:C3:7:LEU:HB3    | 2.13                     | 0.48              |
| 1:CU:102:LEU:CD2 | 1:CY:104:LEU:HD13 | 2.42                     | 0.48              |
| 1:C4:45:ASN:C    | 1:C4:47:ILE:H     | 2.21                     | 0.48              |
| 1:C4:88:TYR:C    | 1:C4:88:TYR:CD2   | 2.91                     | 0.48              |
| 1:AD:98:GLY:O    | 1:AD:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:AJ:16:VAL:HG22 | 1:AJ:49:VAL:HG22  | 1.94                     | 0.48              |
| 1:AP:125:GLU:CA  | 1:AP:129:THR:OG1  | 2.57                     | 0.48              |
| 1:AX:18:VAL:HG12 | 1:AX:77:LEU:CB    | 2.37                     | 0.48              |
| 1:AX:98:GLY:O    | 1:AX:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:A3:6:HIS:CE1   | 1:A3:8:VAL:HB     | 2.47                     | 0.48              |
| 1:BJ:45:ASN:C    | 1:BJ:47:ILE:H     | 2.21                     | 0.48              |
| 1:BN:98:GLY:O    | 1:BN:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:BS:106:THR:O   | 1:BS:107:ASP:HB3  | 2.13                     | 0.48              |
| 1:CB:58:ILE:O    | 1:CB:58:ILE:HG22  | 2.13                     | 0.48              |
| 1:CO:16:VAL:HG22 | 1:CO:49:VAL:HG22  | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CQ:65:MET:O    | 1:CQ:68:SER:HB3   | 2.13                     | 0.48              |
| 1:C1:12:LEU:HD11 | 1:C1:143:ILE:HG23 | 1.95                     | 0.48              |
| 1:AC:17:VAL:HG21 | 1:AC:62:ALA:HA    | 1.95                     | 0.48              |
| 1:AD:106:THR:O   | 1:AD:107:ASP:HB3  | 2.13                     | 0.48              |
| 1:AH:17:VAL:HG21 | 1:AH:62:ALA:HA    | 1.95                     | 0.48              |
| 1:AX:6:HIS:CE1   | 1:AX:8:VAL:HB     | 2.47                     | 0.48              |
| 1:A2:82:ARG:CG   | 1:A2:82:ARG:NH1   | 2.73                     | 0.48              |
| 1:BD:18:VAL:HG12 | 1:BD:77:LEU:CB    | 2.37                     | 0.48              |
| 1:BN:116:THR:O   | 1:BO:85:THR:HB    | 2.12                     | 0.48              |
| 1:CD:98:GLY:O    | 1:CD:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:CJ:82:ARG:HG3  | 1:CJ:118:GLU:OE2  | 2.12                     | 0.48              |
| 1:CV:65:MET:O    | 1:CV:68:SER:HB3   | 2.13                     | 0.48              |
| 1:AB:12:LEU:HD11 | 1:AB:143:ILE:HG23 | 1.95                     | 0.48              |
| 1:AB:97:LYS:HE3  | 1:AC:97:LYS:HZ3   | 1.75                     | 0.48              |
| 1:AD:39:ARG:O    | 1:AJ:7:LEU:HB3    | 2.13                     | 0.48              |
| 1:AG:65:MET:O    | 1:AG:68:SER:HB3   | 2.13                     | 0.48              |
| 1:AI:98:GLY:O    | 1:AI:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:AN:66:ALA:HB2  | 1:AN:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:AS:106:THR:O   | 1:AS:107:ASP:HB3  | 2.13                     | 0.48              |
| 1:AT:45:ASN:C    | 1:AT:47:ILE:H     | 2.21                     | 0.48              |
| 1:AX:66:ALA:HB2  | 1:AX:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:A2:18:VAL:HG22 | 1:A2:77:LEU:HB2   | 1.94                     | 0.48              |
| 1:BD:66:ALA:HB2  | 1:BD:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:BE:16:VAL:HG22 | 1:BE:49:VAL:HG22  | 1.94                     | 0.48              |
| 1:BG:65:MET:O    | 1:BG:68:SER:HB3   | 2.13                     | 0.48              |
| 1:BI:52:VAL:CG1  | 1:BI:61:ILE:HD12  | 2.35                     | 0.48              |
| 1:BJ:88:TYR:C    | 1:BJ:88:TYR:CD2   | 2.91                     | 0.48              |
| 1:BO:53:PRO:HD2  | 1:BO:57:GLU:HB2   | 1.93                     | 0.48              |
| 1:BY:106:THR:O   | 1:BY:107:ASP:C    | 2.57                     | 0.48              |
| 1:BZ:58:ILE:O    | 1:BZ:58:ILE:HG22  | 2.11                     | 0.48              |
| 1:B2:18:VAL:HG22 | 1:B2:77:LEU:HB2   | 1.95                     | 0.48              |
| 1:CE:52:VAL:HB   | 1:CE:53:PRO:CD    | 2.35                     | 0.48              |
| 1:CG:65:MET:O    | 1:CG:68:SER:HB3   | 2.13                     | 0.48              |
| 1:CH:97:LYS:HE3  | 1:CI:97:LYS:HZ3   | 1.78                     | 0.48              |
| 1:CS:66:ALA:HB2  | 1:CS:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:C1:65:MET:O    | 1:C1:68:SER:HB3   | 2.13                     | 0.48              |
| 1:AS:149:SER:HB3 | 1:AS:152:TRP:CZ2  | 2.49                     | 0.48              |
| 1:BA:18:VAL:HG21 | 1:BA:30:LEU:HD13  | 1.94                     | 0.48              |
| 1:BC:17:VAL:HG21 | 1:BC:62:ALA:HA    | 1.95                     | 0.48              |
| 1:BE:88:TYR:CD2  | 1:BE:88:TYR:C     | 2.91                     | 0.48              |
| 1:BF:58:ILE:O    | 1:BF:58:ILE:HG22  | 2.11                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BJ:82:ARG:HG3   | 1:BJ:118:GLU:OE2  | 2.12                     | 0.48              |
| 1:BS:98:GLY:O     | 1:BS:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:BT:121:GLU:O    | 1:BT:125:GLU:HB2  | 2.14                     | 0.48              |
| 1:BV:12:LEU:HB2   | 1:BV:42:VAL:HG13  | 1.96                     | 0.48              |
| 1:BY:18:VAL:HG23  | 1:BY:51:TRP:CE3   | 2.48                     | 0.48              |
| 1:B4:18:VAL:HG23  | 1:B4:51:TRP:CE3   | 2.48                     | 0.48              |
| 1:CJ:18:VAL:HG23  | 1:CJ:51:TRP:CE3   | 2.48                     | 0.48              |
| 1:CN:30:LEU:HA    | 1:CN:77:LEU:HD23  | 1.96                     | 0.48              |
| 1:CO:121:GLU:O    | 1:CO:125:GLU:HB2  | 2.14                     | 0.48              |
| 1:CR:18:VAL:HG22  | 1:CR:77:LEU:HB2   | 1.95                     | 0.48              |
| 1:C3:66:ALA:HB2   | 1:C3:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:AE:52:VAL:CB    | 1:AE:53:PRO:HD2   | 2.34                     | 0.48              |
| 1:AF:58:ILE:O     | 1:AF:58:ILE:HG22  | 2.12                     | 0.48              |
| 1:AQ:12:LEU:HB2   | 1:AQ:42:VAL:HG13  | 1.96                     | 0.48              |
| 1:AS:66:ALA:HB2   | 1:AS:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:A4:106:THR:O    | 1:A4:107:ASP:C    | 2.57                     | 0.48              |
| 1:BD:6:HIS:CE1    | 1:BD:8:VAL:HB     | 2.47                     | 0.48              |
| 1:BE:121:GLU:O    | 1:BE:125:GLU:HB2  | 2.14                     | 0.48              |
| 1:BF:28:LYS:CE    | 1:BR:28:LYS:NZ    | 2.76                     | 0.48              |
| 1:BM:52:VAL:CG1   | 1:BM:61:ILE:HD12  | 2.35                     | 0.48              |
| 1:BN:149:SER:HB3  | 1:BN:152:TRP:CZ2  | 2.49                     | 0.48              |
| 1:BO:82:ARG:HG3   | 1:BO:118:GLU:OE2  | 2.12                     | 0.48              |
| 1:BQ:65:MET:O     | 1:BQ:68:SER:HB3   | 2.13                     | 0.48              |
| 1:BR:106:THR:HG23 | 1:BR:108:ILE:H    | 1.79                     | 0.48              |
| 1:B1:58:ILE:O     | 1:B1:58:ILE:HG22  | 2.13                     | 0.48              |
| 1:B3:66:ALA:HB2   | 1:B3:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:B4:121:GLU:O    | 1:B4:125:GLU:HB2  | 2.14                     | 0.48              |
| 1:CF:18:VAL:HG21  | 1:CF:30:LEU:HD13  | 1.94                     | 0.48              |
| 1:CF:58:ILE:O     | 1:CF:58:ILE:HG22  | 2.11                     | 0.48              |
| 1:CL:12:LEU:HD11  | 1:CL:143:ILE:HG23 | 1.95                     | 0.48              |
| 1:CS:52:VAL:CG1   | 1:CS:61:ILE:HD12  | 2.35                     | 0.48              |
| 1:CX:149:SER:HB3  | 1:CX:152:TRP:CZ2  | 2.49                     | 0.48              |
| 1:AL:116:THR:O    | 1:AM:85:THR:HB    | 2.14                     | 0.48              |
| 1:AN:98:GLY:O     | 1:AN:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:AO:106:THR:O    | 1:AO:107:ASP:C    | 2.57                     | 0.48              |
| 1:AV:65:MET:O     | 1:AV:68:SER:HB3   | 2.13                     | 0.48              |
| 1:AV:116:THR:O    | 1:AW:85:THR:HB    | 2.14                     | 0.48              |
| 1:A3:149:SER:HB3  | 1:A3:152:TRP:CZ2  | 2.49                     | 0.48              |
| 1:BI:39:ARG:O     | 1:BO:7:LEU:HB3    | 2.14                     | 0.48              |
| 1:BI:98:GLY:O     | 1:BI:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:BL:65:MET:O     | 1:BL:68:SER:HB3   | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BO:88:TYR:C     | 1:BO:88:TYR:CD2  | 2.91                     | 0.48              |
| 1:BX:66:ALA:HB2   | 1:BX:74:VAL:HG21 | 1.96                     | 0.48              |
| 1:B4:88:TYR:CD2   | 1:B4:88:TYR:C    | 2.91                     | 0.48              |
| 1:CI:149:SER:HB3  | 1:CI:152:TRP:CZ2 | 2.49                     | 0.48              |
| 1:CM:17:VAL:HG21  | 1:CM:62:ALA:HA   | 1.95                     | 0.48              |
| 1:CV:116:THR:O    | 1:CW:85:THR:HB   | 2.14                     | 0.48              |
| 1:AB:65:MET:O     | 1:AB:68:SER:HB3  | 2.13                     | 0.48              |
| 1:AJ:121:GLU:O    | 1:AJ:125:GLU:HB2 | 2.14                     | 0.48              |
| 1:AN:149:SER:HB3  | 1:AN:152:TRP:CZ2 | 2.49                     | 0.48              |
| 1:AW:17:VAL:HG21  | 1:AW:62:ALA:HA   | 1.95                     | 0.48              |
| 1:A1:58:ILE:O     | 1:A1:58:ILE:HG22 | 2.13                     | 0.48              |
| 1:A4:121:GLU:O    | 1:A4:125:GLU:HB2 | 2.14                     | 0.48              |
| 1:BD:106:THR:O    | 1:BD:107:ASP:HB3 | 2.13                     | 0.48              |
| 1:BH:18:VAL:HG22  | 1:BH:77:LEU:HB2  | 1.94                     | 0.48              |
| 1:BO:121:GLU:O    | 1:BO:125:GLU:HB2 | 2.14                     | 0.48              |
| 1:BR:18:VAL:HG22  | 1:BR:77:LEU:HB2  | 1.94                     | 0.48              |
| 1:BS:66:ALA:HB2   | 1:BS:74:VAL:HG21 | 1.96                     | 0.48              |
| 1:BS:116:THR:O    | 1:BT:85:THR:HB   | 2.12                     | 0.48              |
| 1:BS:149:SER:HB3  | 1:BS:152:TRP:CZ2 | 2.49                     | 0.48              |
| 1:BW:17:VAL:HG21  | 1:BW:62:ALA:HA   | 1.95                     | 0.48              |
| 1:BW:18:VAL:HG22  | 1:BW:77:LEU:HB2  | 1.94                     | 0.48              |
| 1:BX:98:GLY:O     | 1:BX:102:LEU:HB2 | 2.13                     | 0.48              |
| 1:BX:149:SER:HB3  | 1:BX:152:TRP:CZ2 | 2.49                     | 0.48              |
| 1:CB:12:LEU:HB2   | 1:CB:42:VAL:HG13 | 1.96                     | 0.48              |
| 1:CB:65:MET:O     | 1:CB:68:SER:HB3  | 2.13                     | 0.48              |
| 1:CH:24:PHE:CE1   | 1:CU:28:LYS:HD2  | 2.49                     | 0.48              |
| 1:CO:88:TYR:C     | 1:CO:88:TYR:CD2  | 2.91                     | 0.48              |
| 1:CT:88:TYR:C     | 1:CT:88:TYR:CD2  | 2.91                     | 0.48              |
| 1:CT:106:THR:O    | 1:CT:107:ASP:C   | 2.57                     | 0.48              |
| 1:CY:88:TYR:C     | 1:CY:88:TYR:CD2  | 2.91                     | 0.48              |
| 1:C4:106:THR:O    | 1:C4:107:ASP:C   | 2.57                     | 0.48              |
| 1:AB:116:THR:O    | 1:AC:85:THR:HB   | 2.14                     | 0.48              |
| 1:AB:144:GLU:OE2  | 1:AC:20:ARG:HD2  | 2.14                     | 0.48              |
| 1:AI:106:THR:O    | 1:AI:107:ASP:HB3 | 2.13                     | 0.48              |
| 1:AJ:18:VAL:HG23  | 1:AJ:51:TRP:CE3  | 2.48                     | 0.48              |
| 1:AM:17:VAL:HG21  | 1:AM:62:ALA:HA   | 1.95                     | 0.48              |
| 1:AM:106:THR:HG23 | 1:AM:108:ILE:H   | 1.79                     | 0.48              |
| 1:AO:18:VAL:HG23  | 1:AO:51:TRP:CE3  | 2.48                     | 0.48              |
| 1:A1:144:GLU:OE2  | 1:A2:20:ARG:HD2  | 2.14                     | 0.48              |
| 1:BB:97:LYS:HE3   | 1:BC:97:LYS:HZ3  | 1.77                     | 0.48              |
| 1:BB:116:THR:O    | 1:BC:85:THR:HB   | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BC:38:LYS:HZ2   | 1:BC:44:GLU:HA    | 1.79                     | 0.48              |
| 1:BI:149:SER:HB3  | 1:BI:152:TRP:CZ2  | 2.49                     | 0.48              |
| 1:BM:45:ASN:HD22  | 1:BM:45:ASN:HA    | 1.64                     | 0.48              |
| 1:BP:18:VAL:HG21  | 1:BP:30:LEU:HD13  | 1.94                     | 0.48              |
| 1:BS:137:GLU:O    | 1:BS:140:VAL:HG12 | 2.14                     | 0.48              |
| 1:BV:65:MET:O     | 1:BV:68:SER:HB3   | 2.13                     | 0.48              |
| 1:B1:12:LEU:HB2   | 1:B1:42:VAL:HG13  | 1.96                     | 0.48              |
| 1:B3:149:SER:HB3  | 1:B3:152:TRP:CZ2  | 2.49                     | 0.48              |
| 1:CD:28:LYS:HZ3   | 1:CF:28:LYS:NZ    | 2.10                     | 0.48              |
| 1:CN:66:ALA:HB2   | 1:CN:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:C4:121:GLU:O    | 1:C4:125:GLU:HB2  | 2.14                     | 0.48              |
| 1:AL:58:ILE:O     | 1:AL:58:ILE:HG22  | 2.13                     | 0.48              |
| 1:AQ:12:LEU:HD11  | 1:AQ:143:ILE:HG23 | 1.95                     | 0.48              |
| 1:AR:18:VAL:HG22  | 1:AR:77:LEU:HB2   | 1.94                     | 0.48              |
| 1:AX:137:GLU:O    | 1:AX:140:VAL:HG12 | 2.14                     | 0.48              |
| 1:A3:66:ALA:HB2   | 1:A3:74:VAL:HG21  | 1.96                     | 0.48              |
| 1:A3:137:GLU:O    | 1:A3:140:VAL:HG12 | 2.14                     | 0.48              |
| 1:BE:45:ASN:C     | 1:BE:47:ILE:H     | 2.21                     | 0.48              |
| 1:BG:12:LEU:HB2   | 1:BG:42:VAL:HG13  | 1.96                     | 0.48              |
| 1:BG:116:THR:O    | 1:BH:85:THR:HB    | 2.14                     | 0.48              |
| 1:BH:106:THR:HG23 | 1:BH:108:ILE:H    | 1.79                     | 0.48              |
| 1:BL:13:LYS:HD2   | 1:BL:46:ASP:OD2   | 2.14                     | 0.48              |
| 1:BL:116:THR:O    | 1:BM:85:THR:HB    | 2.14                     | 0.48              |
| 1:BM:17:VAL:HG21  | 1:BM:62:ALA:HA    | 1.95                     | 0.48              |
| 1:BM:97:LYS:HE3   | 1:BN:97:LYS:HZ3   | 1.78                     | 0.48              |
| 1:BT:88:TYR:C     | 1:BT:88:TYR:CD2   | 2.91                     | 0.48              |
| 1:B2:106:THR:HG23 | 1:B2:108:ILE:H    | 1.79                     | 0.48              |
| 1:B3:98:GLY:O     | 1:B3:102:LEU:HB2  | 2.13                     | 0.48              |
| 1:B4:45:ASN:C     | 1:B4:47:ILE:H     | 2.21                     | 0.48              |
| 1:B4:82:ARG:HG3   | 1:B4:118:GLU:OE2  | 2.12                     | 0.48              |
| 1:CC:39:ARG:O     | 1:CR:7:LEU:HB3    | 2.14                     | 0.48              |
| 1:CG:12:LEU:HD11  | 1:CG:143:ILE:HG23 | 1.95                     | 0.48              |
| 1:CO:52:VAL:CB    | 1:CO:53:PRO:HD2   | 2.34                     | 0.48              |
| 1:CQ:90:TYR:O     | 1:CQ:94:GLU:HG2   | 2.14                     | 0.48              |
| 1:CR:106:THR:HG23 | 1:CR:108:ILE:H    | 1.79                     | 0.48              |
| 1:CV:13:LYS:HD2   | 1:CV:46:ASP:OD2   | 2.14                     | 0.48              |
| 1:C3:106:THR:O    | 1:C3:107:ASP:HB3  | 2.13                     | 0.48              |
| 1:C4:52:VAL:HB    | 1:C4:53:PRO:CD    | 2.35                     | 0.48              |
| 1:AB:13:LYS:HD2   | 1:AB:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:AD:66:ALA:HB2   | 1:AD:74:VAL:HG21  | 1.96                     | 0.47              |
| 1:AD:82:ARG:HG3   | 1:AD:118:GLU:OE2  | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AG:12:LEU:HB2   | 1:AG:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:AH:106:THR:HG23 | 1:AH:108:ILE:H    | 1.79                     | 0.47              |
| 1:AI:137:GLU:O    | 1:AI:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:AN:30:LEU:HA    | 1:AN:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:AS:116:THR:O    | 1:AT:85:THR:HB    | 2.12                     | 0.47              |
| 1:BA:65:MET:HE2   | 1:BA:65:MET:HB3   | 1.80                     | 0.47              |
| 1:BB:65:MET:O     | 1:BB:68:SER:HB3   | 2.13                     | 0.47              |
| 1:BD:98:GLY:O     | 1:BD:102:LEU:HB2  | 2.13                     | 0.47              |
| 1:BH:38:LYS:HZ2   | 1:BH:44:GLU:HA    | 1.79                     | 0.47              |
| 1:BI:66:ALA:HB2   | 1:BI:74:VAL:HG21  | 1.96                     | 0.47              |
| 1:BT:45:ASN:C     | 1:BT:47:ILE:H     | 2.21                     | 0.47              |
| 1:BV:144:GLU:OE2  | 1:BW:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:BW:106:THR:HG23 | 1:BW:108:ILE:H    | 1.79                     | 0.47              |
| 1:BX:30:LEU:HA    | 1:BX:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:BX:106:THR:O    | 1:BX:107:ASP:HB3  | 2.13                     | 0.47              |
| 1:BX:137:GLU:O    | 1:BX:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:B1:12:LEU:HD11  | 1:B1:143:ILE:HG23 | 1.95                     | 0.47              |
| 1:CA:121:GLU:O    | 1:CA:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:CD:137:GLU:O    | 1:CD:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:CE:88:TYR:C     | 1:CE:88:TYR:CD2   | 2.91                     | 0.47              |
| 1:CL:58:ILE:O     | 1:CL:58:ILE:HG22  | 2.13                     | 0.47              |
| 1:AE:7:LEU:HB3    | 1:AN:39:ARG:O     | 2.13                     | 0.47              |
| 1:AI:30:LEU:HA    | 1:AI:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:AV:12:LEU:HB2   | 1:AV:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:AX:52:VAL:CG1   | 1:AX:61:ILE:HD12  | 2.35                     | 0.47              |
| 1:AY:71:TYR:O     | 1:AY:150:LYS:NZ   | 2.44                     | 0.47              |
| 1:AY:121:GLU:O    | 1:AY:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:A3:106:THR:O    | 1:A3:107:ASP:HB3  | 2.13                     | 0.47              |
| 1:BB:13:LYS:HD2   | 1:BB:46:ASP:OD2   | 2.15                     | 0.47              |
| 1:BB:152:TRP:CD1  | 1:BB:152:TRP:O    | 2.67                     | 0.47              |
| 1:BG:13:LYS:HD2   | 1:BG:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:BG:144:GLU:OE2  | 1:BH:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:BO:45:ASN:C     | 1:BO:47:ILE:H     | 2.21                     | 0.47              |
| 1:BP:121:GLU:O    | 1:BP:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:BV:116:THR:O    | 1:BW:85:THR:HB    | 2.14                     | 0.47              |
| 1:CB:13:LYS:HD2   | 1:CB:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:CC:18:VAL:HG22  | 1:CC:77:LEU:HB2   | 1.94                     | 0.47              |
| 1:CE:71:TYR:O     | 1:CE:150:LYS:NZ   | 2.44                     | 0.47              |
| 1:CH:82:ARG:CG    | 1:CH:82:ARG:NH1   | 2.73                     | 0.47              |
| 1:CL:13:LYS:HD2   | 1:CL:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:CO:106:THR:O    | 1:CO:107:ASP:C    | 2.57                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CQ:12:LEU:HB2   | 1:CQ:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:CS:30:LEU:HA    | 1:CS:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:C2:106:THR:HG23 | 1:C2:108:ILE:H    | 1.79                     | 0.47              |
| 1:C3:98:GLY:O     | 1:C3:102:LEU:HB2  | 2.13                     | 0.47              |
| 1:AE:45:ASN:C     | 1:AE:47:ILE:H     | 2.21                     | 0.47              |
| 1:AE:88:TYR:CD2   | 1:AE:88:TYR:C     | 2.91                     | 0.47              |
| 1:AE:121:GLU:O    | 1:AE:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:AG:13:LYS:HD2   | 1:AG:46:ASP:OD2   | 2.15                     | 0.47              |
| 1:AH:70:LYS:HB2   | 1:AH:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:AI:52:VAL:CG1   | 1:AI:61:ILE:HD12  | 2.35                     | 0.47              |
| 1:AI:128:GLY:O    | 1:AK:22:ASN:HA    | 2.14                     | 0.47              |
| 1:AJ:83:GLY:HA3   | 2:AJ:1001:PO4:O2  | 2.14                     | 0.47              |
| 1:AJ:106:THR:O    | 1:AJ:107:ASP:C    | 2.57                     | 0.47              |
| 1:AL:12:LEU:HB2   | 1:AL:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:AL:152:TRP:CD1  | 1:AL:152:TRP:O    | 2.68                     | 0.47              |
| 1:AN:18:VAL:HG12  | 1:AN:77:LEU:CB    | 2.37                     | 0.47              |
| 1:AS:30:LEU:HA    | 1:AS:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:AX:149:SER:HB3  | 1:AX:152:TRP:CZ2  | 2.49                     | 0.47              |
| 1:BE:106:THR:O    | 1:BE:107:ASP:C    | 2.57                     | 0.47              |
| 1:BH:17:VAL:HG21  | 1:BH:62:ALA:HA    | 1.94                     | 0.47              |
| 1:BK:121:GLU:O    | 1:BK:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:BL:152:TRP:CD1  | 1:BL:152:TRP:O    | 2.67                     | 0.47              |
| 1:BM:106:THR:HG23 | 1:BM:108:ILE:H    | 1.79                     | 0.47              |
| 1:BZ:125:GLU:CA   | 1:BZ:129:THR:OG1  | 2.57                     | 0.47              |
| 1:CB:55:ALA:HB1   | 1:CB:95:VAL:CG2   | 2.40                     | 0.47              |
| 1:CE:45:ASN:C     | 1:CE:47:ILE:H     | 2.21                     | 0.47              |
| 1:CG:152:TRP:CD1  | 1:CG:152:TRP:O    | 2.67                     | 0.47              |
| 1:CO:83:GLY:HA3   | 2:CO:4201:PO4:O2  | 2.15                     | 0.47              |
| 1:CQ:12:LEU:HD11  | 1:CQ:143:ILE:HG23 | 1.95                     | 0.47              |
| 1:CQ:13:LYS:HD2   | 1:CQ:46:ASP:OD2   | 2.15                     | 0.47              |
| 1:CS:98:GLY:O     | 1:CS:102:LEU:HB2  | 2.13                     | 0.47              |
| 1:CV:144:GLU:OE2  | 1:CW:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:CY:106:THR:O    | 1:CY:107:ASP:C    | 2.57                     | 0.47              |
| 1:CY:121:GLU:O    | 1:CY:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:C3:30:LEU:HA    | 1:C3:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:AB:152:TRP:CD1  | 1:AB:152:TRP:O    | 2.68                     | 0.47              |
| 1:AD:149:SER:HB3  | 1:AD:152:TRP:CZ2  | 2.49                     | 0.47              |
| 1:AE:106:THR:O    | 1:AE:107:ASP:C    | 2.57                     | 0.47              |
| 1:AL:13:LYS:HD2   | 1:AL:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:AO:83:GLY:HA3   | 2:AO:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:AQ:58:ILE:O     | 1:AQ:58:ILE:HG22  | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AQ:90:TYR:O     | 1:AQ:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:AQ:144:GLU:OE2  | 1:AR:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:AQ:152:TRP:CD1  | 1:AQ:152:TRP:O    | 2.68                     | 0.47              |
| 1:AT:106:THR:O    | 1:AT:107:ASP:C    | 2.57                     | 0.47              |
| 1:AT:121:GLU:O    | 1:AT:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:AW:106:THR:HG23 | 1:AW:108:ILE:H    | 1.79                     | 0.47              |
| 1:AY:106:THR:O    | 1:AY:107:ASP:C    | 2.57                     | 0.47              |
| 1:A3:82:ARG:HG3   | 1:A3:118:GLU:OE2  | 2.15                     | 0.47              |
| 1:A3:98:GLY:O     | 1:A3:102:LEU:HB2  | 2.13                     | 0.47              |
| 1:A4:83:GLY:HA3   | 2:A4:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:BG:152:TRP:CD1  | 1:BG:152:TRP:O    | 2.68                     | 0.47              |
| 1:BI:82:ARG:HG3   | 1:BI:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:BL:12:LEU:HD11  | 1:BL:143:ILE:HG23 | 1.95                     | 0.47              |
| 1:BL:90:TYR:O     | 1:BL:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:CB:152:TRP:CD1  | 1:CB:152:TRP:O    | 2.68                     | 0.47              |
| 1:CC:106:THR:HG23 | 1:CC:108:ILE:H    | 1.79                     | 0.47              |
| 1:CI:98:GLY:O     | 1:CI:102:LEU:HB2  | 2.13                     | 0.47              |
| 1:CJ:83:GLY:HA3   | 2:CJ:4201:PO4:O2  | 2.15                     | 0.47              |
| 1:CJ:106:THR:O    | 1:CJ:107:ASP:C    | 2.57                     | 0.47              |
| 1:CL:90:TYR:O     | 1:CL:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:CV:12:LEU:HB2   | 1:CV:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:CW:70:LYS:HB2   | 1:CW:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:CX:120:ILE:HG12 | 1:C2:129:THR:HG21 | 1.97                     | 0.47              |
| 1:C1:12:LEU:HB2   | 1:C1:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:C1:152:TRP:CD1  | 1:C1:152:TRP:O    | 2.67                     | 0.47              |
| 1:AE:83:GLY:HA3   | 2:AE:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:AG:152:TRP:CD1  | 1:AG:152:TRP:O    | 2.68                     | 0.47              |
| 1:AL:37:LEU:O     | 1:AL:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:AM:70:LYS:HB2   | 1:AM:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:AU:121:GLU:O    | 1:AU:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:BC:70:LYS:HB2   | 1:BC:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:BG:90:TYR:O     | 1:BG:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:BM:70:LYS:HB2   | 1:BM:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:BO:106:THR:O    | 1:BO:107:ASP:C    | 2.57                     | 0.47              |
| 1:BR:30:LEU:HA    | 1:BR:77:LEU:HD23  | 1.97                     | 0.47              |
| 1:BR:70:LYS:HB2   | 1:BR:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:BS:82:ARG:HG3   | 1:BS:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:B2:70:LYS:HB2   | 1:B2:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:B3:82:ARG:HG3   | 1:B3:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:CB:37:LEU:O     | 1:CB:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:CE:106:THR:O    | 1:CE:107:ASP:C    | 2.57                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CF:121:GLU:O    | 1:CF:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:CF:125:GLU:CA   | 1:CF:129:THR:OG1  | 2.57                     | 0.47              |
| 1:CG:130:LYS:HG3  | 1:CV:120:ILE:HD11 | 1.95                     | 0.47              |
| 1:CI:137:GLU:O    | 1:CI:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:CL:65:MET:O     | 1:CL:68:SER:HB3   | 2.13                     | 0.47              |
| 1:CL:116:THR:O    | 1:CM:85:THR:HB    | 2.14                     | 0.47              |
| 1:CL:144:GLU:OE2  | 1:CM:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:CN:82:ARG:HG3   | 1:CN:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:CQ:144:GLU:OE2  | 1:CR:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:CU:121:GLU:O    | 1:CU:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:CV:58:ILE:O     | 1:CV:58:ILE:HG22  | 2.13                     | 0.47              |
| 1:CV:90:TYR:O     | 1:CV:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:CV:152:TRP:CD1  | 1:CV:152:TRP:O    | 2.68                     | 0.47              |
| 1:CW:106:THR:HG23 | 1:CW:108:ILE:H    | 1.79                     | 0.47              |
| 1:C1:13:LYS:HD2   | 1:C1:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:C1:106:THR:O    | 1:C1:107:ASP:HB3  | 2.15                     | 0.47              |
| 1:AD:30:LEU:HA    | 1:AD:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:AG:116:THR:O    | 1:AH:85:THR:HB    | 2.14                     | 0.47              |
| 1:AI:66:ALA:HB2   | 1:AI:74:VAL:HG21  | 1.96                     | 0.47              |
| 1:AK:58:ILE:O     | 1:AK:58:ILE:HG22  | 2.11                     | 0.47              |
| 1:AL:90:TYR:O     | 1:AL:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:AQ:13:LYS:HD2   | 1:AQ:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:AQ:37:LEU:O     | 1:AQ:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:AV:90:TYR:O     | 1:AV:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:AW:30:LEU:HA    | 1:AW:77:LEU:HD23  | 1.97                     | 0.47              |
| 1:A1:116:THR:O    | 1:A2:85:THR:HB    | 2.14                     | 0.47              |
| 1:BB:90:TYR:O     | 1:BB:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:BD:30:LEU:HA    | 1:BD:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:BQ:58:ILE:O     | 1:BQ:58:ILE:HG22  | 2.13                     | 0.47              |
| 1:BT:83:GLY:HA3   | 2:BT:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:BW:70:LYS:HB2   | 1:BW:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:BY:121:GLU:O    | 1:BY:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:B1:116:THR:O    | 1:B2:85:THR:HB    | 2.14                     | 0.47              |
| 1:B1:129:THR:CG2  | 1:B1:130:LYS:H    | 2.28                     | 0.47              |
| 1:B3:30:LEU:HA    | 1:B3:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:B3:137:GLU:O    | 1:B3:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:CD:149:SER:HB3  | 1:CD:152:TRP:CZ2  | 2.49                     | 0.47              |
| 1:CG:58:ILE:O     | 1:CG:58:ILE:HG22  | 2.13                     | 0.47              |
| 1:CI:30:LEU:HA    | 1:CI:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:CL:12:LEU:HB2   | 1:CL:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:CM:75:ILE:HG22  | 1:CM:77:LEU:HD13  | 1.97                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CR:70:LYS:HB2   | 1:CR:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:CV:129:THR:CG2  | 1:CV:130:LYS:H    | 2.28                     | 0.47              |
| 1:CX:52:VAL:CG1   | 1:CX:61:ILE:HD12  | 2.35                     | 0.47              |
| 1:AB:90:TYR:O     | 1:AB:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:AM:38:LYS:HZ2   | 1:AM:44:GLU:HA    | 1.79                     | 0.47              |
| 1:AN:137:GLU:O    | 1:AN:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:AR:70:LYS:HB2   | 1:AR:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:AR:75:ILE:HG22  | 1:AR:77:LEU:HD13  | 1.97                     | 0.47              |
| 1:AT:83:GLY:HA3   | 2:AT:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:AV:37:LEU:O     | 1:AV:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:AW:70:LYS:HB2   | 1:AW:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:AW:82:ARG:CG    | 1:AW:82:ARG:NH1   | 2.73                     | 0.47              |
| 1:AZ:58:ILE:O     | 1:AZ:58:ILE:HG22  | 2.12                     | 0.47              |
| 1:AZ:121:GLU:O    | 1:AZ:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:A2:106:THR:HG23 | 1:A2:108:ILE:H    | 1.79                     | 0.47              |
| 1:BB:144:GLU:OE2  | 1:BC:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:BC:30:LEU:HA    | 1:BC:77:LEU:HD23  | 1.97                     | 0.47              |
| 1:BD:149:SER:HB3  | 1:BD:152:TRP:CZ2  | 2.49                     | 0.47              |
| 1:BE:83:GLY:HA3   | 2:BE:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:BF:39:ARG:NH2   | 1:BQ:144:GLU:CD   | 2.73                     | 0.47              |
| 1:BH:30:LEU:HA    | 1:BH:77:LEU:HD23  | 1.97                     | 0.47              |
| 1:BI:137:GLU:O    | 1:BI:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:BJ:121:GLU:O    | 1:BJ:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:BL:12:LEU:HB2   | 1:BL:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:BN:66:ALA:HB2   | 1:BN:74:VAL:HG21  | 1.96                     | 0.47              |
| 1:BN:137:GLU:O    | 1:BN:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:BQ:144:GLU:OE2  | 1:BR:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:BT:106:THR:O    | 1:BT:107:ASP:C    | 2.57                     | 0.47              |
| 1:BU:121:GLU:O    | 1:BU:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:BV:13:LYS:HD2   | 1:BV:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:BV:37:LEU:O     | 1:BV:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:BX:82:ARG:HG3   | 1:BX:118:GLU:OE2  | 2.15                     | 0.47              |
| 1:B4:83:GLY:HA3   | 2:B4:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:B4:106:THR:O    | 1:B4:107:ASP:C    | 2.57                     | 0.47              |
| 1:CB:106:THR:O    | 1:CB:107:ASP:HB3  | 2.15                     | 0.47              |
| 1:CB:116:THR:O    | 1:CC:85:THR:HB    | 2.14                     | 0.47              |
| 1:CC:30:LEU:HA    | 1:CC:77:LEU:HD23  | 1.97                     | 0.47              |
| 1:CC:70:LYS:HB2   | 1:CC:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:CE:121:GLU:O    | 1:CE:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:CG:116:THR:O    | 1:CH:85:THR:HB    | 2.14                     | 0.47              |
| 1:CH:106:THR:HG23 | 1:CH:108:ILE:H    | 1.79                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CI:66:ALA:HB2   | 1:CI:74:VAL:HG21  | 1.96                     | 0.47              |
| 1:CJ:121:GLU:O    | 1:CJ:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:CL:106:THR:O    | 1:CL:107:ASP:HB3  | 2.15                     | 0.47              |
| 1:CR:38:LYS:HZ2   | 1:CR:44:GLU:HA    | 1.80                     | 0.47              |
| 1:CR:75:ILE:HG22  | 1:CR:77:LEU:HD13  | 1.97                     | 0.47              |
| 1:CS:106:THR:O    | 1:CS:107:ASP:HB3  | 2.13                     | 0.47              |
| 1:CT:7:LEU:CB     | 1:C3:39:ARG:O     | 2.63                     | 0.47              |
| 1:CT:45:ASN:C     | 1:CT:47:ILE:H     | 2.21                     | 0.47              |
| 1:CX:82:ARG:HG3   | 1:CX:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:CX:98:GLY:O     | 1:CX:102:LEU:HB2  | 2.13                     | 0.47              |
| 1:CY:83:GLY:HA3   | 2:CY:4201:PO4:O2  | 2.15                     | 0.47              |
| 1:C1:37:LEU:O     | 1:C1:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:C1:116:THR:O    | 1:C2:85:THR:HB    | 2.14                     | 0.47              |
| 1:C2:70:LYS:HB2   | 1:C2:71:TYR:CD1   | 2.50                     | 0.47              |
| 1:AC:75:ILE:HG22  | 1:AC:77:LEU:HD13  | 1.97                     | 0.47              |
| 1:AC:106:THR:HG23 | 1:AC:108:ILE:H    | 1.79                     | 0.47              |
| 1:AG:90:TYR:O     | 1:AG:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:AG:144:GLU:OE2  | 1:AH:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:AH:45:ASN:HD22  | 1:AH:45:ASN:HA    | 1.64                     | 0.47              |
| 1:AN:82:ARG:HG3   | 1:AN:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:AR:106:THR:HG23 | 1:AR:108:ILE:H    | 1.79                     | 0.47              |
| 1:AR:148:LEU:HA   | 1:AR:148:LEU:HD23 | 1.79                     | 0.47              |
| 1:AV:58:ILE:O     | 1:AV:58:ILE:HG22  | 2.13                     | 0.47              |
| 1:AV:152:TRP:CD1  | 1:AV:152:TRP:O    | 2.67                     | 0.47              |
| 1:AY:83:GLY:HA3   | 2:AY:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:A1:152:TRP:CD1  | 1:A1:152:TRP:O    | 2.67                     | 0.47              |
| 1:BB:12:LEU:HB2   | 1:BB:42:VAL:HG13  | 1.96                     | 0.47              |
| 1:BB:37:LEU:O     | 1:BB:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:BD:117:THR:HG22 | 1:BE:85:THR:HG21  | 1.97                     | 0.47              |
| 1:BL:144:GLU:OE2  | 1:BM:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:BN:30:LEU:HA    | 1:BN:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:BO:83:GLY:HA3   | 2:BO:1001:PO4:O2  | 2.15                     | 0.47              |
| 1:BR:75:ILE:HG22  | 1:BR:77:LEU:HD13  | 1.97                     | 0.47              |
| 1:CB:144:GLU:OE2  | 1:CC:20:ARG:HD2   | 2.14                     | 0.47              |
| 1:CD:82:ARG:HG3   | 1:CD:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:CG:37:LEU:O     | 1:CG:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:CG:106:THR:O    | 1:CG:107:ASP:HB3  | 2.15                     | 0.47              |
| 1:CH:38:LYS:HZ2   | 1:CH:44:GLU:HA    | 1.79                     | 0.47              |
| 1:CI:40:HIS:CE1   | 1:CO:7:LEU:HD23   | 2.50                     | 0.47              |
| 1:CP:121:GLU:O    | 1:CP:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:CT:83:GLY:HA3   | 2:CT:4201:PO4:O2  | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CX:106:THR:O    | 1:CX:107:ASP:HB3  | 2.13                     | 0.47              |
| 1:C3:117:THR:HG22 | 1:C4:85:THR:HG21  | 1.97                     | 0.47              |
| 1:AA:121:GLU:O    | 1:AA:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:AE:29:LEU:HD11  | 1:AE:134:LYS:HB3  | 1.97                     | 0.47              |
| 1:AE:71:TYR:O     | 1:AE:150:LYS:NZ   | 2.44                     | 0.47              |
| 1:AI:149:SER:HB3  | 1:AI:152:TRP:CZ2  | 2.49                     | 0.47              |
| 1:AL:100:ALA:CA   | 1:AM:56:PHE:HZ    | 2.28                     | 0.47              |
| 1:AN:117:THR:HG22 | 1:AO:85:THR:HG21  | 1.97                     | 0.47              |
| 1:AX:30:LEU:HA    | 1:AX:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:AX:117:THR:HG22 | 1:AY:85:THR:HG21  | 1.97                     | 0.47              |
| 1:AY:29:LEU:HD11  | 1:AY:134:LYS:HB3  | 1.97                     | 0.47              |
| 1:A1:13:LYS:HD2   | 1:A1:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:A2:75:ILE:HG22  | 1:A2:77:LEU:HD13  | 1.97                     | 0.47              |
| 1:A3:30:LEU:HA    | 1:A3:77:LEU:HD23  | 1.96                     | 0.47              |
| 1:BE:29:LEU:HD11  | 1:BE:134:LYS:HB3  | 1.97                     | 0.47              |
| 1:BF:121:GLU:O    | 1:BF:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:BG:37:LEU:O     | 1:BG:42:VAL:HG23  | 2.15                     | 0.47              |
| 1:BJ:106:THR:O    | 1:BJ:107:ASP:C    | 2.57                     | 0.47              |
| 1:BM:82:ARG:CG    | 1:BM:82:ARG:NH1   | 2.73                     | 0.47              |
| 1:BQ:13:LYS:HD2   | 1:BQ:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:BQ:116:THR:O    | 1:BR:85:THR:HB    | 2.14                     | 0.47              |
| 1:B1:152:TRP:CD1  | 1:B1:152:TRP:O    | 2.68                     | 0.47              |
| 1:CG:90:TYR:O     | 1:CG:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:CI:117:THR:HG22 | 1:CJ:85:THR:HG21  | 1.97                     | 0.47              |
| 1:CJ:71:TYR:O     | 1:CJ:150:LYS:NZ   | 2.44                     | 0.47              |
| 1:CL:152:TRP:CD1  | 1:CL:152:TRP:O    | 2.67                     | 0.47              |
| 1:CP:58:ILE:H     | 1:CP:59:PRO:HD2   | 1.80                     | 0.47              |
| 1:CQ:152:TRP:CD1  | 1:CQ:152:TRP:O    | 2.68                     | 0.47              |
| 1:CX:137:GLU:O    | 1:CX:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:CZ:65:MET:HE2   | 1:CZ:65:MET:HB3   | 1.80                     | 0.47              |
| 1:C1:58:ILE:O     | 1:C1:58:ILE:HG22  | 2.13                     | 0.47              |
| 1:AF:121:GLU:O    | 1:AF:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:AJ:45:ASN:C     | 1:AJ:47:ILE:H     | 2.21                     | 0.47              |
| 1:AM:30:LEU:HA    | 1:AM:77:LEU:HD23  | 1.97                     | 0.47              |
| 1:AO:121:GLU:O    | 1:AO:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:AS:117:THR:HG22 | 1:AT:85:THR:HG21  | 1.97                     | 0.47              |
| 1:AS:137:GLU:O    | 1:AS:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:AV:13:LYS:HD2   | 1:AV:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:AW:75:ILE:HG22  | 1:AW:77:LEU:HD13  | 1.97                     | 0.47              |
| 1:BB:106:THR:O    | 1:BB:107:ASP:HB3  | 2.15                     | 0.47              |
| 1:BD:137:GLU:O    | 1:BD:140:VAL:HG12 | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BG:106:THR:O    | 1:BG:107:ASP:HB3  | 2.15                     | 0.47              |
| 1:BJ:71:TYR:O     | 1:BJ:150:LYS:NZ   | 2.44                     | 0.47              |
| 1:BO:29:LEU:HD11  | 1:BO:134:LYS:HB3  | 1.97                     | 0.47              |
| 1:BS:48:ASP:HB2   | 1:BS:71:TYR:CE1   | 2.50                     | 0.47              |
| 1:BX:117:THR:HG22 | 1:BY:85:THR:HG21  | 1.97                     | 0.47              |
| 1:B1:13:LYS:HD2   | 1:B1:46:ASP:OD2   | 2.14                     | 0.47              |
| 1:CD:66:ALA:HB2   | 1:CD:74:VAL:HG21  | 1.96                     | 0.47              |
| 1:CI:82:ARG:HG3   | 1:CI:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:CK:121:GLU:O    | 1:CK:125:GLU:HG3  | 2.14                     | 0.47              |
| 1:CO:29:LEU:HD11  | 1:CO:134:LYS:HB3  | 1.97                     | 0.47              |
| 1:CQ:100:ALA:CA   | 1:CR:56:PHE:HZ    | 2.28                     | 0.47              |
| 1:CS:82:ARG:HG3   | 1:CS:118:GLU:OE2  | 2.14                     | 0.47              |
| 1:CS:149:SER:HB3  | 1:CS:152:TRP:CZ2  | 2.49                     | 0.47              |
| 1:CT:121:GLU:O    | 1:CT:125:GLU:HB2  | 2.14                     | 0.47              |
| 1:CW:9:GLY:HA3    | 1:CW:12:LEU:HD12  | 1.97                     | 0.47              |
| 1:CX:48:ASP:HB2   | 1:CX:71:TYR:CE1   | 2.50                     | 0.47              |
| 1:CX:66:ALA:HB2   | 1:CX:74:VAL:HG21  | 1.96                     | 0.47              |
| 1:C1:90:TYR:O     | 1:C1:94:GLU:HG2   | 2.14                     | 0.47              |
| 1:C3:137:GLU:O    | 1:C3:140:VAL:HG12 | 2.14                     | 0.47              |
| 1:AB:12:LEU:HB2   | 1:AB:42:VAL:HG13  | 1.96                     | 0.46              |
| 1:AG:37:LEU:O     | 1:AG:42:VAL:HG23  | 2.15                     | 0.46              |
| 1:AH:30:LEU:HA    | 1:AH:77:LEU:HD23  | 1.97                     | 0.46              |
| 1:AM:52:VAL:CG1   | 1:AM:61:ILE:HD12  | 2.35                     | 0.46              |
| 1:AQ:116:THR:O    | 1:AR:85:THR:HB    | 2.14                     | 0.46              |
| 1:BJ:83:GLY:HA3   | 2:BJ:1001:PO4:O2  | 2.15                     | 0.46              |
| 1:BQ:12:LEU:HB2   | 1:BQ:42:VAL:HG13  | 1.96                     | 0.46              |
| 1:BQ:152:TRP:CD1  | 1:BQ:152:TRP:O    | 2.68                     | 0.46              |
| 1:BT:71:TYR:O     | 1:BT:150:LYS:NZ   | 2.44                     | 0.46              |
| 1:BV:58:ILE:O     | 1:BV:58:ILE:HG22  | 2.13                     | 0.46              |
| 1:BV:129:THR:CG2  | 1:BV:130:LYS:H    | 2.28                     | 0.46              |
| 1:BY:29:LEU:HD11  | 1:BY:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:BY:83:GLY:HA3   | 2:BY:1001:PO4:O2  | 2.15                     | 0.46              |
| 1:BZ:121:GLU:O    | 1:BZ:125:GLU:HG3  | 2.14                     | 0.46              |
| 1:B1:90:TYR:O     | 1:B1:94:GLU:HG2   | 2.14                     | 0.46              |
| 1:CH:104:LEU:HD13 | 1:CI:102:LEU:HG   | 1.98                     | 0.46              |
| 1:CM:106:THR:HG23 | 1:CM:108:ILE:H    | 1.79                     | 0.46              |
| 1:CN:117:THR:HG22 | 1:CO:85:THR:HG21  | 1.97                     | 0.46              |
| 1:CS:117:THR:HG22 | 1:CT:85:THR:HG21  | 1.97                     | 0.46              |
| 1:CS:137:GLU:O    | 1:CS:140:VAL:HG12 | 2.14                     | 0.46              |
| 1:CV:37:LEU:O     | 1:CV:42:VAL:HG23  | 2.15                     | 0.46              |
| 1:C2:30:LEU:HA    | 1:C2:77:LEU:HD23  | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C3:149:SER:HB3  | 1:C3:152:TRP:CZ2  | 2.49                     | 0.46              |
| 1:AB:100:ALA:CA   | 1:AC:56:PHE:HZ    | 2.28                     | 0.46              |
| 1:AG:129:THR:CG2  | 1:AG:130:LYS:H    | 2.28                     | 0.46              |
| 1:AQ:69:GLY:C     | 1:BU:10:THR:CG2   | 2.86                     | 0.46              |
| 1:AS:82:ARG:HG3   | 1:AS:118:GLU:OE2  | 2.14                     | 0.46              |
| 1:AV:144:GLU:OE2  | 1:AW:20:ARG:HD2   | 2.14                     | 0.46              |
| 1:AZ:106:THR:C    | 1:AZ:108:ILE:H    | 2.23                     | 0.46              |
| 1:A1:12:LEU:HB2   | 1:A1:42:VAL:HG13  | 1.96                     | 0.46              |
| 1:BC:106:THR:HG23 | 1:BC:108:ILE:H    | 1.79                     | 0.46              |
| 1:BN:117:THR:HG22 | 1:BO:85:THR:HG21  | 1.97                     | 0.46              |
| 1:BT:29:LEU:HD11  | 1:BT:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:BU:106:THR:C    | 1:BU:108:ILE:H    | 2.23                     | 0.46              |
| 1:BV:90:TYR:O     | 1:BV:94:GLU:HG2   | 2.14                     | 0.46              |
| 1:B2:104:LEU:HD13 | 1:B3:102:LEU:HG   | 1.98                     | 0.46              |
| 1:CC:9:GLY:HA3    | 1:CC:12:LEU:HD12  | 1.97                     | 0.46              |
| 1:CH:75:ILE:HG22  | 1:CH:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:CN:137:GLU:O    | 1:CN:140:VAL:HG12 | 2.14                     | 0.46              |
| 1:CN:149:SER:HB3  | 1:CN:152:TRP:CZ2  | 2.49                     | 0.46              |
| 1:CO:45:ASN:C     | 1:CO:47:ILE:H     | 2.21                     | 0.46              |
| 1:CQ:58:ILE:O     | 1:CQ:58:ILE:HG22  | 2.13                     | 0.46              |
| 1:CW:45:ASN:HD22  | 1:CW:45:ASN:HA    | 1.64                     | 0.46              |
| 1:CZ:106:THR:C    | 1:CZ:108:ILE:H    | 2.24                     | 0.46              |
| 1:CZ:125:GLU:CA   | 1:CZ:129:THR:OG1  | 2.57                     | 0.46              |
| 1:C1:100:ALA:CA   | 1:C2:56:PHE:HZ    | 2.28                     | 0.46              |
| 1:C4:83:GLY:HA3   | 2:C4:4201:PO4:O2  | 2.15                     | 0.46              |
| 1:AL:129:THR:CG2  | 1:AL:130:LYS:H    | 2.28                     | 0.46              |
| 1:AQ:129:THR:CG2  | 1:AQ:130:LYS:H    | 2.28                     | 0.46              |
| 1:AT:29:LEU:HD11  | 1:AT:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:A1:100:ALA:CA   | 1:A2:56:PHE:HZ    | 2.28                     | 0.46              |
| 1:A2:70:LYS:HB2   | 1:A2:71:TYR:CD1   | 2.50                     | 0.46              |
| 1:A3:117:THR:HG22 | 1:A4:85:THR:HG21  | 1.97                     | 0.46              |
| 1:BH:52:VAL:CG1   | 1:BH:61:ILE:HD12  | 2.35                     | 0.46              |
| 1:BH:70:LYS:HB2   | 1:BH:71:TYR:CD1   | 2.50                     | 0.46              |
| 1:BI:117:THR:HG22 | 1:BJ:85:THR:HG21  | 1.97                     | 0.46              |
| 1:BL:37:LEU:O     | 1:BL:42:VAL:HG23  | 2.15                     | 0.46              |
| 1:BQ:90:TYR:O     | 1:BQ:94:GLU:HG2   | 2.14                     | 0.46              |
| 1:BY:71:TYR:O     | 1:BY:150:LYS:NZ   | 2.44                     | 0.46              |
| 1:B1:144:GLU:OE2  | 1:B2:20:ARG:HD2   | 2.14                     | 0.46              |
| 1:B2:75:ILE:HG22  | 1:B2:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:B3:117:THR:HG22 | 1:B4:85:THR:HG21  | 1.97                     | 0.46              |
| 1:CF:58:ILE:H     | 1:CF:59:PRO:HD2   | 1.80                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CH:30:LEU:HA    | 1:CH:77:LEU:HD23  | 1.97                     | 0.46              |
| 1:CH:70:LYS:HB2   | 1:CH:71:TYR:CD1   | 2.50                     | 0.46              |
| 1:CJ:45:ASN:C     | 1:CJ:47:ILE:H     | 2.21                     | 0.46              |
| 1:CQ:37:LEU:O     | 1:CQ:42:VAL:HG23  | 2.15                     | 0.46              |
| 1:CQ:116:THR:O    | 1:CR:85:THR:HB    | 2.14                     | 0.46              |
| 1:CV:106:THR:O    | 1:CV:107:ASP:HB3  | 2.15                     | 0.46              |
| 1:CW:75:ILE:HG22  | 1:CW:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:C2:104:LEU:HD13 | 1:C3:102:LEU:HG   | 1.98                     | 0.46              |
| 1:AC:70:LYS:HB2   | 1:AC:71:TYR:CD1   | 2.50                     | 0.46              |
| 1:AC:104:LEU:HD13 | 1:AD:102:LEU:HG   | 1.98                     | 0.46              |
| 1:AK:121:GLU:O    | 1:AK:125:GLU:HG3  | 2.14                     | 0.46              |
| 1:AL:144:GLU:OE2  | 1:AM:20:ARG:HD2   | 2.14                     | 0.46              |
| 1:AP:121:GLU:O    | 1:AP:125:GLU:HG3  | 2.14                     | 0.46              |
| 1:BJ:29:LEU:HD11  | 1:BJ:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:BM:30:LEU:HA    | 1:BM:77:LEU:HD23  | 1.97                     | 0.46              |
| 1:BV:152:TRP:CD1  | 1:BV:152:TRP:O    | 2.67                     | 0.46              |
| 1:BX:18:VAL:HG12  | 1:BX:77:LEU:CB    | 2.37                     | 0.46              |
| 1:CD:30:LEU:HA    | 1:CD:77:LEU:HD23  | 1.96                     | 0.46              |
| 1:CG:13:LYS:HD2   | 1:CG:46:ASP:OD2   | 2.14                     | 0.46              |
| 1:CG:144:GLU:OE2  | 1:CH:20:ARG:HD2   | 2.14                     | 0.46              |
| 1:CM:70:LYS:HB2   | 1:CM:71:TYR:CD1   | 2.50                     | 0.46              |
| 1:CQ:106:THR:O    | 1:CQ:107:ASP:HB3  | 2.15                     | 0.46              |
| 1:C1:144:GLU:OE2  | 1:C2:20:ARG:HD2   | 2.14                     | 0.46              |
| 1:AC:30:LEU:HA    | 1:AC:77:LEU:HD23  | 1.97                     | 0.46              |
| 1:AD:137:GLU:O    | 1:AD:140:VAL:HG12 | 2.14                     | 0.46              |
| 1:AF:106:THR:C    | 1:AF:108:ILE:H    | 2.23                     | 0.46              |
| 1:AI:82:ARG:HG3   | 1:AI:118:GLU:OE2  | 2.14                     | 0.46              |
| 1:AN:75:ILE:HG22  | 1:AN:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:AO:29:LEU:HD11  | 1:AO:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:AX:75:ILE:HG22  | 1:AX:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:AX:82:ARG:HG3   | 1:AX:118:GLU:OE2  | 2.15                     | 0.46              |
| 1:A1:37:LEU:O     | 1:A1:42:VAL:HG23  | 2.15                     | 0.46              |
| 1:A3:18:VAL:HG11  | 1:A3:30:LEU:HD13  | 1.98                     | 0.46              |
| 1:BC:75:ILE:HG22  | 1:BC:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:BI:30:LEU:HA    | 1:BI:77:LEU:HD23  | 1.96                     | 0.46              |
| 1:BL:106:THR:O    | 1:BL:107:ASP:HB3  | 2.15                     | 0.46              |
| 1:BM:75:ILE:HG22  | 1:BM:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:BN:82:ARG:HG3   | 1:BN:118:GLU:OE2  | 2.14                     | 0.46              |
| 1:BQ:106:THR:O    | 1:BQ:107:ASP:HB3  | 2.15                     | 0.46              |
| 1:B1:37:LEU:O     | 1:B1:42:VAL:HG23  | 2.15                     | 0.46              |
| 1:CE:83:GLY:HA3   | 2:CE:1001:PO4:O2  | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CH:52:VAL:CG1   | 1:CH:61:ILE:HD12  | 2.35                     | 0.46              |
| 1:CK:58:ILE:H     | 1:CK:59:PRO:HD2   | 1.80                     | 0.46              |
| 1:CM:30:LEU:HA    | 1:CM:77:LEU:HD23  | 1.97                     | 0.46              |
| 1:CT:29:LEU:HD11  | 1:CT:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:CX:75:ILE:HG22  | 1:CX:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:CX:120:ILE:HD11 | 1:C2:129:THR:HG21 | 1.97                     | 0.46              |
| 1:CZ:121:GLU:O    | 1:CZ:125:GLU:HG3  | 2.14                     | 0.46              |
| 1:C2:45:ASN:HD22  | 1:C2:45:ASN:HA    | 1.63                     | 0.46              |
| 1:C3:75:ILE:HG22  | 1:C3:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:AA:58:ILE:O     | 1:AA:62:ALA:CB    | 2.64                     | 0.46              |
| 1:AM:75:ILE:HG22  | 1:AM:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:AP:106:THR:C    | 1:AP:108:ILE:H    | 2.24                     | 0.46              |
| 1:AZ:58:ILE:H     | 1:AZ:59:PRO:HD2   | 1.80                     | 0.46              |
| 1:A1:90:TYR:O     | 1:A1:94:GLU:HG2   | 2.14                     | 0.46              |
| 1:A2:104:LEU:HD13 | 1:A3:102:LEU:HG   | 1.98                     | 0.46              |
| 1:A4:45:ASN:C     | 1:A4:47:ILE:H     | 2.21                     | 0.46              |
| 1:BA:121:GLU:O    | 1:BA:125:GLU:HG3  | 2.14                     | 0.46              |
| 1:BB:129:THR:CG2  | 1:BB:130:LYS:H    | 2.28                     | 0.46              |
| 1:BD:9:GLY:HA2    | 1:BD:147:HIS:HE1  | 1.81                     | 0.46              |
| 1:BD:82:ARG:HG3   | 1:BD:118:GLU:OE2  | 2.14                     | 0.46              |
| 1:BE:39:ARG:O     | 1:BN:7:LEU:HB3    | 2.16                     | 0.46              |
| 1:BS:30:LEU:HA    | 1:BS:77:LEU:HD23  | 1.96                     | 0.46              |
| 1:BS:117:THR:HG22 | 1:BT:85:THR:HG21  | 1.97                     | 0.46              |
| 1:BW:9:GLY:HA3    | 1:BW:12:LEU:HD12  | 1.98                     | 0.46              |
| 1:BX:18:VAL:HG11  | 1:BX:30:LEU:HD13  | 1.98                     | 0.46              |
| 1:BY:129:THR:O    | 1:BY:130:LYS:C    | 2.59                     | 0.46              |
| 1:B2:30:LEU:HA    | 1:B2:77:LEU:HD23  | 1.97                     | 0.46              |
| 1:CD:117:THR:HG22 | 1:CE:85:THR:HG21  | 1.97                     | 0.46              |
| 1:CG:12:LEU:HB2   | 1:CG:42:VAL:HG13  | 1.96                     | 0.46              |
| 1:CM:9:GLY:HA3    | 1:CM:12:LEU:HD12  | 1.97                     | 0.46              |
| 1:CP:7:LEU:HD23   | 1:CV:40:HIS:CE1   | 2.51                     | 0.46              |
| 1:CU:106:THR:C    | 1:CU:108:ILE:H    | 2.23                     | 0.46              |
| 1:CY:71:TYR:O     | 1:CY:150:LYS:NZ   | 2.44                     | 0.46              |
| 1:C3:82:ARG:HG3   | 1:C3:118:GLU:OE2  | 2.15                     | 0.46              |
| 1:AJ:29:LEU:HD11  | 1:AJ:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:AK:58:ILE:O     | 1:AK:62:ALA:CB    | 2.64                     | 0.46              |
| 1:AM:9:GLY:HA3    | 1:AM:12:LEU:HD12  | 1.97                     | 0.46              |
| 1:AQ:70:LYS:HE3   | 1:BU:43:GLU:CD    | 2.41                     | 0.46              |
| 1:AR:9:GLY:HA3    | 1:AR:12:LEU:HD12  | 1.98                     | 0.46              |
| 1:AX:9:GLY:HA2    | 1:AX:147:HIS:HE1  | 1.81                     | 0.46              |
| 1:A4:29:LEU:HD11  | 1:A4:134:LYS:HB3  | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BD:13:LYS:NZ    | 1:CM:13:LYS:HD3   | 2.30                     | 0.46              |
| 1:BF:106:THR:C    | 1:BF:108:ILE:H    | 2.24                     | 0.46              |
| 1:BI:18:VAL:HG11  | 1:BI:30:LEU:HD13  | 1.98                     | 0.46              |
| 1:BI:75:ILE:HG22  | 1:BI:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:BS:75:ILE:HG22  | 1:BS:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:BW:75:ILE:HG22  | 1:BW:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:BX:75:ILE:HG22  | 1:BX:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:BZ:58:ILE:O     | 1:BZ:62:ALA:CB    | 2.64                     | 0.46              |
| 1:B3:18:VAL:HG11  | 1:B3:30:LEU:HD13  | 1.98                     | 0.46              |
| 1:CC:75:ILE:HG22  | 1:CC:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:CD:75:ILE:HG22  | 1:CD:77:LEU:HD13  | 1.98                     | 0.46              |
| 1:CE:129:THR:O    | 1:CE:130:LYS:C    | 2.59                     | 0.46              |
| 1:CJ:29:LEU:HD11  | 1:CJ:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:CK:58:ILE:O     | 1:CK:62:ALA:CB    | 2.64                     | 0.46              |
| 1:CN:9:GLY:HA2    | 1:CN:147:HIS:HE1  | 1.81                     | 0.46              |
| 1:CR:30:LEU:HA    | 1:CR:77:LEU:HD23  | 1.97                     | 0.46              |
| 1:CX:9:GLY:HA2    | 1:CX:147:HIS:HE1  | 1.81                     | 0.46              |
| 1:CY:129:THR:O    | 1:CY:130:LYS:C    | 2.59                     | 0.46              |
| 1:C4:129:THR:O    | 1:C4:130:LYS:C    | 2.59                     | 0.46              |
| 1:AB:37:LEU:O     | 1:AB:42:VAL:HG23  | 2.15                     | 0.46              |
| 1:AD:9:GLY:HA2    | 1:AD:147:HIS:HE1  | 1.81                     | 0.46              |
| 1:AF:58:ILE:H     | 1:AF:59:PRO:HD2   | 1.80                     | 0.46              |
| 1:AH:75:ILE:HG22  | 1:AH:77:LEU:HD13  | 1.97                     | 0.46              |
| 1:AI:40:HIS:CE1   | 1:AO:7:LEU:HD23   | 2.51                     | 0.46              |
| 1:AK:106:THR:C    | 1:AK:108:ILE:H    | 2.23                     | 0.46              |
| 1:AR:104:LEU:HD13 | 1:AS:102:LEU:HG   | 1.98                     | 0.46              |
| 1:A2:45:ASN:HD22  | 1:A2:45:ASN:HA    | 1.64                     | 0.46              |
| 1:BD:48:ASP:HB2   | 1:BD:71:TYR:CE1   | 2.50                     | 0.46              |
| 1:BD:120:ILE:HD13 | 1:BR:129:THR:HG21 | 1.96                     | 0.46              |
| 1:BJ:129:THR:O    | 1:BJ:130:LYS:C    | 2.59                     | 0.46              |
| 1:BW:104:LEU:HD13 | 1:BX:102:LEU:HG   | 1.97                     | 0.46              |
| 1:BX:9:GLY:HA2    | 1:BX:147:HIS:HE1  | 1.81                     | 0.46              |
| 1:B3:48:ASP:HB2   | 1:B3:71:TYR:CE1   | 2.50                     | 0.46              |
| 1:B4:29:LEU:HD11  | 1:B4:134:LYS:HB3  | 1.97                     | 0.46              |
| 1:B4:71:TYR:O     | 1:B4:150:LYS:NZ   | 2.44                     | 0.46              |
| 1:CH:9:GLY:HA3    | 1:CH:12:LEU:HD12  | 1.98                     | 0.46              |
| 1:CM:52:VAL:CG1   | 1:CM:61:ILE:HD12  | 2.35                     | 0.46              |
| 1:CQ:129:THR:CG2  | 1:CQ:130:LYS:H    | 2.28                     | 0.46              |
| 1:CX:30:LEU:HA    | 1:CX:77:LEU:HD23  | 1.96                     | 0.46              |
| 1:CZ:58:ILE:O     | 1:CZ:58:ILE:HG22  | 2.11                     | 0.46              |
| 1:CZ:58:ILE:O     | 1:CZ:62:ALA:CB    | 2.64                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C3:18:VAL:HG11  | 1:C3:30:LEU:HD13 | 1.98                     | 0.46              |
| 1:C4:29:LEU:HD11  | 1:C4:134:LYS:HB3 | 1.97                     | 0.46              |
| 1:AA:65:MET:HE2   | 1:AA:65:MET:HB3  | 1.80                     | 0.46              |
| 1:AI:117:THR:HG22 | 1:AJ:85:THR:HG21 | 1.97                     | 0.46              |
| 1:AX:7:LEU:HB3    | 1:A4:39:ARG:O    | 2.16                     | 0.46              |
| 1:AZ:58:ILE:O     | 1:AZ:62:ALA:CB   | 2.64                     | 0.46              |
| 1:A3:75:ILE:HG22  | 1:A3:77:LEU:HD13 | 1.98                     | 0.46              |
| 1:A4:129:THR:O    | 1:A4:130:LYS:C   | 2.59                     | 0.46              |
| 1:BD:75:ILE:HG22  | 1:BD:77:LEU:HD13 | 1.98                     | 0.46              |
| 1:BD:148:LEU:HD23 | 1:BD:148:LEU:HA  | 1.82                     | 0.46              |
| 1:BQ:100:ALA:CA   | 1:BR:56:PHE:HZ   | 2.28                     | 0.46              |
| 1:BR:67:ASN:HD22  | 1:BR:67:ASN:HA   | 1.59                     | 0.46              |
| 1:BX:48:ASP:HB2   | 1:BX:71:TYR:CE1  | 2.50                     | 0.46              |
| 1:B3:9:GLY:HA2    | 1:B3:147:HIS:HE1 | 1.81                     | 0.46              |
| 1:CA:106:THR:C    | 1:CA:108:ILE:H   | 2.24                     | 0.46              |
| 1:CB:90:TYR:O     | 1:CB:94:GLU:HG2  | 2.14                     | 0.46              |
| 1:CK:58:ILE:O     | 1:CK:58:ILE:HG22 | 2.11                     | 0.46              |
| 1:CS:75:ILE:HG22  | 1:CS:77:LEU:HD13 | 1.98                     | 0.46              |
| 1:CW:104:LEU:HD13 | 1:CX:102:LEU:HG  | 1.98                     | 0.46              |
| 1:CY:29:LEU:HD11  | 1:CY:134:LYS:HB3 | 1.97                     | 0.46              |
| 1:AB:129:THR:CG2  | 1:AB:130:LYS:H   | 2.28                     | 0.46              |
| 1:AC:83:GLY:HA3   | 2:AC:1001:PO4:O4 | 2.16                     | 0.46              |
| 1:AH:9:GLY:HA3    | 1:AH:12:LEU:HD12 | 1.97                     | 0.46              |
| 1:AI:75:ILE:HG22  | 1:AI:77:LEU:HD13 | 1.98                     | 0.46              |
| 1:BA:58:ILE:O     | 1:BA:62:ALA:CB   | 2.64                     | 0.46              |
| 1:BA:106:THR:C    | 1:BA:108:ILE:H   | 2.24                     | 0.46              |
| 1:BO:109:PRO:HG3  | 1:BO:149:SER:CB  | 2.46                     | 0.46              |
| 1:BP:58:ILE:H     | 1:BP:59:PRO:HD2  | 1.80                     | 0.46              |
| 1:BQ:37:LEU:O     | 1:BQ:42:VAL:HG23 | 2.15                     | 0.46              |
| 1:BV:100:ALA:CA   | 1:BW:56:PHE:HZ   | 2.28                     | 0.46              |
| 1:CD:20:ARG:CZ    | 1:CR:39:ARG:NE   | 2.78                     | 0.46              |
| 1:CF:58:ILE:O     | 1:CF:62:ALA:CB   | 2.64                     | 0.46              |
| 1:CI:75:ILE:HG22  | 1:CI:77:LEU:HD13 | 1.98                     | 0.46              |
| 1:CK:106:THR:C    | 1:CK:108:ILE:H   | 2.24                     | 0.46              |
| 1:CN:18:VAL:HG11  | 1:CN:30:LEU:HD13 | 1.98                     | 0.46              |
| 1:CN:75:ILE:HG22  | 1:CN:77:LEU:HD13 | 1.98                     | 0.46              |
| 1:CR:83:GLY:HA3   | 2:CR:2201:PO4:O4 | 2.16                     | 0.46              |
| 1:CU:58:ILE:O     | 1:CU:58:ILE:HG22 | 2.11                     | 0.46              |
| 1:CU:58:ILE:O     | 1:CU:62:ALA:CB   | 2.64                     | 0.46              |
| 1:AA:106:THR:C    | 1:AA:108:ILE:H   | 2.23                     | 0.45              |
| 1:AD:48:ASP:HB2   | 1:AD:71:TYR:CE1  | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AU:32:GLY:HA3   | 1:AU:135:GLY:C    | 2.42                     | 0.45              |
| 1:A2:30:LEU:HA    | 1:A2:77:LEU:HD23  | 1.97                     | 0.45              |
| 1:BH:75:ILE:HG22  | 1:BH:77:LEU:HD13  | 1.97                     | 0.45              |
| 1:BJ:109:PRO:HG3  | 1:BJ:149:SER:CB   | 2.46                     | 0.45              |
| 1:BL:65:MET:HE3   | 1:BL:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:BL:100:ALA:CA   | 1:BM:56:PHE:HZ    | 2.28                     | 0.45              |
| 1:BN:75:ILE:HG22  | 1:BN:77:LEU:HD13  | 1.98                     | 0.45              |
| 1:BP:106:THR:C    | 1:BP:108:ILE:H    | 2.23                     | 0.45              |
| 1:BT:129:THR:O    | 1:BT:130:LYS:C    | 2.59                     | 0.45              |
| 1:BV:106:THR:O    | 1:BV:107:ASP:HB3  | 2.15                     | 0.45              |
| 1:BW:30:LEU:HA    | 1:BW:77:LEU:HD23  | 1.97                     | 0.45              |
| 1:CB:100:ALA:CA   | 1:CC:56:PHE:HZ    | 2.28                     | 0.45              |
| 1:CL:37:LEU:O     | 1:CL:42:VAL:HG23  | 2.15                     | 0.45              |
| 1:CM:83:GLY:HA3   | 2:CM:2201:PO4:O4  | 2.16                     | 0.45              |
| 1:CQ:70:LYS:O     | 1:CQ:70:LYS:HG2   | 2.17                     | 0.45              |
| 1:C2:9:GLY:HA3    | 1:C2:12:LEU:HD12  | 1.98                     | 0.45              |
| 1:AD:24:PHE:CD1   | 1:AR:28:LYS:HG3   | 2.52                     | 0.45              |
| 1:AE:129:THR:O    | 1:AE:130:LYS:C    | 2.59                     | 0.45              |
| 1:AH:104:LEU:HD13 | 1:AI:102:LEU:HG   | 1.98                     | 0.45              |
| 1:AJ:129:THR:O    | 1:AJ:130:LYS:C    | 2.59                     | 0.45              |
| 1:AM:108:ILE:O    | 1:AM:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:AT:109:PRO:HG3  | 1:AT:149:SER:CB   | 2.46                     | 0.45              |
| 1:AZ:7:LEU:HD12   | 1:AZ:7:LEU:HA     | 1.84                     | 0.45              |
| 1:BC:108:ILE:O    | 1:BC:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:BD:18:VAL:HG11  | 1:BD:30:LEU:HD13  | 1.98                     | 0.45              |
| 1:BF:58:ILE:H     | 1:BF:59:PRO:HD2   | 1.80                     | 0.45              |
| 1:BG:65:MET:HE3   | 1:BG:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:BR:45:ASN:HD22  | 1:BR:45:ASN:HA    | 1.63                     | 0.45              |
| 1:BU:58:ILE:O     | 1:BU:58:ILE:HG22  | 2.11                     | 0.45              |
| 1:BZ:106:THR:C    | 1:BZ:108:ILE:H    | 2.23                     | 0.45              |
| 1:B1:4:GLU:CG     | 1:B2:51:TRP:HD1   | 2.29                     | 0.45              |
| 1:CF:106:THR:C    | 1:CF:108:ILE:H    | 2.24                     | 0.45              |
| 1:CH:148:LEU:HD23 | 1:CH:148:LEU:HA   | 1.80                     | 0.45              |
| 1:CN:48:ASP:HB2   | 1:CN:71:TYR:CE1   | 2.50                     | 0.45              |
| 1:CP:58:ILE:O     | 1:CP:62:ALA:CB    | 2.64                     | 0.45              |
| 1:CP:106:THR:C    | 1:CP:108:ILE:H    | 2.23                     | 0.45              |
| 1:CS:48:ASP:HB2   | 1:CS:71:TYR:CE1   | 2.50                     | 0.45              |
| 1:C1:65:MET:HE3   | 1:C1:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:C2:83:GLY:HA3   | 2:C2:2201:PO4:O4  | 2.16                     | 0.45              |
| 1:AI:18:VAL:HG11  | 1:AI:30:LEU:HD13  | 1.98                     | 0.45              |
| 1:AN:9:GLY:HA2    | 1:AN:147:HIS:HE1  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AN:18:VAL:HG11  | 1:AN:30:LEU:HD13  | 1.98                     | 0.45              |
| 1:AO:109:PRO:HG3  | 1:AO:149:SER:CB   | 2.46                     | 0.45              |
| 1:A1:65:MET:HE3   | 1:A1:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:A4:109:PRO:HG3  | 1:A4:149:SER:CB   | 2.46                     | 0.45              |
| 1:BB:58:ILE:O     | 1:BB:58:ILE:HG22  | 2.13                     | 0.45              |
| 1:BC:52:VAL:CG1   | 1:BC:61:ILE:HD12  | 2.35                     | 0.45              |
| 1:BF:58:ILE:O     | 1:BF:62:ALA:CB    | 2.64                     | 0.45              |
| 1:BK:58:ILE:O     | 1:BK:62:ALA:CB    | 2.64                     | 0.45              |
| 1:BR:108:ILE:O    | 1:BR:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:BS:18:VAL:HG23  | 1:BS:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:BU:58:ILE:O     | 1:BU:62:ALA:CB    | 2.64                     | 0.45              |
| 1:BV:4:GLU:CG     | 1:BW:51:TRP:HD1   | 2.29                     | 0.45              |
| 1:CA:58:ILE:O     | 1:CA:62:ALA:CB    | 2.64                     | 0.45              |
| 1:CC:83:GLY:HA3   | 2:CC:1001:PO4:O4  | 2.16                     | 0.45              |
| 1:CD:18:VAL:HG11  | 1:CD:30:LEU:HD13  | 1.98                     | 0.45              |
| 1:CD:52:VAL:CG1   | 1:CD:61:ILE:HD12  | 2.35                     | 0.45              |
| 1:CE:109:PRO:HG3  | 1:CE:149:SER:CB   | 2.46                     | 0.45              |
| 1:CL:70:LYS:O     | 1:CL:70:LYS:HG2   | 2.16                     | 0.45              |
| 1:CR:9:GLY:HA3    | 1:CR:12:LEU:HD12  | 1.98                     | 0.45              |
| 1:CR:104:LEU:HD13 | 1:CS:102:LEU:HG   | 1.98                     | 0.45              |
| 1:CR:108:ILE:O    | 1:CR:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:CU:58:ILE:H     | 1:CU:59:PRO:HD2   | 1.80                     | 0.45              |
| 1:CW:30:LEU:HA    | 1:CW:77:LEU:HD23  | 1.97                     | 0.45              |
| 1:CX:18:VAL:HG11  | 1:CX:30:LEU:HD13  | 1.98                     | 0.45              |
| 1:CZ:32:GLY:HA3   | 1:CZ:135:GLY:C    | 2.42                     | 0.45              |
| 1:AD:18:VAL:HG11  | 1:AD:30:LEU:HD13  | 1.98                     | 0.45              |
| 1:AK:32:GLY:HA3   | 1:AK:135:GLY:C    | 2.42                     | 0.45              |
| 1:AQ:65:MET:HE3   | 1:AQ:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:AQ:100:ALA:CA   | 1:AR:56:PHE:HZ    | 2.28                     | 0.45              |
| 1:AR:30:LEU:HA    | 1:AR:77:LEU:HD23  | 1.97                     | 0.45              |
| 1:AR:83:GLY:HA3   | 2:AR:1001:PO4:O4  | 2.16                     | 0.45              |
| 1:AU:106:THR:C    | 1:AU:108:ILE:H    | 2.24                     | 0.45              |
| 1:AV:65:MET:HE3   | 1:AV:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:A3:9:GLY:HA2    | 1:A3:147:HIS:HE1  | 1.81                     | 0.45              |
| 1:BC:104:LEU:HD13 | 1:BD:102:LEU:HG   | 1.98                     | 0.45              |
| 1:BH:67:ASN:HD22  | 1:BH:67:ASN:HA    | 1.60                     | 0.45              |
| 1:BV:65:MET:HE3   | 1:BV:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:BX:18:VAL:HG23  | 1:BX:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:B2:9:GLY:HA3    | 1:B2:12:LEU:HD12  | 1.97                     | 0.45              |
| 1:CA:28:LYS:NZ    | 1:CN:28:LYS:NZ    | 2.65                     | 0.45              |
| 1:CI:9:GLY:HA2    | 1:CI:147:HIS:HE1  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CP:32:GLY:HA3   | 1:CP:135:GLY:C    | 2.42                     | 0.45              |
| 1:CY:109:PRO:HG3  | 1:CY:149:SER:CB   | 2.46                     | 0.45              |
| 1:AB:65:MET:HE3   | 1:AB:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:AF:58:ILE:O     | 1:AF:62:ALA:CB    | 2.64                     | 0.45              |
| 1:AG:58:ILE:O     | 1:AG:58:ILE:HG22  | 2.13                     | 0.45              |
| 1:AH:108:ILE:O    | 1:AH:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:AQ:70:LYS:HG2   | 1:AQ:70:LYS:O     | 2.16                     | 0.45              |
| 1:AR:45:ASN:HD22  | 1:AR:45:ASN:HA    | 1.63                     | 0.45              |
| 1:A3:148:LEU:HD23 | 1:A3:148:LEU:HA   | 1.82                     | 0.45              |
| 1:BG:58:ILE:O     | 1:BG:58:ILE:HG22  | 2.13                     | 0.45              |
| 1:BN:9:GLY:HA2    | 1:BN:147:HIS:HE1  | 1.81                     | 0.45              |
| 1:BN:18:VAL:HG23  | 1:BN:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:BQ:6:HIS:HB3    | 1:BQ:147:HIS:CG   | 2.52                     | 0.45              |
| 1:BS:149:SER:HB3  | 1:BS:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:BT:109:PRO:HG3  | 1:BT:149:SER:CB   | 2.46                     | 0.45              |
| 1:BW:108:ILE:O    | 1:BW:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:B2:83:GLY:HA3   | 2:B2:1001:PO4:O4  | 2.16                     | 0.45              |
| 1:CD:9:GLY:HA2    | 1:CD:147:HIS:HE1  | 1.81                     | 0.45              |
| 1:CD:48:ASP:HB2   | 1:CD:71:TYR:CE1   | 2.50                     | 0.45              |
| 1:CF:32:GLY:HA3   | 1:CF:135:GLY:C    | 2.42                     | 0.45              |
| 1:CG:55:ALA:CB    | 1:CG:95:VAL:HG21  | 2.40                     | 0.45              |
| 1:CL:65:MET:HE3   | 1:CL:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:CM:104:LEU:HD13 | 1:CN:102:LEU:HG   | 1.98                     | 0.45              |
| 1:CN:149:SER:HB3  | 1:CN:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:CO:129:THR:O    | 1:CO:130:LYS:C    | 2.59                     | 0.45              |
| 1:CU:32:GLY:HA3   | 1:CU:135:GLY:C    | 2.42                     | 0.45              |
| 1:C2:75:ILE:HG22  | 1:C2:77:LEU:HD13  | 1.97                     | 0.45              |
| 1:AH:67:ASN:HD22  | 1:AH:67:ASN:HA    | 1.59                     | 0.45              |
| 1:AR:108:ILE:O    | 1:AR:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:AV:9:GLY:HA3    | 1:AV:12:LEU:HD12  | 1.99                     | 0.45              |
| 1:AV:100:ALA:CA   | 1:AW:56:PHE:HZ    | 2.28                     | 0.45              |
| 1:AW:9:GLY:HA3    | 1:AW:12:LEU:HD12  | 1.97                     | 0.45              |
| 1:AX:48:ASP:HB2   | 1:AX:71:TYR:CE1   | 2.50                     | 0.45              |
| 1:BA:58:ILE:HG21  | 1:BA:76:THR:OG1   | 2.17                     | 0.45              |
| 1:BB:4:GLU:CG     | 1:BC:51:TRP:HD1   | 2.29                     | 0.45              |
| 1:BD:18:VAL:HG23  | 1:BD:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:BG:6:HIS:HB3    | 1:BG:147:HIS:CG   | 2.52                     | 0.45              |
| 1:BG:97:LYS:N     | 1:BG:100:ALA:HB2  | 2.31                     | 0.45              |
| 1:BH:9:GLY:HA3    | 1:BH:12:LEU:HD12  | 1.98                     | 0.45              |
| 1:BI:149:SER:HB3  | 1:BI:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:BL:58:ILE:O     | 1:BL:58:ILE:HG22  | 2.13                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BP:58:ILE:HG21  | 1:BP:76:THR:OG1   | 2.17                     | 0.45              |
| 1:BQ:70:LYS:O     | 1:BQ:70:LYS:HG2   | 2.17                     | 0.45              |
| 1:BY:109:PRO:HG3  | 1:BY:149:SER:CB   | 2.46                     | 0.45              |
| 1:B1:106:THR:O    | 1:B1:107:ASP:HB3  | 2.15                     | 0.45              |
| 1:B2:108:ILE:O    | 1:B2:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:B3:149:SER:HB3  | 1:B3:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:CA:22:ASN:HA    | 1:CN:128:GLY:O    | 2.17                     | 0.45              |
| 1:CI:52:VAL:CG1   | 1:CI:61:ILE:HD12  | 2.35                     | 0.45              |
| 1:CK:32:GLY:HA3   | 1:CK:135:GLY:C    | 2.42                     | 0.45              |
| 1:CK:58:ILE:HG21  | 1:CK:76:THR:OG1   | 2.17                     | 0.45              |
| 1:CL:6:HIS:HB3    | 1:CL:147:HIS:CG   | 2.52                     | 0.45              |
| 1:CQ:4:GLU:CG     | 1:CR:51:TRP:HD1   | 2.29                     | 0.45              |
| 1:CQ:65:MET:HE3   | 1:CQ:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:CX:117:THR:HG22 | 1:CY:85:THR:HG21  | 1.97                     | 0.45              |
| 1:AG:6:HIS:HB3    | 1:AG:147:HIS:CG   | 2.52                     | 0.45              |
| 1:AH:83:GLY:HA3   | 2:AH:1001:PO4:O4  | 2.17                     | 0.45              |
| 1:AI:18:VAL:HG23  | 1:AI:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:AI:149:SER:HB3  | 1:AI:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:AJ:109:PRO:HG3  | 1:AJ:149:SER:CB   | 2.46                     | 0.45              |
| 1:AL:97:LYS:N     | 1:AL:100:ALA:HB2  | 2.31                     | 0.45              |
| 1:AN:18:VAL:HG23  | 1:AN:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:AO:129:THR:O    | 1:AO:130:LYS:C    | 2.59                     | 0.45              |
| 1:AU:58:ILE:HG21  | 1:AU:76:THR:OG1   | 2.17                     | 0.45              |
| 1:A2:9:GLY:HA3    | 1:A2:12:LEU:HD12  | 1.98                     | 0.45              |
| 1:A3:48:ASP:HB2   | 1:A3:71:TYR:CE1   | 2.50                     | 0.45              |
| 1:A4:71:TYR:O     | 1:A4:150:LYS:NZ   | 2.44                     | 0.45              |
| 1:BB:6:HIS:HB3    | 1:BB:147:HIS:CG   | 2.52                     | 0.45              |
| 1:BH:108:ILE:O    | 1:BH:110:VAL:HG23 | 2.16                     | 0.45              |
| 1:BL:70:LYS:O     | 1:BL:70:LYS:HG2   | 2.17                     | 0.45              |
| 1:BO:129:THR:O    | 1:BO:130:LYS:C    | 2.59                     | 0.45              |
| 1:BV:55:ALA:CB    | 1:BV:95:VAL:HG21  | 2.40                     | 0.45              |
| 1:BW:97:LYS:HE3   | 1:BX:97:LYS:HZ1   | 1.82                     | 0.45              |
| 1:BZ:58:ILE:HG21  | 1:BZ:76:THR:OG1   | 2.17                     | 0.45              |
| 1:B3:75:ILE:HG22  | 1:B3:77:LEU:HD13  | 1.98                     | 0.45              |
| 1:CB:65:MET:HE3   | 1:CB:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:CC:104:LEU:HD13 | 1:CD:102:LEU:HG   | 1.98                     | 0.45              |
| 1:CD:149:SER:HB3  | 1:CD:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:CE:29:LEU:HD11  | 1:CE:134:LYS:HB3  | 1.97                     | 0.45              |
| 1:CM:97:LYS:HE3   | 1:CN:97:LYS:HZ1   | 1.82                     | 0.45              |
| 1:CT:129:THR:O    | 1:CT:130:LYS:C    | 2.59                     | 0.45              |
| 1:C3:9:GLY:HA2    | 1:C3:147:HIS:HE1  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C3:149:SER:HB3  | 1:C3:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:AC:52:VAL:CG1   | 1:AC:61:ILE:HD12  | 2.35                     | 0.45              |
| 1:AC:97:LYS:HE3   | 1:AD:97:LYS:NZ    | 2.32                     | 0.45              |
| 1:AD:117:THR:HG22 | 1:AE:85:THR:HG21  | 1.97                     | 0.45              |
| 1:AL:6:HIS:HB3    | 1:AL:147:HIS:CG   | 2.52                     | 0.45              |
| 1:AN:34:LEU:O     | 1:AN:38:LYS:HG3   | 2.17                     | 0.45              |
| 1:AN:149:SER:HB3  | 1:AN:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:AU:58:ILE:O     | 1:AU:62:ALA:CB    | 2.64                     | 0.45              |
| 1:AV:6:HIS:HB3    | 1:AV:147:HIS:CG   | 2.52                     | 0.45              |
| 1:AX:18:VAL:HG23  | 1:AX:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:AY:129:THR:O    | 1:AY:130:LYS:C    | 2.59                     | 0.45              |
| 1:A2:108:ILE:O    | 1:A2:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:BC:83:GLY:HA3   | 2:BC:1001:PO4:O4  | 2.16                     | 0.45              |
| 1:BF:32:GLY:HA3   | 1:BF:135:GLY:C    | 2.42                     | 0.45              |
| 1:BH:83:GLY:HA3   | 2:BH:1001:PO4:O4  | 2.16                     | 0.45              |
| 1:BS:148:LEU:HD23 | 1:BS:148:LEU:HA   | 1.82                     | 0.45              |
| 1:BU:32:GLY:HA3   | 1:BU:135:GLY:C    | 2.42                     | 0.45              |
| 1:BX:75:ILE:HD13  | 1:BX:139:ALA:HA   | 1.99                     | 0.45              |
| 1:CG:4:GLU:CG     | 1:CH:51:TRP:HD1   | 2.29                     | 0.45              |
| 1:CO:109:PRO:HG3  | 1:CO:149:SER:CB   | 2.47                     | 0.45              |
| 1:CV:9:GLY:HA3    | 1:CV:12:LEU:HD12  | 1.99                     | 0.45              |
| 1:CW:83:GLY:HA3   | 2:CW:2201:PO4:O4  | 2.16                     | 0.45              |
| 1:C1:97:LYS:N     | 1:C1:100:ALA:HB2  | 2.31                     | 0.45              |
| 1:C2:108:ILE:O    | 1:C2:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:C3:18:VAL:HG23  | 1:C3:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:AA:32:GLY:HA3   | 1:AA:135:GLY:C    | 2.42                     | 0.45              |
| 1:AA:58:ILE:HG21  | 1:AA:76:THR:OG1   | 2.17                     | 0.45              |
| 1:AD:18:VAL:HG23  | 1:AD:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:AD:22:ASN:HA    | 1:AR:128:GLY:O    | 2.17                     | 0.45              |
| 1:AE:109:PRO:HG3  | 1:AE:149:SER:CB   | 2.46                     | 0.45              |
| 1:AG:55:ALA:HB1   | 1:AG:95:VAL:CG2   | 2.40                     | 0.45              |
| 1:AG:65:MET:HE3   | 1:AG:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:AG:97:LYS:N     | 1:AG:100:ALA:HB2  | 2.31                     | 0.45              |
| 1:AI:34:LEU:O     | 1:AI:38:LYS:HG3   | 2.17                     | 0.45              |
| 1:AO:71:TYR:O     | 1:AO:150:LYS:NZ   | 2.44                     | 0.45              |
| 1:AP:58:ILE:O     | 1:AP:62:ALA:CB    | 2.64                     | 0.45              |
| 1:AS:48:ASP:HB2   | 1:AS:71:TYR:CE1   | 2.50                     | 0.45              |
| 1:AT:129:THR:O    | 1:AT:130:LYS:C    | 2.59                     | 0.45              |
| 1:AX:34:LEU:O     | 1:AX:38:LYS:HG3   | 2.17                     | 0.45              |
| 1:BA:32:GLY:HA3   | 1:BA:135:GLY:C    | 2.42                     | 0.45              |
| 1:BD:34:LEU:O     | 1:BD:38:LYS:HG3   | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BD:75:ILE:HD13  | 1:BD:139:ALA:HA   | 1.99                     | 0.45              |
| 1:BP:58:ILE:O     | 1:BP:62:ALA:CB    | 2.64                     | 0.45              |
| 1:BR:9:GLY:HA3    | 1:BR:12:LEU:HD12  | 1.97                     | 0.45              |
| 1:BR:52:VAL:CG1   | 1:BR:61:ILE:HD12  | 2.35                     | 0.45              |
| 1:BW:83:GLY:HA3   | 2:BW:1001:PO4:O4  | 2.16                     | 0.45              |
| 1:B1:65:MET:HE3   | 1:B1:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:B4:129:THR:O    | 1:B4:130:LYS:C    | 2.59                     | 0.45              |
| 1:CA:7:LEU:HD12   | 1:CA:7:LEU:HA     | 1.84                     | 0.45              |
| 1:CC:7:LEU:CD2    | 1:CR:40:HIS:CE1   | 2.97                     | 0.45              |
| 1:CC:82:ARG:CG    | 1:CC:82:ARG:NH1   | 2.73                     | 0.45              |
| 1:CG:70:LYS:HG2   | 1:CG:70:LYS:O     | 2.17                     | 0.45              |
| 1:CI:7:LEU:HD23   | 1:CO:40:HIS:CE1   | 2.52                     | 0.45              |
| 1:CI:18:VAL:HG11  | 1:CI:30:LEU:HD13  | 1.98                     | 0.45              |
| 1:CJ:129:THR:O    | 1:CJ:130:LYS:C    | 2.59                     | 0.45              |
| 1:CL:4:GLU:CG     | 1:CM:51:TRP:HD1   | 2.29                     | 0.45              |
| 1:CN:34:LEU:O     | 1:CN:38:LYS:HG3   | 2.17                     | 0.45              |
| 1:CO:53:PRO:CG    | 1:CO:57:GLU:CG    | 2.46                     | 0.45              |
| 1:CV:65:MET:HE3   | 1:CV:71:TYR:CZ    | 2.52                     | 0.45              |
| 1:CX:18:VAL:HG23  | 1:CX:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:CX:149:SER:HB3  | 1:CX:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:CZ:58:ILE:HG21  | 1:CZ:76:THR:OG1   | 2.17                     | 0.45              |
| 1:AA:7:LEU:HD12   | 1:AA:7:LEU:HA     | 1.84                     | 0.45              |
| 1:AD:149:SER:HB3  | 1:AD:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:AE:4:GLU:C      | 1:AE:148:LEU:HD21 | 2.42                     | 0.45              |
| 1:AI:9:GLY:HA2    | 1:AI:147:HIS:HE1  | 1.81                     | 0.45              |
| 1:AK:58:ILE:H     | 1:AK:59:PRO:HD2   | 1.80                     | 0.45              |
| 1:AM:66:ALA:HB2   | 1:AM:74:VAL:HG21  | 1.99                     | 0.45              |
| 1:AM:104:LEU:HD13 | 1:AN:102:LEU:HG   | 1.97                     | 0.45              |
| 1:AS:9:GLY:HA2    | 1:AS:147:HIS:HE1  | 1.81                     | 0.45              |
| 1:AS:75:ILE:HG22  | 1:AS:77:LEU:HD13  | 1.98                     | 0.45              |
| 1:AX:149:SER:HB3  | 1:AX:152:TRP:CH2  | 2.52                     | 0.45              |
| 1:A2:83:GLY:HA3   | 2:A2:1001:PO4:O4  | 2.16                     | 0.45              |
| 1:A3:18:VAL:HG23  | 1:A3:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:BE:129:THR:O    | 1:BE:130:LYS:C    | 2.59                     | 0.45              |
| 1:BG:70:LYS:O     | 1:BG:70:LYS:HG2   | 2.17                     | 0.45              |
| 1:BH:97:LYS:HE3   | 1:BI:97:LYS:NZ    | 2.32                     | 0.45              |
| 1:BH:104:LEU:HD13 | 1:BI:102:LEU:HG   | 1.98                     | 0.45              |
| 1:BK:106:THR:C    | 1:BK:108:ILE:H    | 2.23                     | 0.45              |
| 1:BL:6:HIS:HB3    | 1:BL:147:HIS:CG   | 2.52                     | 0.45              |
| 1:BL:129:THR:CG2  | 1:BL:130:LYS:H    | 2.28                     | 0.45              |
| 1:BM:104:LEU:HD13 | 1:BN:102:LEU:HG   | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BP:32:GLY:HA3  | 1:BP:135:GLY:C    | 2.42                     | 0.45              |
| 1:BU:7:LEU:HD12  | 1:BU:7:LEU:HA     | 1.85                     | 0.45              |
| 1:BV:6:HIS:HB3   | 1:BV:147:HIS:CG   | 2.52                     | 0.45              |
| 1:BW:45:ASN:HD22 | 1:BW:45:ASN:HA    | 1.64                     | 0.45              |
| 1:BX:39:ARG:O    | 1:B4:7:LEU:HB3    | 2.17                     | 0.45              |
| 1:CC:34:LEU:HD22 | 1:CC:38:LYS:CE    | 2.43                     | 0.45              |
| 1:CD:18:VAL:HG23 | 1:CD:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:CH:83:GLY:HA3  | 2:CH:2201:PO4:O4  | 2.16                     | 0.45              |
| 1:CK:65:MET:HE3  | 1:CK:71:TYR:CE2   | 2.52                     | 0.45              |
| 1:CM:66:ALA:HB2  | 1:CM:74:VAL:HG21  | 1.99                     | 0.45              |
| 1:CN:18:VAL:HG23 | 1:CN:51:TRP:CE3   | 2.52                     | 0.45              |
| 1:CQ:97:LYS:N    | 1:CQ:100:ALA:HB2  | 2.31                     | 0.45              |
| 1:CR:67:ASN:HD22 | 1:CR:67:ASN:HA    | 1.60                     | 0.45              |
| 1:CU:58:ILE:HG21 | 1:CU:76:THR:OG1   | 2.17                     | 0.45              |
| 1:CW:108:ILE:O   | 1:CW:110:VAL:HG23 | 2.17                     | 0.45              |
| 1:C3:48:ASP:HB2  | 1:C3:71:TYR:CE1   | 2.50                     | 0.45              |
| 1:AC:9:GLY:HA3   | 1:AC:12:LEU:HD12  | 1.98                     | 0.44              |
| 1:AD:75:ILE:HG22 | 1:AD:77:LEU:HD13  | 1.98                     | 0.44              |
| 1:AH:34:LEU:HD22 | 1:AH:38:LYS:CE    | 2.43                     | 0.44              |
| 1:AK:58:ILE:HG21 | 1:AK:76:THR:OG1   | 2.17                     | 0.44              |
| 1:AK:65:MET:HE3  | 1:AK:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:AQ:6:HIS:HB3   | 1:AQ:147:HIS:CG   | 2.52                     | 0.44              |
| 1:AQ:55:ALA:HB1  | 1:AQ:95:VAL:CG2   | 2.40                     | 0.44              |
| 1:AR:67:ASN:HD22 | 1:AR:67:ASN:HA    | 1.59                     | 0.44              |
| 1:AS:18:VAL:HG11 | 1:AS:30:LEU:HD13  | 1.98                     | 0.44              |
| 1:AS:18:VAL:HG23 | 1:AS:51:TRP:CE3   | 2.52                     | 0.44              |
| 1:AT:71:TYR:O    | 1:AT:150:LYS:NZ   | 2.44                     | 0.44              |
| 1:AW:66:ALA:HB2  | 1:AW:74:VAL:HG21  | 1.99                     | 0.44              |
| 1:AW:97:LYS:HE3  | 1:AX:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:AW:108:ILE:O   | 1:AW:110:VAL:HG23 | 2.17                     | 0.44              |
| 1:A2:97:LYS:HE3  | 1:A3:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:BB:9:GLY:HA3   | 1:BB:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:BC:9:GLY:HA3   | 1:BC:12:LEU:HD12  | 1.98                     | 0.44              |
| 1:BH:66:ALA:HB2  | 1:BH:74:VAL:HG21  | 1.99                     | 0.44              |
| 1:BK:65:MET:HE3  | 1:BK:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:BL:9:GLY:HA3   | 1:BL:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:BM:9:GLY:HA3   | 1:BM:12:LEU:HD12  | 1.97                     | 0.44              |
| 1:BM:83:GLY:HA3  | 2:BM:1001:PO4:O4  | 2.16                     | 0.44              |
| 1:BN:18:VAL:HG11 | 1:BN:30:LEU:HD13  | 1.98                     | 0.44              |
| 1:BQ:65:MET:HE3  | 1:BQ:71:TYR:CZ    | 2.52                     | 0.44              |
| 1:BS:18:VAL:HG11 | 1:BS:30:LEU:HD13  | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BU:58:ILE:HG21 | 1:BU:76:THR:OG1   | 2.17                     | 0.44              |
| 1:BZ:65:MET:HE3  | 1:BZ:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:B1:97:LYS:N    | 1:B1:100:ALA:HB2  | 2.31                     | 0.44              |
| 1:B1:100:ALA:CA  | 1:B2:56:PHE:HZ    | 2.28                     | 0.44              |
| 1:B3:34:LEU:O    | 1:B3:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:CA:32:GLY:HA3  | 1:CA:135:GLY:C    | 2.42                     | 0.44              |
| 1:CC:97:LYS:HE3  | 1:CD:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:CE:4:GLU:C     | 1:CE:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:CF:58:ILE:HG21 | 1:CF:76:THR:OG1   | 2.17                     | 0.44              |
| 1:CJ:4:GLU:C     | 1:CJ:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:CL:9:GLY:HA3   | 1:CL:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:CM:108:ILE:O   | 1:CM:110:VAL:HG23 | 2.17                     | 0.44              |
| 1:CN:121:GLU:O   | 1:CN:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:CU:144:GLU:O   | 1:CU:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:CV:70:LYS:O    | 1:CV:70:LYS:HG2   | 2.17                     | 0.44              |
| 1:CW:97:LYS:HE3  | 1:CX:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:C3:34:LEU:O    | 1:C3:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:AG:70:LYS:O    | 1:AG:70:LYS:HG2   | 2.17                     | 0.44              |
| 1:AI:28:LYS:NZ   | 1:AK:28:LYS:HZ2   | 2.15                     | 0.44              |
| 1:AL:58:ILE:O    | 1:AL:58:ILE:CG2   | 2.65                     | 0.44              |
| 1:AM:82:ARG:HG3  | 1:AM:118:GLU:OE2  | 2.17                     | 0.44              |
| 1:AM:83:GLY:HA3  | 2:AM:1001:PO4:O4  | 2.16                     | 0.44              |
| 1:AP:144:GLU:O   | 1:AP:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:AU:58:ILE:O    | 1:AU:62:ALA:HB2   | 2.17                     | 0.44              |
| 1:AU:58:ILE:H    | 1:AU:59:PRO:HD2   | 1.80                     | 0.44              |
| 1:AV:58:ILE:O    | 1:AV:58:ILE:CG2   | 2.65                     | 0.44              |
| 1:AV:70:LYS:O    | 1:AV:70:LYS:HG2   | 2.17                     | 0.44              |
| 1:AW:83:GLY:HA3  | 2:AW:201:PO4:O4   | 2.16                     | 0.44              |
| 1:AX:18:VAL:HG11 | 1:AX:30:LEU:HD13  | 1.98                     | 0.44              |
| 1:AZ:58:ILE:O    | 1:AZ:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:A1:6:HIS:HB3   | 1:A1:147:HIS:CG   | 2.52                     | 0.44              |
| 1:BC:82:ARG:HG3  | 1:BC:118:GLU:OE2  | 2.18                     | 0.44              |
| 1:BC:97:LYS:HE3  | 1:BD:97:LYS:HZ3   | 1.82                     | 0.44              |
| 1:BF:65:MET:HE3  | 1:BF:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:BI:9:GLY:HA2   | 1:BI:147:HIS:HE1  | 1.81                     | 0.44              |
| 1:BJ:4:GLU:C     | 1:BJ:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:BK:58:ILE:O    | 1:BK:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:BK:144:GLU:O   | 1:BK:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:BL:97:LYS:N    | 1:BL:100:ALA:HB2  | 2.31                     | 0.44              |
| 1:BN:34:LEU:O    | 1:BN:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:BN:75:ILE:HD13 | 1:BN:139:ALA:HA   | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B1:6:HIS:HB3    | 1:B1:147:HIS:CG   | 2.52                     | 0.44              |
| 1:B2:97:LYS:HE3   | 1:B3:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:B4:109:PRO:HG3  | 1:B4:149:SER:CB   | 2.46                     | 0.44              |
| 1:CA:58:ILE:HG21  | 1:CA:76:THR:OG1   | 2.17                     | 0.44              |
| 1:CB:6:HIS:HB3    | 1:CB:147:HIS:CG   | 2.52                     | 0.44              |
| 1:CC:82:ARG:HG3   | 1:CC:118:GLU:OE2  | 2.17                     | 0.44              |
| 1:CF:58:ILE:O     | 1:CF:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:CF:144:GLU:O    | 1:CF:148:LEU:HB2  | 2.17                     | 0.44              |
| 1:CH:24:PHE:CD1   | 1:CU:28:LYS:HD2   | 2.52                     | 0.44              |
| 1:CH:108:ILE:O    | 1:CH:110:VAL:HG23 | 2.17                     | 0.44              |
| 1:CJ:109:PRO:HG3  | 1:CJ:149:SER:CB   | 2.46                     | 0.44              |
| 1:CU:58:ILE:O     | 1:CU:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:CV:6:HIS:HB3    | 1:CV:147:HIS:CG   | 2.52                     | 0.44              |
| 1:CW:82:ARG:HG3   | 1:CW:118:GLU:OE2  | 2.17                     | 0.44              |
| 1:C4:4:GLU:C      | 1:C4:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:AB:55:ALA:CB    | 1:AB:95:VAL:HG21  | 2.40                     | 0.44              |
| 1:AD:121:GLU:O    | 1:AD:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:AF:32:GLY:HA3   | 1:AF:135:GLY:C    | 2.42                     | 0.44              |
| 1:AH:82:ARG:HG3   | 1:AH:118:GLU:OE2  | 2.17                     | 0.44              |
| 1:AN:121:GLU:O    | 1:AN:125:GLU:HG3  | 2.17                     | 0.44              |
| 1:AR:97:LYS:HE3   | 1:AS:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:AS:149:SER:HB3  | 1:AS:152:TRP:CH2  | 2.52                     | 0.44              |
| 1:AT:4:GLU:C      | 1:AT:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:AU:65:MET:HE2   | 1:AU:65:MET:HB3   | 1.80                     | 0.44              |
| 1:AW:104:LEU:HD13 | 1:AX:102:LEU:HG   | 1.98                     | 0.44              |
| 1:AX:75:ILE:HD13  | 1:AX:139:ALA:HA   | 1.99                     | 0.44              |
| 1:AZ:144:GLU:O    | 1:AZ:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:A1:70:LYS:O     | 1:A1:70:LYS:HG2   | 2.17                     | 0.44              |
| 1:A3:75:ILE:HD13  | 1:A3:139:ALA:HA   | 1.99                     | 0.44              |
| 1:A3:121:GLU:O    | 1:A3:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:BC:67:ASN:HD22  | 1:BC:67:ASN:HA    | 1.59                     | 0.44              |
| 1:BI:121:GLU:O    | 1:BI:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:BP:65:MET:HE3   | 1:BP:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:BQ:9:GLY:HA3    | 1:BQ:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:BR:66:ALA:HB2   | 1:BR:74:VAL:HG21  | 1.99                     | 0.44              |
| 1:BR:104:LEU:HD13 | 1:BS:102:LEU:HG   | 1.98                     | 0.44              |
| 1:BS:9:GLY:HA2    | 1:BS:147:HIS:HE1  | 1.81                     | 0.44              |
| 1:B3:121:GLU:O    | 1:B3:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:CH:104:LEU:CD2  | 1:CI:60:LEU:HA    | 2.48                     | 0.44              |
| 1:CI:18:VAL:HG23  | 1:CI:51:TRP:CE3   | 2.52                     | 0.44              |
| 1:CM:82:ARG:HG3   | 1:CM:118:GLU:OE2  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CM:97:LYS:HE3   | 1:CN:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:CQ:6:HIS:HB3    | 1:CQ:147:HIS:CG   | 2.52                     | 0.44              |
| 1:CU:98:GLY:O     | 1:CU:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:CZ:65:MET:HE3   | 1:CZ:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:C1:4:GLU:CG     | 1:C2:51:TRP:HD1   | 2.29                     | 0.44              |
| 1:AA:58:ILE:O     | 1:AA:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:AB:58:ILE:O     | 1:AB:58:ILE:HG22  | 2.13                     | 0.44              |
| 1:AB:144:GLU:CD   | 1:AU:39:ARG:NH2   | 2.76                     | 0.44              |
| 1:AD:75:ILE:HD13  | 1:AD:139:ALA:HA   | 1.99                     | 0.44              |
| 1:AG:9:GLY:HA3    | 1:AG:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:AJ:4:GLU:C      | 1:AJ:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:A2:67:ASN:HD22  | 1:A2:67:ASN:HA    | 1.59                     | 0.44              |
| 1:BB:70:LYS:HG2   | 1:BB:70:LYS:O     | 2.17                     | 0.44              |
| 1:BF:58:ILE:O     | 1:BF:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:BH:104:LEU:CD2  | 1:BI:60:LEU:HA    | 2.48                     | 0.44              |
| 1:BI:18:VAL:HG23  | 1:BI:51:TRP:CE3   | 2.52                     | 0.44              |
| 1:BN:148:LEU:HD23 | 1:BN:148:LEU:HA   | 1.82                     | 0.44              |
| 1:BU:58:ILE:O     | 1:BU:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:BX:149:SER:HB3  | 1:BX:152:TRP:CH2  | 2.52                     | 0.44              |
| 1:B1:129:THR:HG22 | 1:B1:130:LYS:N    | 2.33                     | 0.44              |
| 1:B2:66:ALA:HB2   | 1:B2:74:VAL:HG21  | 1.99                     | 0.44              |
| 1:B2:82:ARG:HG3   | 1:B2:118:GLU:OE2  | 2.18                     | 0.44              |
| 1:CC:8:VAL:CG2    | 1:CR:8:VAL:HG13   | 2.48                     | 0.44              |
| 1:CC:108:ILE:O    | 1:CC:110:VAL:HG23 | 2.17                     | 0.44              |
| 1:CD:75:ILE:HD13  | 1:CD:139:ALA:HA   | 1.99                     | 0.44              |
| 1:CG:7:LEU:HD23   | 1:CU:40:HIS:CE1   | 2.52                     | 0.44              |
| 1:CG:65:MET:HE3   | 1:CG:71:TYR:CZ    | 2.52                     | 0.44              |
| 1:CQ:58:ILE:O     | 1:CQ:58:ILE:CG2   | 2.65                     | 0.44              |
| 1:CS:34:LEU:O     | 1:CS:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:CU:65:MET:HE3   | 1:CU:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:CY:4:GLU:C      | 1:CY:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:C1:6:HIS:HB3    | 1:C1:147:HIS:CG   | 2.52                     | 0.44              |
| 1:AB:6:HIS:HB3    | 1:AB:147:HIS:CG   | 2.52                     | 0.44              |
| 1:AB:58:ILE:O     | 1:AB:58:ILE:CG2   | 2.65                     | 0.44              |
| 1:AF:58:ILE:HG21  | 1:AF:76:THR:OG1   | 2.17                     | 0.44              |
| 1:AK:20:ARG:HH12  | 1:AO:144:GLU:CD   | 2.26                     | 0.44              |
| 1:AK:144:GLU:O    | 1:AK:148:LEU:HB2  | 2.17                     | 0.44              |
| 1:AL:65:MET:HE3   | 1:AL:71:TYR:CZ    | 2.52                     | 0.44              |
| 1:AO:64:LYS:HD3   | 1:AO:64:LYS:HA    | 1.85                     | 0.44              |
| 1:AU:65:MET:HE3   | 1:AU:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:AU:98:GLY:O     | 1:AU:102:LEU:HB2  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A1:9:GLY:HA3    | 1:A1:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:A3:149:SER:HB3  | 1:A3:152:TRP:CH2  | 2.52                     | 0.44              |
| 1:BA:58:ILE:H     | 1:BA:59:PRO:HD2   | 1.80                     | 0.44              |
| 1:BA:144:GLU:O    | 1:BA:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:BC:66:ALA:HB2   | 1:BC:74:VAL:HG21  | 1.99                     | 0.44              |
| 1:BC:104:LEU:CD2  | 1:BD:60:LEU:HA    | 2.48                     | 0.44              |
| 1:BI:75:ILE:HD13  | 1:BI:139:ALA:HA   | 1.99                     | 0.44              |
| 1:BK:58:ILE:HG21  | 1:BK:76:THR:OG1   | 2.17                     | 0.44              |
| 1:BM:97:LYS:HE3   | 1:BN:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:BQ:52:VAL:O     | 1:BQ:53:PRO:C     | 2.61                     | 0.44              |
| 1:BR:83:GLY:HA3   | 2:BR:1001:PO4:O4  | 2.16                     | 0.44              |
| 1:BR:97:LYS:HE3   | 1:BS:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:BS:121:GLU:O    | 1:BS:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:BT:4:GLU:C      | 1:BT:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:BU:90:TYR:O     | 1:BU:94:GLU:HG2   | 2.18                     | 0.44              |
| 1:BW:82:ARG:HG3   | 1:BW:118:GLU:OE2  | 2.18                     | 0.44              |
| 1:B3:75:ILE:HD13  | 1:B3:139:ALA:HA   | 1.99                     | 0.44              |
| 1:CH:82:ARG:HG3   | 1:CH:118:GLU:OE2  | 2.17                     | 0.44              |
| 1:CP:58:ILE:HG21  | 1:CP:76:THR:OG1   | 2.17                     | 0.44              |
| 1:CT:4:GLU:C      | 1:CT:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:CV:129:THR:HG22 | 1:CV:130:LYS:N    | 2.33                     | 0.44              |
| 1:C1:55:ALA:CB    | 1:C1:95:VAL:HG21  | 2.40                     | 0.44              |
| 1:C2:104:LEU:CD2  | 1:C3:60:LEU:HA    | 2.48                     | 0.44              |
| 1:C4:71:TYR:O     | 1:C4:150:LYS:NZ   | 2.44                     | 0.44              |
| 1:C4:109:PRO:HG3  | 1:C4:149:SER:CB   | 2.46                     | 0.44              |
| 1:AF:58:ILE:O     | 1:AF:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:AP:20:ARG:HH12  | 1:AT:144:GLU:CD   | 2.26                     | 0.44              |
| 1:AP:98:GLY:O     | 1:AP:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:AW:104:LEU:CD2  | 1:AX:60:LEU:HA    | 2.48                     | 0.44              |
| 1:AX:121:GLU:O    | 1:AX:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:AY:109:PRO:HG3  | 1:AY:149:SER:CB   | 2.46                     | 0.44              |
| 1:AZ:98:GLY:O     | 1:AZ:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:BC:28:LYS:NZ    | 1:BU:28:LYS:CE    | 2.81                     | 0.44              |
| 1:BE:109:PRO:HG3  | 1:BE:149:SER:CB   | 2.46                     | 0.44              |
| 1:BF:90:TYR:O     | 1:BF:94:GLU:HG2   | 2.18                     | 0.44              |
| 1:BG:129:THR:CG2  | 1:BG:130:LYS:H    | 2.28                     | 0.44              |
| 1:BH:97:LYS:HE3   | 1:BI:97:LYS:HZ3   | 1.82                     | 0.44              |
| 1:BL:129:THR:HG22 | 1:BL:130:LYS:N    | 2.33                     | 0.44              |
| 1:BX:17:VAL:HG13  | 1:BX:65:MET:CE    | 2.48                     | 0.44              |
| 1:BZ:58:ILE:H     | 1:BZ:59:PRO:HD2   | 1.80                     | 0.44              |
| 1:BZ:98:GLY:O     | 1:BZ:102:LEU:HB2  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:144:GLU:O    | 1:CA:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:CD:34:LEU:O     | 1:CD:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:CD:58:ILE:HB    | 1:CD:59:PRO:HD3   | 2.00                     | 0.44              |
| 1:CG:6:HIS:HB3    | 1:CG:147:HIS:CG   | 2.52                     | 0.44              |
| 1:CG:9:GLY:HA3    | 1:CG:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:CH:97:LYS:HE3   | 1:CI:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:CK:98:GLY:O     | 1:CK:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:CP:58:ILE:O     | 1:CP:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:CP:65:MET:HE3   | 1:CP:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:CP:98:GLY:O     | 1:CP:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:CR:82:ARG:HG3   | 1:CR:118:GLU:OE2  | 2.17                     | 0.44              |
| 1:CR:104:LEU:CD2  | 1:CS:60:LEU:HA    | 2.48                     | 0.44              |
| 1:CS:9:GLY:HA2    | 1:CS:147:HIS:HE1  | 1.81                     | 0.44              |
| 1:CS:18:VAL:HG23  | 1:CS:51:TRP:CE3   | 2.52                     | 0.44              |
| 1:CS:75:ILE:HD13  | 1:CS:139:ALA:HA   | 1.99                     | 0.44              |
| 1:CU:20:ARG:HH12  | 1:CY:144:GLU:CD   | 2.26                     | 0.44              |
| 1:CY:106:THR:O    | 1:CY:107:ASP:OD1  | 2.36                     | 0.44              |
| 1:C3:121:GLU:O    | 1:C3:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:AA:90:TYR:O     | 1:AA:94:GLU:HG2   | 2.18                     | 0.44              |
| 1:AA:98:GLY:O     | 1:AA:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:AC:108:ILE:O    | 1:AC:110:VAL:HG23 | 2.17                     | 0.44              |
| 1:AK:90:TYR:O     | 1:AK:94:GLU:HG2   | 2.18                     | 0.44              |
| 1:AL:70:LYS:HG2   | 1:AL:70:LYS:O     | 2.17                     | 0.44              |
| 1:AN:75:ILE:HD13  | 1:AN:139:ALA:HA   | 1.99                     | 0.44              |
| 1:AO:4:GLU:C      | 1:AO:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:AQ:9:GLY:HA3    | 1:AQ:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:AR:52:VAL:CG1   | 1:AR:61:ILE:HD12  | 2.35                     | 0.44              |
| 1:AZ:32:GLY:HA3   | 1:AZ:135:GLY:C    | 2.42                     | 0.44              |
| 1:A2:104:LEU:CD2  | 1:A3:60:LEU:HA    | 2.48                     | 0.44              |
| 1:A3:17:VAL:HG13  | 1:A3:65:MET:CE    | 2.48                     | 0.44              |
| 1:BB:52:VAL:O     | 1:BB:53:PRO:C     | 2.61                     | 0.44              |
| 1:BB:58:ILE:O     | 1:BB:58:ILE:CG2   | 2.65                     | 0.44              |
| 1:BD:17:VAL:HG13  | 1:BD:65:MET:CE    | 2.48                     | 0.44              |
| 1:BF:98:GLY:O     | 1:BF:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:BG:104:LEU:HD23 | 1:BH:60:LEU:HD13  | 2.00                     | 0.44              |
| 1:BL:104:LEU:HD23 | 1:BM:60:LEU:HD13  | 2.00                     | 0.44              |
| 1:BO:4:GLU:C      | 1:BO:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:BP:98:GLY:O     | 1:BP:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:BU:20:ARG:HH12  | 1:BY:144:GLU:CD   | 2.26                     | 0.44              |
| 1:BU:98:GLY:O     | 1:BU:102:LEU:HB2  | 2.18                     | 0.44              |
| 1:BV:9:GLY:HA3    | 1:BV:12:LEU:HD12  | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BV:70:LYS:HG2   | 1:BV:70:LYS:O     | 2.17                     | 0.44              |
| 1:BZ:32:GLY:HA3   | 1:BZ:135:GLY:C    | 2.42                     | 0.44              |
| 1:CA:65:MET:HE3   | 1:CA:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:CI:148:LEU:HD23 | 1:CI:148:LEU:HA   | 1.82                     | 0.44              |
| 1:CI:149:SER:HB3  | 1:CI:152:TRP:CH2  | 2.52                     | 0.44              |
| 1:CN:150:LYS:H    | 1:CN:150:LYS:HG3  | 1.33                     | 0.44              |
| 1:CQ:52:VAL:O     | 1:CQ:53:PRO:C     | 2.61                     | 0.44              |
| 1:CQ:129:THR:HG22 | 1:CQ:130:LYS:N    | 2.33                     | 0.44              |
| 1:CS:18:VAL:HG11  | 1:CS:30:LEU:HD13  | 1.98                     | 0.44              |
| 1:CS:121:GLU:O    | 1:CS:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:CT:109:PRO:HG3  | 1:CT:149:SER:CB   | 2.46                     | 0.44              |
| 1:CW:148:LEU:HD23 | 1:CW:148:LEU:HA   | 1.80                     | 0.44              |
| 1:CX:121:GLU:O    | 1:CX:125:GLU:HG3  | 2.18                     | 0.44              |
| 1:C1:70:LYS:HG2   | 1:C1:70:LYS:O     | 2.17                     | 0.44              |
| 1:C4:106:THR:O    | 1:C4:107:ASP:OD1  | 2.36                     | 0.44              |
| 1:AA:144:GLU:O    | 1:AA:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:AB:129:THR:HG22 | 1:AB:130:LYS:N    | 2.33                     | 0.44              |
| 1:AD:7:LEU:HD23   | 1:AJ:40:HIS:CE1   | 2.53                     | 0.44              |
| 1:AF:65:MET:HE3   | 1:AF:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:AH:66:ALA:HB2   | 1:AH:74:VAL:HG21  | 1.99                     | 0.44              |
| 1:AK:58:ILE:O     | 1:AK:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:AL:9:GLY:HA3    | 1:AL:12:LEU:HD12  | 1.99                     | 0.44              |
| 1:AP:32:GLY:HA3   | 1:AP:135:GLY:C    | 2.42                     | 0.44              |
| 1:AP:58:ILE:HG21  | 1:AP:76:THR:OG1   | 2.17                     | 0.44              |
| 1:AR:82:ARG:HG3   | 1:AR:118:GLU:OE2  | 2.18                     | 0.44              |
| 1:AZ:34:LEU:C     | 1:AZ:36:GLY:N     | 2.76                     | 0.44              |
| 1:A1:52:VAL:O     | 1:A1:53:PRO:C     | 2.61                     | 0.44              |
| 1:A3:34:LEU:O     | 1:A3:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:BI:34:LEU:O     | 1:BI:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:BN:58:ILE:HB    | 1:BN:59:PRO:HD3   | 2.00                     | 0.44              |
| 1:BR:104:LEU:CD2  | 1:BS:60:LEU:HA    | 2.48                     | 0.44              |
| 1:BS:34:LEU:O     | 1:BS:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:BT:106:THR:O    | 1:BT:107:ASP:OD1  | 2.36                     | 0.44              |
| 1:BZ:58:ILE:O     | 1:BZ:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:B1:52:VAL:O     | 1:B1:53:PRO:C     | 2.61                     | 0.44              |
| 1:B3:17:VAL:HG13  | 1:B3:65:MET:CE    | 2.48                     | 0.44              |
| 1:B4:4:GLU:C      | 1:B4:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:CB:52:VAL:O     | 1:CB:53:PRO:C     | 2.61                     | 0.44              |
| 1:CC:66:ALA:HB2   | 1:CC:74:VAL:HG21  | 1.99                     | 0.44              |
| 1:CD:121:GLU:O    | 1:CD:125:GLU:HG3  | 2.17                     | 0.44              |
| 1:CI:75:ILE:HD13  | 1:CI:139:ALA:HA   | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CJ:106:THR:O    | 1:CJ:107:ASP:OD1  | 2.36                     | 0.44              |
| 1:CK:58:ILE:O     | 1:CK:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:CM:45:ASN:HD22  | 1:CM:45:ASN:HA    | 1.63                     | 0.44              |
| 1:CR:45:ASN:HD22  | 1:CR:45:ASN:HA    | 1.63                     | 0.44              |
| 1:CR:97:LYS:HE3   | 1:CS:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:CV:55:ALA:HB1   | 1:CV:95:VAL:CG2   | 2.40                     | 0.44              |
| 1:CX:34:LEU:O     | 1:CX:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:CZ:20:ARG:HH12  | 1:C4:144:GLU:CD   | 2.26                     | 0.44              |
| 1:C1:104:LEU:HD23 | 1:C2:60:LEU:HD13  | 2.00                     | 0.44              |
| 1:AD:58:ILE:HB    | 1:AD:59:PRO:HD3   | 2.00                     | 0.44              |
| 1:AF:20:ARG:HH12  | 1:AJ:144:GLU:CD   | 2.26                     | 0.44              |
| 1:AF:90:TYR:O     | 1:AF:94:GLU:HG2   | 2.18                     | 0.44              |
| 1:AG:129:THR:HG22 | 1:AG:130:LYS:N    | 2.33                     | 0.44              |
| 1:AL:52:VAL:O     | 1:AL:53:PRO:C     | 2.61                     | 0.44              |
| 1:AP:58:ILE:O     | 1:AP:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:AP:58:ILE:H     | 1:AP:59:PRO:HD2   | 1.80                     | 0.44              |
| 1:AP:65:MET:HE3   | 1:AP:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:AP:90:TYR:O     | 1:AP:94:GLU:HG2   | 2.18                     | 0.44              |
| 1:AS:17:VAL:HG13  | 1:AS:65:MET:CE    | 2.48                     | 0.44              |
| 1:AS:34:LEU:O     | 1:AS:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:AY:106:THR:O    | 1:AY:107:ASP:OD1  | 2.36                     | 0.44              |
| 1:AZ:51:TRP:O     | 1:A4:148:LEU:HD11 | 2.18                     | 0.44              |
| 1:A1:97:LYS:HA    | 1:A1:100:ALA:HB3  | 2.00                     | 0.44              |
| 1:A2:52:VAL:CG1   | 1:A2:61:ILE:HD12  | 2.35                     | 0.44              |
| 1:A2:82:ARG:HG3   | 1:A2:118:GLU:OE2  | 2.18                     | 0.44              |
| 1:A3:58:ILE:HB    | 1:A3:59:PRO:HD3   | 2.00                     | 0.44              |
| 1:BA:34:LEU:C     | 1:BA:36:GLY:N     | 2.76                     | 0.44              |
| 1:BA:58:ILE:O     | 1:BA:62:ALA:HB2   | 2.18                     | 0.44              |
| 1:BC:97:LYS:HE3   | 1:BD:97:LYS:NZ    | 2.32                     | 0.44              |
| 1:BE:106:THR:O    | 1:BE:107:ASP:OD1  | 2.36                     | 0.44              |
| 1:BN:17:VAL:HG13  | 1:BN:65:MET:CE    | 2.48                     | 0.44              |
| 1:BP:90:TYR:O     | 1:BP:94:GLU:HG2   | 2.18                     | 0.44              |
| 1:BP:144:GLU:O    | 1:BP:148:LEU:HB2  | 2.18                     | 0.44              |
| 1:BQ:58:ILE:O     | 1:BQ:58:ILE:CG2   | 2.65                     | 0.44              |
| 1:BS:75:ILE:HD13  | 1:BS:139:ALA:HA   | 1.99                     | 0.44              |
| 1:BU:65:MET:HE3   | 1:BU:71:TYR:CE2   | 2.52                     | 0.44              |
| 1:BV:104:LEU:HD23 | 1:BW:60:LEU:HD13  | 2.00                     | 0.44              |
| 1:B1:70:LYS:HG2   | 1:B1:70:LYS:O     | 2.17                     | 0.44              |
| 1:B2:104:LEU:CD2  | 1:B3:60:LEU:HA    | 2.48                     | 0.44              |
| 1:B3:18:VAL:HG23  | 1:B3:51:TRP:CE3   | 2.52                     | 0.44              |
| 1:CB:13:LYS:HG2   | 1:CB:70:LYS:O     | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CD:17:VAL:HG13  | 1:CD:65:MET:CE    | 2.48                     | 0.44              |
| 1:CG:52:VAL:O     | 1:CG:53:PRO:C     | 2.61                     | 0.44              |
| 1:CG:100:ALA:CA   | 1:CH:56:PHE:HZ    | 2.28                     | 0.44              |
| 1:CI:34:LEU:O     | 1:CI:38:LYS:HG3   | 2.17                     | 0.44              |
| 1:CO:4:GLU:C      | 1:CO:148:LEU:HD21 | 2.42                     | 0.44              |
| 1:CQ:13:LYS:HG2   | 1:CQ:70:LYS:O     | 2.18                     | 0.44              |
| 1:CS:149:SER:HB3  | 1:CS:152:TRP:CH2  | 2.52                     | 0.44              |
| 1:CV:13:LYS:HG2   | 1:CV:70:LYS:O     | 2.18                     | 0.44              |
| 1:CX:75:ILE:HD13  | 1:CX:139:ALA:HA   | 1.99                     | 0.44              |
| 1:AA:20:ARG:HH12  | 1:AE:144:GLU:CD   | 2.26                     | 0.43              |
| 1:AF:144:GLU:O    | 1:AF:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:AH:97:LYS:HE3   | 1:AI:97:LYS:NZ    | 2.32                     | 0.43              |
| 1:AM:97:LYS:HE3   | 1:AN:97:LYS:NZ    | 2.32                     | 0.43              |
| 1:AO:108:ILE:CG1  | 1:AO:150:LYS:HE3  | 2.42                     | 0.43              |
| 1:AQ:13:LYS:HG2   | 1:AQ:70:LYS:O     | 2.18                     | 0.43              |
| 1:AQ:129:THR:HG22 | 1:AQ:130:LYS:N    | 2.33                     | 0.43              |
| 1:AV:13:LYS:HG2   | 1:AV:70:LYS:O     | 2.18                     | 0.43              |
| 1:A1:129:THR:HG22 | 1:A1:130:LYS:N    | 2.33                     | 0.43              |
| 1:BA:65:MET:HE3   | 1:BA:71:TYR:CE2   | 2.52                     | 0.43              |
| 1:BB:65:MET:HE3   | 1:BB:71:TYR:CZ    | 2.52                     | 0.43              |
| 1:BC:82:ARG:CG    | 1:BC:82:ARG:NH1   | 2.73                     | 0.43              |
| 1:BD:121:GLU:O    | 1:BD:125:GLU:HG3  | 2.18                     | 0.43              |
| 1:BD:149:SER:HB3  | 1:BD:152:TRP:CH2  | 2.52                     | 0.43              |
| 1:BE:4:GLU:C      | 1:BE:148:LEU:HD21 | 2.42                     | 0.43              |
| 1:BK:32:GLY:HA3   | 1:BK:135:GLY:C    | 2.42                     | 0.43              |
| 1:BK:58:ILE:H     | 1:BK:59:PRO:HD2   | 1.80                     | 0.43              |
| 1:BK:98:GLY:O     | 1:BK:102:LEU:HB2  | 2.18                     | 0.43              |
| 1:BP:20:ARG:HH12  | 1:BT:144:GLU:CD   | 2.26                     | 0.43              |
| 1:BV:97:LYS:HA    | 1:BV:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:BX:121:GLU:O    | 1:BX:125:GLU:HG3  | 2.18                     | 0.43              |
| 1:BY:90:TYR:O     | 1:BY:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BZ:65:MET:HE2   | 1:BZ:65:MET:HB3   | 1.80                     | 0.43              |
| 1:BZ:90:TYR:O     | 1:BZ:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BZ:144:GLU:O    | 1:BZ:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:CA:20:ARG:HH12  | 1:CE:144:GLU:CD   | 2.26                     | 0.43              |
| 1:CA:58:ILE:O     | 1:CA:62:ALA:HB2   | 2.18                     | 0.43              |
| 1:CB:70:LYS:O     | 1:CB:70:LYS:HG2   | 2.16                     | 0.43              |
| 1:CE:106:THR:O    | 1:CE:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:CI:17:VAL:HG13  | 1:CI:65:MET:CE    | 2.48                     | 0.43              |
| 1:CK:144:GLU:O    | 1:CK:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:CN:75:ILE:HD13  | 1:CN:139:ALA:HA   | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CP:51:TRP:O     | 1:CT:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:CQ:104:LEU:HD23 | 1:CR:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:CU:90:TYR:O     | 1:CU:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CV:52:VAL:O     | 1:CV:53:PRO:C     | 2.61                     | 0.43              |
| 1:CX:58:ILE:HB    | 1:CX:59:PRO:HD3   | 2.00                     | 0.43              |
| 1:CZ:98:GLY:O     | 1:CZ:102:LEU:HB2  | 2.18                     | 0.43              |
| 1:C1:9:GLY:HA3    | 1:C1:12:LEU:HD12  | 1.99                     | 0.43              |
| 1:AA:65:MET:HE3   | 1:AA:71:TYR:CE2   | 2.52                     | 0.43              |
| 1:AA:65:MET:HE3   | 1:AA:71:TYR:CZ    | 2.53                     | 0.43              |
| 1:AB:70:LYS:O     | 1:AB:70:LYS:HG2   | 2.17                     | 0.43              |
| 1:AE:90:TYR:O     | 1:AE:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:AG:52:VAL:O     | 1:AG:53:PRO:C     | 2.61                     | 0.43              |
| 1:AG:100:ALA:CA   | 1:AH:56:PHE:HZ    | 2.28                     | 0.43              |
| 1:AI:58:ILE:HB    | 1:AI:59:PRO:HD3   | 2.00                     | 0.43              |
| 1:AI:121:GLU:O    | 1:AI:125:GLU:HG3  | 2.18                     | 0.43              |
| 1:AJ:106:THR:O    | 1:AJ:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:A1:104:LEU:HD23 | 1:A2:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:BB:100:ALA:CA   | 1:BC:56:PHE:HZ    | 2.28                     | 0.43              |
| 1:BF:28:LYS:HD2   | 1:BR:24:PHE:CE1   | 2.53                     | 0.43              |
| 1:BG:129:THR:HG22 | 1:BG:130:LYS:N    | 2.33                     | 0.43              |
| 1:BI:17:VAL:HG13  | 1:BI:65:MET:CE    | 2.48                     | 0.43              |
| 1:BI:58:ILE:HB    | 1:BI:59:PRO:HD3   | 2.00                     | 0.43              |
| 1:BK:90:TYR:O     | 1:BK:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BM:104:LEU:CD2  | 1:BN:60:LEU:HA    | 2.48                     | 0.43              |
| 1:BM:108:ILE:O    | 1:BM:110:VAL:HG23 | 2.17                     | 0.43              |
| 1:BU:65:MET:HE3   | 1:BU:71:TYR:CZ    | 2.54                     | 0.43              |
| 1:BV:52:VAL:O     | 1:BV:53:PRO:C     | 2.61                     | 0.43              |
| 1:BW:104:LEU:CD2  | 1:BX:60:LEU:HA    | 2.48                     | 0.43              |
| 1:B1:13:LYS:HG2   | 1:B1:70:LYS:O     | 2.18                     | 0.43              |
| 1:B4:90:TYR:O     | 1:B4:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CA:98:GLY:O     | 1:CA:102:LEU:HB2  | 2.18                     | 0.43              |
| 1:CB:129:THR:CG2  | 1:CB:130:LYS:H    | 2.28                     | 0.43              |
| 1:CC:67:ASN:HD22  | 1:CC:67:ASN:HA    | 1.59                     | 0.43              |
| 1:CE:90:TYR:O     | 1:CE:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CF:65:MET:HE3   | 1:CF:71:TYR:CE2   | 2.52                     | 0.43              |
| 1:CF:90:TYR:O     | 1:CF:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CG:55:ALA:HB1   | 1:CG:95:VAL:CG2   | 2.40                     | 0.43              |
| 1:CG:104:LEU:HD23 | 1:CH:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:CK:20:ARG:HH12  | 1:CO:144:GLU:CD   | 2.26                     | 0.43              |
| 1:CL:13:LYS:HG2   | 1:CL:70:LYS:O     | 2.18                     | 0.43              |
| 1:CY:15:GLY:O     | 1:CY:74:VAL:HA    | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CZ:90:TYR:O     | 1:CZ:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CZ:144:GLU:O    | 1:CZ:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:C2:66:ALA:HB2   | 1:C2:74:VAL:HG21  | 1.99                     | 0.43              |
| 1:C2:82:ARG:HG3   | 1:C2:118:GLU:OE2  | 2.18                     | 0.43              |
| 1:AA:51:TRP:O     | 1:AE:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:AC:104:LEU:CD2  | 1:AD:60:LEU:HA    | 2.48                     | 0.43              |
| 1:AK:51:TRP:O     | 1:AO:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:AL:95:VAL:C     | 1:AL:97:LYS:H     | 2.27                     | 0.43              |
| 1:AR:66:ALA:HB2   | 1:AR:74:VAL:HG21  | 1.99                     | 0.43              |
| 1:AU:7:LEU:HA     | 1:AU:7:LEU:HD12   | 1.84                     | 0.43              |
| 1:AU:90:TYR:O     | 1:AU:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:AX:17:VAL:HG13  | 1:AX:65:MET:CE    | 2.48                     | 0.43              |
| 1:AY:4:GLU:C      | 1:AY:148:LEU:HD21 | 2.42                     | 0.43              |
| 1:AZ:65:MET:HE3   | 1:AZ:71:TYR:CE2   | 2.52                     | 0.43              |
| 1:AZ:90:TYR:O     | 1:AZ:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:A1:55:ALA:CB    | 1:A1:95:VAL:HG21  | 2.40                     | 0.43              |
| 1:A1:58:ILE:O     | 1:A1:58:ILE:CG2   | 2.65                     | 0.43              |
| 1:A2:125:GLU:HA   | 1:A2:129:THR:HB   | 2.01                     | 0.43              |
| 1:BE:90:TYR:O     | 1:BE:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BF:7:LEU:HA     | 1:BF:7:LEU:HD12   | 1.84                     | 0.43              |
| 1:BF:58:ILE:HG21  | 1:BF:76:THR:OG1   | 2.17                     | 0.43              |
| 1:BJ:106:THR:O    | 1:BJ:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:BK:20:ARG:HH12  | 1:BO:144:GLU:CD   | 2.26                     | 0.43              |
| 1:BM:82:ARG:HG3   | 1:BM:118:GLU:OE2  | 2.17                     | 0.43              |
| 1:BN:149:SER:HB3  | 1:BN:152:TRP:CH2  | 2.52                     | 0.43              |
| 1:BO:106:THR:O    | 1:BO:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:BQ:129:THR:HG22 | 1:BQ:130:LYS:N    | 2.33                     | 0.43              |
| 1:BT:90:TYR:O     | 1:BT:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BU:144:GLU:O    | 1:BU:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:BY:4:GLU:C      | 1:BY:148:LEU:HD21 | 2.42                     | 0.43              |
| 1:CB:9:GLY:HA3    | 1:CB:12:LEU:HD12  | 1.99                     | 0.43              |
| 1:CC:104:LEU:CD2  | 1:CD:60:LEU:HA    | 2.48                     | 0.43              |
| 1:CF:65:MET:HE2   | 1:CF:65:MET:HB3   | 1.80                     | 0.43              |
| 1:CG:97:LYS:N     | 1:CG:100:ALA:HB2  | 2.31                     | 0.43              |
| 1:CK:51:TRP:O     | 1:CO:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:CL:104:LEU:HD23 | 1:CM:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:CV:58:ILE:O     | 1:CV:58:ILE:CG2   | 2.65                     | 0.43              |
| 1:CV:97:LYS:HA    | 1:CV:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:C4:15:GLY:O     | 1:C4:74:VAL:HA    | 2.19                     | 0.43              |
| 1:AB:9:GLY:HA3    | 1:AB:12:LEU:HD12  | 1.99                     | 0.43              |
| 1:AG:65:MET:HE2   | 1:AG:65:MET:HB3   | 1.95                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AH:97:LYS:HE3   | 1:AI:97:LYS:HZ3   | 1.83                     | 0.43              |
| 1:AI:75:ILE:HD13  | 1:AI:139:ALA:HA   | 1.99                     | 0.43              |
| 1:AL:13:LYS:HG2   | 1:AL:70:LYS:O     | 2.18                     | 0.43              |
| 1:AQ:58:ILE:O     | 1:AQ:58:ILE:CG2   | 2.65                     | 0.43              |
| 1:AS:75:ILE:HD13  | 1:AS:139:ALA:HA   | 1.99                     | 0.43              |
| 1:AS:121:GLU:O    | 1:AS:125:GLU:HG3  | 2.17                     | 0.43              |
| 1:AW:82:ARG:HG3   | 1:AW:118:GLU:OE2  | 2.17                     | 0.43              |
| 1:A2:66:ALA:HB2   | 1:A2:74:VAL:HG21  | 1.99                     | 0.43              |
| 1:BB:97:LYS:HA    | 1:BB:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:BI:75:ILE:HG22  | 1:BI:77:LEU:CD1   | 2.48                     | 0.43              |
| 1:BL:58:ILE:O     | 1:BL:58:ILE:CG2   | 2.65                     | 0.43              |
| 1:BN:48:ASP:HB2   | 1:BN:71:TYR:CE1   | 2.50                     | 0.43              |
| 1:BN:121:GLU:O    | 1:BN:125:GLU:HG3  | 2.18                     | 0.43              |
| 1:BQ:95:VAL:C     | 1:BQ:97:LYS:H     | 2.27                     | 0.43              |
| 1:BQ:104:LEU:HD23 | 1:BR:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:BT:15:GLY:O     | 1:BT:74:VAL:HA    | 2.18                     | 0.43              |
| 1:BV:129:THR:HG22 | 1:BV:130:LYS:N    | 2.33                     | 0.43              |
| 1:CA:90:TYR:O     | 1:CA:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CF:20:ARG:HH12  | 1:CJ:144:GLU:CD   | 2.26                     | 0.43              |
| 1:CF:98:GLY:O     | 1:CF:102:LEU:HB2  | 2.18                     | 0.43              |
| 1:CG:129:THR:HG22 | 1:CG:130:LYS:N    | 2.33                     | 0.43              |
| 1:CI:75:ILE:HG22  | 1:CI:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:CK:34:LEU:C     | 1:CK:36:GLY:N     | 2.76                     | 0.43              |
| 1:CN:17:VAL:HG13  | 1:CN:65:MET:CE    | 2.48                     | 0.43              |
| 1:CQ:55:ALA:HB1   | 1:CQ:95:VAL:CG2   | 2.40                     | 0.43              |
| 1:CS:17:VAL:HG13  | 1:CS:65:MET:CE    | 2.48                     | 0.43              |
| 1:CT:15:GLY:O     | 1:CT:74:VAL:HA    | 2.19                     | 0.43              |
| 1:CT:106:THR:O    | 1:CT:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:CU:7:LEU:HD12   | 1:CU:7:LEU:HA     | 1.84                     | 0.43              |
| 1:CX:17:VAL:HG13  | 1:CX:65:MET:CE    | 2.48                     | 0.43              |
| 1:CZ:58:ILE:O     | 1:CZ:62:ALA:HB2   | 2.18                     | 0.43              |
| 1:C1:13:LYS:HG2   | 1:C1:70:LYS:O     | 2.18                     | 0.43              |
| 1:C1:52:VAL:O     | 1:C1:53:PRO:C     | 2.61                     | 0.43              |
| 1:C2:34:LEU:HD22  | 1:C2:38:LYS:CE    | 2.43                     | 0.43              |
| 1:C2:97:LYS:HE3   | 1:C3:97:LYS:NZ    | 2.32                     | 0.43              |
| 1:C3:17:VAL:HG13  | 1:C3:65:MET:CE    | 2.48                     | 0.43              |
| 1:AB:97:LYS:N     | 1:AB:100:ALA:HB2  | 2.31                     | 0.43              |
| 1:AC:34:LEU:C     | 1:AC:36:GLY:N     | 2.77                     | 0.43              |
| 1:AC:82:ARG:HG3   | 1:AC:118:GLU:OE2  | 2.17                     | 0.43              |
| 1:AE:7:LEU:HD11   | 1:AE:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:AF:51:TRP:O     | 1:AJ:148:LEU:HD11 | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AF:98:GLY:O     | 1:AF:102:LEU:HB2  | 2.18                     | 0.43              |
| 1:AG:104:LEU:HD23 | 1:AH:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:AK:98:GLY:O     | 1:AK:102:LEU:HB2  | 2.18                     | 0.43              |
| 1:AT:106:THR:O    | 1:AT:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:AU:144:GLU:O    | 1:AU:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:AV:52:VAL:O     | 1:AV:53:PRO:C     | 2.61                     | 0.43              |
| 1:A4:4:GLU:C      | 1:A4:148:LEU:HD21 | 2.42                     | 0.43              |
| 1:BA:51:TRP:O     | 1:BE:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:BA:98:GLY:O     | 1:BA:102:LEU:HB2  | 2.18                     | 0.43              |
| 1:BB:129:THR:HG22 | 1:BB:130:LYS:N    | 2.33                     | 0.43              |
| 1:BE:15:GLY:O     | 1:BE:74:VAL:HA    | 2.18                     | 0.43              |
| 1:BE:21:PHE:O     | 1:BE:22:ASN:HB2   | 2.19                     | 0.43              |
| 1:BG:97:LYS:HA    | 1:BG:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:BH:82:ARG:HG3   | 1:BH:118:GLU:OE2  | 2.18                     | 0.43              |
| 1:BK:34:LEU:C     | 1:BK:36:GLY:N     | 2.76                     | 0.43              |
| 1:BM:125:GLU:HA   | 1:BM:129:THR:HB   | 2.01                     | 0.43              |
| 1:BP:58:ILE:O     | 1:BP:62:ALA:HB2   | 2.18                     | 0.43              |
| 1:BQ:13:LYS:HG2   | 1:BQ:70:LYS:O     | 2.18                     | 0.43              |
| 1:BU:51:TRP:O     | 1:BY:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:BW:66:ALA:HB2   | 1:BW:74:VAL:HG21  | 2.00                     | 0.43              |
| 1:BX:34:LEU:O     | 1:BX:38:LYS:HG3   | 2.17                     | 0.43              |
| 1:BY:7:LEU:HD11   | 1:BY:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:BY:106:THR:O    | 1:BY:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:CB:95:VAL:C     | 1:CB:97:LYS:H     | 2.27                     | 0.43              |
| 1:CB:104:LEU:HD23 | 1:CC:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:CO:7:LEU:HD11   | 1:CO:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:CP:65:MET:HE3   | 1:CP:71:TYR:CZ    | 2.53                     | 0.43              |
| 1:CP:144:GLU:O    | 1:CP:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:CR:66:ALA:HB2   | 1:CR:74:VAL:HG21  | 2.00                     | 0.43              |
| 1:CR:125:GLU:HA   | 1:CR:129:THR:HB   | 2.01                     | 0.43              |
| 1:CT:71:TYR:O     | 1:CT:150:LYS:NZ   | 2.44                     | 0.43              |
| 1:CV:100:ALA:CA   | 1:CW:56:PHE:HZ    | 2.28                     | 0.43              |
| 1:C3:52:VAL:CG1   | 1:C3:61:ILE:HD12  | 2.35                     | 0.43              |
| 1:AA:58:ILE:H     | 1:AA:59:PRO:HD2   | 1.80                     | 0.43              |
| 1:AB:104:LEU:HD23 | 1:AC:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:AC:66:ALA:HB2   | 1:AC:74:VAL:HG21  | 1.99                     | 0.43              |
| 1:AD:7:LEU:HB3    | 1:AJ:39:ARG:O     | 2.19                     | 0.43              |
| 1:AH:104:LEU:CD2  | 1:AI:60:LEU:HA    | 2.48                     | 0.43              |
| 1:AK:65:MET:HE3   | 1:AK:71:TYR:CZ    | 2.54                     | 0.43              |
| 1:AL:104:LEU:HD23 | 1:AM:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:AM:34:LEU:C     | 1:AM:36:GLY:N     | 2.77                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AM:125:GLU:HA   | 1:AM:129:THR:HB   | 2.01                     | 0.43              |
| 1:AO:106:THR:O    | 1:AO:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:AR:104:LEU:CD2  | 1:AS:60:LEU:HA    | 2.48                     | 0.43              |
| 1:AT:15:GLY:O     | 1:AT:74:VAL:HA    | 2.18                     | 0.43              |
| 1:AU:34:LEU:C     | 1:AU:36:GLY:N     | 2.76                     | 0.43              |
| 1:AU:51:TRP:O     | 1:AY:148:LEU:HD11 | 2.19                     | 0.43              |
| 1:AV:129:THR:HG22 | 1:AV:130:LYS:N    | 2.33                     | 0.43              |
| 1:BA:20:ARG:HH12  | 1:BE:144:GLU:CD   | 2.26                     | 0.43              |
| 1:BB:95:VAL:C     | 1:BB:97:LYS:H     | 2.27                     | 0.43              |
| 1:BF:20:ARG:HH12  | 1:BJ:144:GLU:CD   | 2.26                     | 0.43              |
| 1:BF:34:LEU:C     | 1:BF:36:GLY:N     | 2.76                     | 0.43              |
| 1:BF:144:GLU:O    | 1:BF:148:LEU:HB2  | 2.18                     | 0.43              |
| 1:BJ:90:TYR:O     | 1:BJ:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BM:66:ALA:HB2   | 1:BM:74:VAL:HG21  | 1.99                     | 0.43              |
| 1:BQ:4:GLU:CG     | 1:BR:51:TRP:HD1   | 2.29                     | 0.43              |
| 1:BR:82:ARG:HG3   | 1:BR:118:GLU:OE2  | 2.18                     | 0.43              |
| 1:CA:58:ILE:O     | 1:CA:58:ILE:HG22  | 2.11                     | 0.43              |
| 1:CB:4:GLU:CG     | 1:CC:51:TRP:HD1   | 2.29                     | 0.43              |
| 1:CC:125:GLU:HA   | 1:CC:129:THR:HB   | 2.01                     | 0.43              |
| 1:CE:21:PHE:O     | 1:CE:22:ASN:HB2   | 2.19                     | 0.43              |
| 1:CF:51:TRP:O     | 1:CJ:148:LEU:HD11 | 2.19                     | 0.43              |
| 1:CJ:21:PHE:O     | 1:CJ:22:ASN:HB2   | 2.19                     | 0.43              |
| 1:CO:106:THR:O    | 1:CO:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:CP:39:ARG:NH1   | 1:CV:7:LEU:HD22   | 2.33                     | 0.43              |
| 1:CQ:24:PHE:CD1   | 1:CV:28:LYS:HG3   | 2.53                     | 0.43              |
| 1:CT:64:LYS:HD3   | 1:CT:64:LYS:HA    | 1.85                     | 0.43              |
| 1:CX:75:ILE:HG22  | 1:CX:77:LEU:CD1   | 2.48                     | 0.43              |
| 1:CZ:34:LEU:C     | 1:CZ:36:GLY:N     | 2.76                     | 0.43              |
| 1:CZ:51:TRP:O     | 1:C4:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:C1:55:ALA:HB1   | 1:C1:95:VAL:CG2   | 2.40                     | 0.43              |
| 1:AD:17:VAL:HG13  | 1:AD:65:MET:CE    | 2.48                     | 0.43              |
| 1:AH:34:LEU:C     | 1:AH:36:GLY:N     | 2.77                     | 0.43              |
| 1:AI:17:VAL:HG13  | 1:AI:65:MET:CE    | 2.48                     | 0.43              |
| 1:AO:7:LEU:HD11   | 1:AO:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:AO:90:TYR:O     | 1:AO:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:AQ:95:VAL:C     | 1:AQ:97:LYS:H     | 2.27                     | 0.43              |
| 1:AW:45:ASN:HD22  | 1:AW:45:ASN:HA    | 1.64                     | 0.43              |
| 1:AX:75:ILE:HG22  | 1:AX:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:AY:90:TYR:O     | 1:AY:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:AZ:58:ILE:HG21  | 1:AZ:76:THR:OG1   | 2.17                     | 0.43              |
| 1:AZ:65:MET:HE3   | 1:AZ:71:TYR:CZ    | 2.54                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:BE:65:MET:HE2  | 1:BE:65:MET:HB3   | 1.91                     | 0.43              |
| 1:BG:9:GLY:HA3   | 1:BG:12:LEU:HD12  | 1.99                     | 0.43              |
| 1:BH:34:LEU:C    | 1:BH:36:GLY:N     | 2.77                     | 0.43              |
| 1:BK:51:TRP:O    | 1:BO:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:BL:4:GLU:CG    | 1:BM:51:TRP:HD1   | 2.29                     | 0.43              |
| 1:BL:13:LYS:HG2  | 1:BL:70:LYS:O     | 2.18                     | 0.43              |
| 1:BL:52:VAL:O    | 1:BL:53:PRO:C     | 2.61                     | 0.43              |
| 1:BO:15:GLY:O    | 1:BO:74:VAL:HA    | 2.19                     | 0.43              |
| 1:BU:65:MET:HE2  | 1:BU:65:MET:HB3   | 1.80                     | 0.43              |
| 1:BV:58:ILE:O    | 1:BV:58:ILE:CG2   | 2.65                     | 0.43              |
| 1:BW:34:LEU:C    | 1:BW:36:GLY:N     | 2.77                     | 0.43              |
| 1:BX:58:ILE:HB   | 1:BX:59:PRO:HD3   | 2.00                     | 0.43              |
| 1:BZ:65:MET:HE3  | 1:BZ:71:TYR:CZ    | 2.54                     | 0.43              |
| 1:B1:95:VAL:C    | 1:B1:97:LYS:H     | 2.27                     | 0.43              |
| 1:B2:18:VAL:HA   | 1:B2:77:LEU:O     | 2.19                     | 0.43              |
| 1:CF:34:LEU:C    | 1:CF:36:GLY:N     | 2.76                     | 0.43              |
| 1:CF:65:MET:HE3  | 1:CF:71:TYR:CZ    | 2.54                     | 0.43              |
| 1:CJ:90:TYR:O    | 1:CJ:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CJ:108:ILE:CG1 | 1:CJ:150:LYS:HE3  | 2.42                     | 0.43              |
| 1:CL:95:VAL:C    | 1:CL:97:LYS:H     | 2.27                     | 0.43              |
| 1:CS:150:LYS:H   | 1:CS:150:LYS:HG3  | 1.33                     | 0.43              |
| 1:CZ:58:ILE:H    | 1:CZ:59:PRO:HD2   | 1.80                     | 0.43              |
| 1:CZ:65:MET:HE3  | 1:CZ:71:TYR:CZ    | 2.54                     | 0.43              |
| 1:C2:125:GLU:HA  | 1:C2:129:THR:HB   | 2.01                     | 0.43              |
| 1:C2:148:LEU:HA  | 1:C2:148:LEU:HD23 | 1.80                     | 0.43              |
| 1:C4:7:LEU:HD11  | 1:C4:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:AB:13:LYS:HG2  | 1:AB:70:LYS:O     | 2.18                     | 0.43              |
| 1:AB:52:VAL:O    | 1:AB:53:PRO:C     | 2.61                     | 0.43              |
| 1:AC:18:VAL:HA   | 1:AC:77:LEU:O     | 2.19                     | 0.43              |
| 1:AD:34:LEU:O    | 1:AD:38:LYS:HG3   | 2.17                     | 0.43              |
| 1:AE:106:THR:O   | 1:AE:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:AH:125:GLU:HA  | 1:AH:129:THR:HB   | 2.01                     | 0.43              |
| 1:AI:75:ILE:HG22 | 1:AI:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:AJ:21:PHE:O    | 1:AJ:22:ASN:HB2   | 2.19                     | 0.43              |
| 1:AJ:90:TYR:O    | 1:AJ:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:AN:75:ILE:HG22 | 1:AN:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:AQ:13:LYS:HZ1  | 1:BU:43:GLU:HB2   | 1.76                     | 0.43              |
| 1:AT:90:TYR:O    | 1:AT:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:AZ:20:ARG:HH12 | 1:A4:144:GLU:CD   | 2.26                     | 0.43              |
| 1:A4:106:THR:O   | 1:A4:107:ASP:OD1  | 2.36                     | 0.43              |
| 1:BA:65:MET:HE3  | 1:BA:71:TYR:CZ    | 2.54                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BO:90:TYR:O     | 1:BO:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BP:51:TRP:O     | 1:BT:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:BP:65:MET:HE3   | 1:BP:71:TYR:CZ    | 2.53                     | 0.43              |
| 1:BR:18:VAL:HA    | 1:BR:77:LEU:O     | 2.19                     | 0.43              |
| 1:BV:95:VAL:C     | 1:BV:97:LYS:H     | 2.27                     | 0.43              |
| 1:B4:7:LEU:HD11   | 1:B4:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:CC:18:VAL:HA    | 1:CC:77:LEU:O     | 2.19                     | 0.43              |
| 1:CI:128:GLY:O    | 1:CK:22:ASN:HA    | 2.19                     | 0.43              |
| 1:CK:90:TYR:O     | 1:CK:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:CL:97:LYS:HA    | 1:CL:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:CN:75:ILE:HG22  | 1:CN:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:CQ:9:GLY:HA3    | 1:CQ:12:LEU:HD12  | 1.99                     | 0.43              |
| 1:CT:8:VAL:CG2    | 1:C3:8:VAL:HG13   | 2.48                     | 0.43              |
| 1:CW:18:VAL:HA    | 1:CW:77:LEU:O     | 2.19                     | 0.43              |
| 1:C1:95:VAL:C     | 1:C1:97:LYS:H     | 2.27                     | 0.43              |
| 1:C3:58:ILE:HB    | 1:C3:59:PRO:HD3   | 2.00                     | 0.43              |
| 1:C3:75:ILE:HG22  | 1:C3:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:AD:75:ILE:HG22  | 1:AD:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:AF:65:MET:HE3   | 1:AF:71:TYR:CZ    | 2.53                     | 0.43              |
| 1:AG:97:LYS:HA    | 1:AG:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:AS:58:ILE:HB    | 1:AS:59:PRO:HD3   | 2.00                     | 0.43              |
| 1:AU:58:ILE:O     | 1:AU:58:ILE:HG22  | 2.11                     | 0.43              |
| 1:AV:95:VAL:C     | 1:AV:97:LYS:H     | 2.27                     | 0.43              |
| 1:AW:148:LEU:HD23 | 1:AW:148:LEU:HA   | 1.80                     | 0.43              |
| 1:A2:18:VAL:HA    | 1:A2:77:LEU:O     | 2.19                     | 0.43              |
| 1:BA:90:TYR:O     | 1:BA:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:BB:13:LYS:HG2   | 1:BB:70:LYS:O     | 2.18                     | 0.43              |
| 1:BB:55:ALA:HB1   | 1:BB:95:VAL:CG2   | 2.40                     | 0.43              |
| 1:BE:7:LEU:HD11   | 1:BE:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:BG:120:ILE:CD1  | 1:BQ:125:GLU:HG2  | 2.49                     | 0.43              |
| 1:BH:34:LEU:HD22  | 1:BH:38:LYS:CE    | 2.43                     | 0.43              |
| 1:BI:150:LYS:H    | 1:BI:150:LYS:HG3  | 1.33                     | 0.43              |
| 1:BU:34:LEU:C     | 1:BU:36:GLY:N     | 2.76                     | 0.43              |
| 1:BX:75:ILE:HG22  | 1:BX:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:BZ:51:TRP:O     | 1:B4:148:LEU:HD11 | 2.19                     | 0.43              |
| 1:B1:9:GLY:HA3    | 1:B1:12:LEU:HD12  | 1.99                     | 0.43              |
| 1:CI:121:GLU:O    | 1:CI:125:GLU:HG3  | 2.18                     | 0.43              |
| 1:CL:100:ALA:CA   | 1:CM:56:PHE:HZ    | 2.28                     | 0.43              |
| 1:CT:7:LEU:HD11   | 1:CT:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:CY:90:TYR:O     | 1:CY:94:GLU:HG2   | 2.18                     | 0.43              |
| 1:AB:97:LYS:HA    | 1:AB:100:ALA:HB3  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AI:148:LEU:HD23 | 1:AI:148:LEU:HA   | 1.82                     | 0.43              |
| 1:AJ:15:GLY:O     | 1:AJ:74:VAL:HA    | 2.18                     | 0.43              |
| 1:AN:48:ASP:HB2   | 1:AN:71:TYR:CE1   | 2.50                     | 0.43              |
| 1:AN:88:TYR:CD2   | 1:AN:88:TYR:C     | 2.97                     | 0.43              |
| 1:AO:15:GLY:O     | 1:AO:74:VAL:HA    | 2.19                     | 0.43              |
| 1:AP:51:TRP:O     | 1:AT:148:LEU:HD11 | 2.18                     | 0.43              |
| 1:AQ:55:ALA:CB    | 1:AQ:95:VAL:HG21  | 2.40                     | 0.43              |
| 1:AQ:97:LYS:HA    | 1:AQ:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:AQ:104:LEU:HD23 | 1:AR:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:AR:91:VAL:O     | 1:AR:95:VAL:HG23  | 2.19                     | 0.43              |
| 1:AT:21:PHE:O     | 1:AT:22:ASN:HB2   | 2.19                     | 0.43              |
| 1:AW:18:VAL:HA    | 1:AW:77:LEU:O     | 2.19                     | 0.43              |
| 1:AY:7:LEU:HD11   | 1:AY:140:VAL:HG22 | 2.01                     | 0.43              |
| 1:BD:75:ILE:HG22  | 1:BD:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:BE:40:HIS:CE1   | 1:BN:7:LEU:HD23   | 2.54                     | 0.43              |
| 1:BJ:15:GLY:O     | 1:BJ:74:VAL:HA    | 2.19                     | 0.43              |
| 1:BP:34:LEU:C     | 1:BP:36:GLY:N     | 2.76                     | 0.43              |
| 1:BR:91:VAL:O     | 1:BR:95:VAL:HG23  | 2.19                     | 0.43              |
| 1:BS:17:VAL:HG13  | 1:BS:65:MET:CE    | 2.48                     | 0.43              |
| 1:BS:75:ILE:HG22  | 1:BS:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:BW:91:VAL:O     | 1:BW:95:VAL:HG23  | 2.19                     | 0.43              |
| 1:B2:125:GLU:HA   | 1:B2:129:THR:HB   | 2.01                     | 0.43              |
| 1:CD:75:ILE:HG22  | 1:CD:77:LEU:CD1   | 2.49                     | 0.43              |
| 1:CK:65:MET:HE3   | 1:CK:71:TYR:CZ    | 2.54                     | 0.43              |
| 1:CQ:55:ALA:CB    | 1:CQ:95:VAL:HG21  | 2.40                     | 0.43              |
| 1:CT:21:PHE:O     | 1:CT:22:ASN:HB2   | 2.19                     | 0.43              |
| 1:C1:97:LYS:HA    | 1:C1:100:ALA:HB3  | 2.00                     | 0.43              |
| 1:C3:75:ILE:HD13  | 1:C3:139:ALA:HA   | 1.99                     | 0.43              |
| 1:C3:88:TYR:CD2   | 1:C3:88:TYR:C     | 2.97                     | 0.43              |
| 1:AH:52:VAL:CG1   | 1:AH:61:ILE:HD12  | 2.35                     | 0.42              |
| 1:AH:91:VAL:O     | 1:AH:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:AK:34:LEU:C     | 1:AK:36:GLY:N     | 2.76                     | 0.42              |
| 1:AM:45:ASN:HD22  | 1:AM:45:ASN:HA    | 1.64                     | 0.42              |
| 1:AM:148:LEU:HD23 | 1:AM:148:LEU:HA   | 1.80                     | 0.42              |
| 1:AR:34:LEU:C     | 1:AR:36:GLY:N     | 2.77                     | 0.42              |
| 1:AU:20:ARG:HH12  | 1:AY:144:GLU:CD   | 2.26                     | 0.42              |
| 1:A2:34:LEU:HD22  | 1:A2:38:LYS:CE    | 2.43                     | 0.42              |
| 1:A4:21:PHE:O     | 1:A4:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:BL:97:LYS:HA    | 1:BL:100:ALA:HB3  | 2.00                     | 0.42              |
| 1:BM:91:VAL:O     | 1:BM:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:BQ:129:THR:CG2  | 1:BQ:130:LYS:H    | 2.28                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BR:34:LEU:C     | 1:BR:36:GLY:N     | 2.77                     | 0.42              |
| 1:BW:18:VAL:HA    | 1:BW:77:LEU:O     | 2.19                     | 0.42              |
| 1:BW:97:LYS:HE3   | 1:BX:97:LYS:NZ    | 2.32                     | 0.42              |
| 1:BX:148:LEU:HD23 | 1:BX:148:LEU:HA   | 1.82                     | 0.42              |
| 1:BZ:20:ARG:HH12  | 1:B4:144:GLU:CD   | 2.26                     | 0.42              |
| 1:CA:51:TRP:O     | 1:CE:148:LEU:HD11 | 2.18                     | 0.42              |
| 1:CB:129:THR:HG22 | 1:CB:130:LYS:N    | 2.33                     | 0.42              |
| 1:CJ:145:MET:O    | 1:CJ:149:SER:HB3  | 2.20                     | 0.42              |
| 1:CL:88:TYR:CD2   | 1:CL:88:TYR:C     | 2.97                     | 0.42              |
| 1:CM:104:LEU:CD2  | 1:CN:60:LEU:HA    | 2.48                     | 0.42              |
| 1:CR:18:VAL:HA    | 1:CR:77:LEU:O     | 2.19                     | 0.42              |
| 1:CR:52:VAL:CG1   | 1:CR:61:ILE:HD12  | 2.35                     | 0.42              |
| 1:CS:58:ILE:HB    | 1:CS:59:PRO:HD3   | 2.00                     | 0.42              |
| 1:CT:90:TYR:O     | 1:CT:94:GLU:HG2   | 2.18                     | 0.42              |
| 1:CT:145:MET:O    | 1:CT:149:SER:HB3  | 2.19                     | 0.42              |
| 1:CU:65:MET:HE2   | 1:CU:65:MET:HB3   | 1.80                     | 0.42              |
| 1:CV:97:LYS:N     | 1:CV:100:ALA:HB2  | 2.31                     | 0.42              |
| 1:CW:66:ALA:HB2   | 1:CW:74:VAL:HG21  | 1.99                     | 0.42              |
| 1:CX:148:LEU:HD23 | 1:CX:148:LEU:HA   | 1.82                     | 0.42              |
| 1:C2:18:VAL:HA    | 1:C2:77:LEU:O     | 2.19                     | 0.42              |
| 1:C4:90:TYR:O     | 1:C4:94:GLU:HG2   | 2.18                     | 0.42              |
| 1:AM:104:LEU:CD2  | 1:AN:60:LEU:HA    | 2.48                     | 0.42              |
| 1:AQ:13:LYS:NZ    | 1:BU:43:GLU:CB    | 2.67                     | 0.42              |
| 1:AR:18:VAL:HA    | 1:AR:77:LEU:O     | 2.19                     | 0.42              |
| 1:AV:97:LYS:HA    | 1:AV:100:ALA:HB3  | 2.00                     | 0.42              |
| 1:A3:75:ILE:HG22  | 1:A3:77:LEU:CD1   | 2.49                     | 0.42              |
| 1:A4:7:LEU:HD11   | 1:A4:140:VAL:HG22 | 2.01                     | 0.42              |
| 1:BF:51:TRP:O     | 1:BJ:148:LEU:HD11 | 2.18                     | 0.42              |
| 1:BF:65:MET:HE2   | 1:BF:65:MET:HB3   | 1.80                     | 0.42              |
| 1:BG:88:TYR:CD2   | 1:BG:88:TYR:C     | 2.97                     | 0.42              |
| 1:BJ:21:PHE:O     | 1:BJ:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:BN:88:TYR:CD2   | 1:BN:88:TYR:C     | 2.97                     | 0.42              |
| 1:BP:58:ILE:O     | 1:BP:58:ILE:HG22  | 2.12                     | 0.42              |
| 1:BV:55:ALA:HB1   | 1:BV:95:VAL:CG2   | 2.40                     | 0.42              |
| 1:BW:125:GLU:HA   | 1:BW:129:THR:HB   | 2.01                     | 0.42              |
| 1:B1:88:TYR:CD2   | 1:B1:88:TYR:C     | 2.97                     | 0.42              |
| 1:B3:75:ILE:HG22  | 1:B3:77:LEU:CD1   | 2.49                     | 0.42              |
| 1:B4:106:THR:O    | 1:B4:107:ASP:OD1  | 2.36                     | 0.42              |
| 1:B4:145:MET:O    | 1:B4:149:SER:HB3  | 2.19                     | 0.42              |
| 1:CB:97:LYS:HA    | 1:CB:100:ALA:HB3  | 2.00                     | 0.42              |
| 1:CD:20:ARG:NH1   | 1:CR:39:ARG:NH1   | 2.67                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CH:66:ALA:HB2   | 1:CH:74:VAL:HG21  | 1.99                     | 0.42              |
| 1:CL:55:ALA:HB1   | 1:CL:95:VAL:CG2   | 2.40                     | 0.42              |
| 1:CO:145:MET:O    | 1:CO:149:SER:HB3  | 2.19                     | 0.42              |
| 1:CQ:95:VAL:C     | 1:CQ:97:LYS:H     | 2.27                     | 0.42              |
| 1:CU:65:MET:HE3   | 1:CU:71:TYR:CZ    | 2.54                     | 0.42              |
| 1:CX:88:TYR:CD2   | 1:CX:88:TYR:C     | 2.97                     | 0.42              |
| 1:AD:120:ILE:CG1  | 1:AR:129:THR:HG21 | 2.49                     | 0.42              |
| 1:AN:17:VAL:HG13  | 1:AN:65:MET:CE    | 2.48                     | 0.42              |
| 1:AO:145:MET:O    | 1:AO:149:SER:HB3  | 2.20                     | 0.42              |
| 1:AR:125:GLU:HA   | 1:AR:129:THR:HB   | 2.01                     | 0.42              |
| 1:AV:88:TYR:CD2   | 1:AV:88:TYR:C     | 2.97                     | 0.42              |
| 1:AV:104:LEU:HD23 | 1:AW:60:LEU:HD13  | 2.00                     | 0.42              |
| 1:AY:21:PHE:O     | 1:AY:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:A1:88:TYR:CD2   | 1:A1:88:TYR:C     | 2.97                     | 0.42              |
| 1:BC:18:VAL:HA    | 1:BC:77:LEU:O     | 2.19                     | 0.42              |
| 1:BD:7:LEU:CB     | 1:BJ:39:ARG:O     | 2.67                     | 0.42              |
| 1:BE:145:MET:O    | 1:BE:149:SER:HB3  | 2.20                     | 0.42              |
| 1:BM:18:VAL:HA    | 1:BM:77:LEU:O     | 2.19                     | 0.42              |
| 1:BT:145:MET:O    | 1:BT:149:SER:HB3  | 2.19                     | 0.42              |
| 1:B2:91:VAL:O     | 1:B2:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:B3:58:ILE:HB    | 1:B3:59:PRO:HD3   | 2.00                     | 0.42              |
| 1:CA:58:ILE:H     | 1:CA:59:PRO:HD2   | 1.80                     | 0.42              |
| 1:CB:58:ILE:O     | 1:CB:58:ILE:CG2   | 2.65                     | 0.42              |
| 1:CG:13:LYS:HG2   | 1:CG:70:LYS:O     | 2.18                     | 0.42              |
| 1:CG:31:GLY:O     | 1:CG:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:CH:125:GLU:HA   | 1:CH:129:THR:HB   | 2.01                     | 0.42              |
| 1:CL:129:THR:HG22 | 1:CL:130:LYS:N    | 2.33                     | 0.42              |
| 1:CM:30:LEU:C     | 1:CM:32:GLY:N     | 2.78                     | 0.42              |
| 1:CM:83:GLY:HA3   | 2:CM:2201:PO4:P   | 2.60                     | 0.42              |
| 1:CO:108:ILE:CG1  | 1:CO:150:LYS:HE3  | 2.42                     | 0.42              |
| 1:CP:18:VAL:HG22  | 1:CP:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:CW:104:LEU:CD2  | 1:CX:60:LEU:HA    | 2.48                     | 0.42              |
| 1:C2:83:GLY:HA3   | 2:C2:2201:PO4:P   | 2.60                     | 0.42              |
| 1:C4:108:ILE:CG1  | 1:C4:150:LYS:HE3  | 2.42                     | 0.42              |
| 1:AA:21:PHE:O     | 1:AA:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:AA:34:LEU:C     | 1:AA:36:GLY:N     | 2.76                     | 0.42              |
| 1:AD:40:HIS:CE1   | 1:AJ:7:LEU:HD23   | 2.54                     | 0.42              |
| 1:AE:95:VAL:HG12  | 1:AE:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:AE:145:MET:O    | 1:AE:149:SER:HB3  | 2.20                     | 0.42              |
| 1:AG:13:LYS:HG2   | 1:AG:70:LYS:O     | 2.18                     | 0.42              |
| 1:AM:91:VAL:O     | 1:AM:95:VAL:HG23  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AQ:65:MET:HE2   | 1:AQ:65:MET:HB3   | 1.95                     | 0.42              |
| 1:AQ:88:TYR:CD2   | 1:AQ:88:TYR:C     | 2.97                     | 0.42              |
| 1:AS:75:ILE:HG22  | 1:AS:77:LEU:CD1   | 2.49                     | 0.42              |
| 1:AT:95:VAL:HG12  | 1:AT:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:AU:65:MET:HE3   | 1:AU:71:TYR:CZ    | 2.54                     | 0.42              |
| 1:AW:30:LEU:C     | 1:AW:32:GLY:N     | 2.78                     | 0.42              |
| 1:AW:91:VAL:O     | 1:AW:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:AY:6:HIS:HB3    | 1:AY:147:HIS:CG   | 2.55                     | 0.42              |
| 1:AZ:18:VAL:HG22  | 1:AZ:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:AZ:21:PHE:O     | 1:AZ:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:A1:13:LYS:HG2   | 1:A1:70:LYS:O     | 2.18                     | 0.42              |
| 1:A1:129:THR:CG2  | 1:A1:130:LYS:H    | 2.28                     | 0.42              |
| 1:A4:15:GLY:O     | 1:A4:74:VAL:HA    | 2.19                     | 0.42              |
| 1:BB:31:GLY:O     | 1:BB:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:BB:104:LEU:HD23 | 1:BC:60:LEU:HD13  | 2.00                     | 0.42              |
| 1:BC:34:LEU:C     | 1:BC:36:GLY:N     | 2.77                     | 0.42              |
| 1:BC:83:GLY:HA3   | 2:BC:1001:PO4:O3  | 2.20                     | 0.42              |
| 1:BC:125:GLU:HA   | 1:BC:129:THR:HB   | 2.01                     | 0.42              |
| 1:BF:65:MET:HE3   | 1:BF:71:TYR:CZ    | 2.54                     | 0.42              |
| 1:BG:13:LYS:HG2   | 1:BG:70:LYS:O     | 2.18                     | 0.42              |
| 1:BG:52:VAL:O     | 1:BG:53:PRO:C     | 2.61                     | 0.42              |
| 1:BG:55:ALA:HB1   | 1:BG:95:VAL:CG2   | 2.40                     | 0.42              |
| 1:BG:58:ILE:O     | 1:BG:58:ILE:CG2   | 2.65                     | 0.42              |
| 1:BJ:65:MET:HE2   | 1:BJ:65:MET:HB3   | 1.91                     | 0.42              |
| 1:BK:65:MET:HE3   | 1:BK:71:TYR:CZ    | 2.54                     | 0.42              |
| 1:BK:65:MET:HE2   | 1:BK:65:MET:HB3   | 1.79                     | 0.42              |
| 1:BO:95:VAL:HG12  | 1:BO:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:BR:125:GLU:HA   | 1:BR:129:THR:HB   | 2.01                     | 0.42              |
| 1:BT:7:LEU:HD11   | 1:BT:140:VAL:HG22 | 2.01                     | 0.42              |
| 1:BU:58:ILE:H     | 1:BU:59:PRO:HD2   | 1.80                     | 0.42              |
| 1:BW:30:LEU:C     | 1:BW:32:GLY:N     | 2.78                     | 0.42              |
| 1:BY:15:GLY:O     | 1:BY:74:VAL:HA    | 2.18                     | 0.42              |
| 1:BY:21:PHE:O     | 1:BY:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:BZ:18:VAL:HG22  | 1:BZ:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:BZ:21:PHE:O     | 1:BZ:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:B1:58:ILE:O     | 1:B1:58:ILE:CG2   | 2.65                     | 0.42              |
| 1:B1:97:LYS:HA    | 1:B1:100:ALA:HB3  | 2.00                     | 0.42              |
| 1:B1:104:LEU:HD23 | 1:B2:60:LEU:HD13  | 2.00                     | 0.42              |
| 1:B2:45:ASN:HD22  | 1:B2:45:ASN:HA    | 1.63                     | 0.42              |
| 1:B4:21:PHE:O     | 1:B4:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:CA:21:PHE:O     | 1:CA:22:ASN:HB2   | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CC:83:GLY:HA3  | 2:CC:1001:PO4:O3  | 2.20                     | 0.42              |
| 1:CD:88:TYR:CD2  | 1:CD:88:TYR:C     | 2.97                     | 0.42              |
| 1:CI:58:ILE:HB   | 1:CI:59:PRO:HD3   | 2.00                     | 0.42              |
| 1:CM:18:VAL:HA   | 1:CM:77:LEU:O     | 2.19                     | 0.42              |
| 1:CN:58:ILE:HB   | 1:CN:59:PRO:HD3   | 2.00                     | 0.42              |
| 1:CO:15:GLY:O    | 1:CO:74:VAL:HA    | 2.19                     | 0.42              |
| 1:CP:7:LEU:HD12  | 1:CP:7:LEU:HA     | 1.84                     | 0.42              |
| 1:CP:21:PHE:O    | 1:CP:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:CS:88:TYR:CD2  | 1:CS:88:TYR:C     | 2.97                     | 0.42              |
| 1:CW:91:VAL:O    | 1:CW:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:CW:125:GLU:HA  | 1:CW:129:THR:HB   | 2.01                     | 0.42              |
| 1:AG:31:GLY:O    | 1:AG:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:AG:58:ILE:O    | 1:AG:58:ILE:CG2   | 2.65                     | 0.42              |
| 1:AG:95:VAL:C    | 1:AG:97:LYS:H     | 2.27                     | 0.42              |
| 1:AH:18:VAL:HA   | 1:AH:77:LEU:O     | 2.19                     | 0.42              |
| 1:AH:83:GLY:HA3  | 2:AH:1001:PO4:O3  | 2.20                     | 0.42              |
| 1:AI:28:LYS:HZ3  | 1:AK:28:LYS:NZ    | 2.17                     | 0.42              |
| 1:AI:88:TYR:CD2  | 1:AI:88:TYR:C     | 2.97                     | 0.42              |
| 1:AJ:145:MET:O   | 1:AJ:149:SER:HB3  | 2.19                     | 0.42              |
| 1:AL:97:LYS:HA   | 1:AL:100:ALA:HB3  | 2.00                     | 0.42              |
| 1:AN:58:ILE:HB   | 1:AN:59:PRO:HD3   | 2.00                     | 0.42              |
| 1:AP:18:VAL:HG22 | 1:AP:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:AR:83:GLY:HA3  | 2:AR:1001:PO4:P   | 2.60                     | 0.42              |
| 1:AS:29:LEU:HD11 | 1:AS:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:AS:88:TYR:CD2  | 1:AS:88:TYR:C     | 2.97                     | 0.42              |
| 1:AV:55:ALA:HB1  | 1:AV:95:VAL:CG2   | 2.40                     | 0.42              |
| 1:AW:30:LEU:C    | 1:AW:32:GLY:H     | 2.28                     | 0.42              |
| 1:A1:31:GLY:O    | 1:A1:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:A2:30:LEU:C    | 1:A2:32:GLY:N     | 2.78                     | 0.42              |
| 1:A4:90:TYR:O    | 1:A4:94:GLU:HG2   | 2.18                     | 0.42              |
| 1:BA:21:PHE:O    | 1:BA:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:BG:95:VAL:C    | 1:BG:97:LYS:H     | 2.27                     | 0.42              |
| 1:BG:100:ALA:CA  | 1:BH:56:PHE:HZ    | 2.28                     | 0.42              |
| 1:BH:83:GLY:HA3  | 2:BH:1001:PO4:O3  | 2.20                     | 0.42              |
| 1:BH:125:GLU:HA  | 1:BH:129:THR:HB   | 2.01                     | 0.42              |
| 1:BI:98:GLY:HA2  | 1:BI:102:LEU:HD23 | 2.02                     | 0.42              |
| 1:BJ:6:HIS:HB3   | 1:BJ:147:HIS:CG   | 2.55                     | 0.42              |
| 1:BJ:145:MET:O   | 1:BJ:149:SER:HB3  | 2.20                     | 0.42              |
| 1:BM:34:LEU:C    | 1:BM:36:GLY:N     | 2.77                     | 0.42              |
| 1:BO:64:LYS:HD3  | 1:BO:64:LYS:HA    | 1.85                     | 0.42              |
| 1:BS:58:ILE:HB   | 1:BS:59:PRO:HD3   | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BU:18:VAL:HG22  | 1:BU:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:BX:52:VAL:CG1   | 1:BX:61:ILE:HD12  | 2.35                     | 0.42              |
| 1:CC:83:GLY:HA3   | 2:CC:1001:PO4:P   | 2.60                     | 0.42              |
| 1:CC:91:VAL:O     | 1:CC:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:CF:28:LYS:HD2   | 1:CR:24:PHE:CD1   | 2.55                     | 0.42              |
| 1:CG:58:ILE:O     | 1:CG:58:ILE:CG2   | 2.65                     | 0.42              |
| 1:CG:97:LYS:HA    | 1:CG:100:ALA:HB3  | 2.00                     | 0.42              |
| 1:CH:83:GLY:HA3   | 2:CH:2201:PO4:P   | 2.60                     | 0.42              |
| 1:CI:48:ASP:HB2   | 1:CI:71:TYR:CE1   | 2.50                     | 0.42              |
| 1:CO:6:HIS:HB3    | 1:CO:147:HIS:CG   | 2.55                     | 0.42              |
| 1:CU:51:TRP:O     | 1:CY:148:LEU:HD11 | 2.19                     | 0.42              |
| 1:CV:95:VAL:C     | 1:CV:97:LYS:H     | 2.27                     | 0.42              |
| 1:CW:39:ARG:CZ    | 1:C3:20:ARG:CZ    | 2.97                     | 0.42              |
| 1:CY:21:PHE:O     | 1:CY:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:C1:88:TYR:CD2   | 1:C1:88:TYR:C     | 2.97                     | 0.42              |
| 1:C2:91:VAL:O     | 1:C2:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:AA:18:VAL:HG22  | 1:AA:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:AD:98:GLY:HA2   | 1:AD:102:LEU:HD23 | 2.02                     | 0.42              |
| 1:AJ:6:HIS:HB3    | 1:AJ:147:HIS:CG   | 2.55                     | 0.42              |
| 1:AJ:7:LEU:HD11   | 1:AJ:140:VAL:HG22 | 2.01                     | 0.42              |
| 1:AN:29:LEU:HD11  | 1:AN:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:AQ:104:LEU:HD13 | 1:AR:102:LEU:CD2  | 2.46                     | 0.42              |
| 1:AW:34:LEU:C     | 1:AW:36:GLY:N     | 2.77                     | 0.42              |
| 1:AX:6:HIS:HB3    | 1:AX:147:HIS:CG   | 2.55                     | 0.42              |
| 1:AX:58:ILE:HB    | 1:AX:59:PRO:HD3   | 2.00                     | 0.42              |
| 1:AY:145:MET:O    | 1:AY:149:SER:HB3  | 2.19                     | 0.42              |
| 1:A4:6:HIS:HB3    | 1:A4:147:HIS:CG   | 2.55                     | 0.42              |
| 1:A4:108:ILE:CG1  | 1:A4:150:LYS:HE3  | 2.42                     | 0.42              |
| 1:BB:97:LYS:N     | 1:BB:100:ALA:HB2  | 2.31                     | 0.42              |
| 1:BC:91:VAL:O     | 1:BC:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:BD:58:ILE:HB    | 1:BD:59:PRO:HD3   | 2.00                     | 0.42              |
| 1:BE:7:LEU:HD12   | 1:BE:7:LEU:HA     | 1.91                     | 0.42              |
| 1:BH:30:LEU:C     | 1:BH:32:GLY:N     | 2.78                     | 0.42              |
| 1:BL:95:VAL:C     | 1:BL:97:LYS:H     | 2.27                     | 0.42              |
| 1:BQ:31:GLY:O     | 1:BQ:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:CA:65:MET:HE3   | 1:CA:71:TYR:CZ    | 2.54                     | 0.42              |
| 1:CC:30:LEU:C     | 1:CC:32:GLY:N     | 2.78                     | 0.42              |
| 1:CG:95:VAL:C     | 1:CG:97:LYS:H     | 2.27                     | 0.42              |
| 1:CK:53:PRO:HD2   | 1:CK:57:GLU:CB    | 2.49                     | 0.42              |
| 1:CN:148:LEU:HD23 | 1:CN:148:LEU:HA   | 1.82                     | 0.42              |
| 1:CO:90:TYR:O     | 1:CO:94:GLU:HG2   | 2.18                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CR:30:LEU:C     | 1:CR:32:GLY:N     | 2.78                     | 0.42              |
| 1:CR:83:GLY:HA3   | 2:CR:2201:PO4:P   | 2.60                     | 0.42              |
| 1:CX:6:HIS:HB3    | 1:CX:147:HIS:CG   | 2.55                     | 0.42              |
| 1:CY:145:MET:O    | 1:CY:149:SER:HB3  | 2.20                     | 0.42              |
| 1:C1:55:ALA:HA    | 1:C1:58:ILE:HG13  | 2.02                     | 0.42              |
| 1:C3:6:HIS:HB3    | 1:C3:147:HIS:CG   | 2.55                     | 0.42              |
| 1:AE:6:HIS:HB3    | 1:AE:147:HIS:CG   | 2.55                     | 0.42              |
| 1:AH:83:GLY:HA3   | 2:AH:1001:PO4:P   | 2.60                     | 0.42              |
| 1:AL:129:THR:HG22 | 1:AL:130:LYS:N    | 2.33                     | 0.42              |
| 1:AM:83:GLY:HA3   | 2:AM:1001:PO4:P   | 2.60                     | 0.42              |
| 1:AQ:31:GLY:O     | 1:AQ:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:AX:98:GLY:HA2   | 1:AX:102:LEU:HD23 | 2.02                     | 0.42              |
| 1:A3:29:LEU:HD11  | 1:A3:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:A3:88:TYR:CD2   | 1:A3:88:TYR:C     | 2.97                     | 0.42              |
| 1:BC:83:GLY:HA3   | 2:BC:1001:PO4:P   | 2.60                     | 0.42              |
| 1:BD:88:TYR:CD2   | 1:BD:88:TYR:C     | 2.97                     | 0.42              |
| 1:BE:6:HIS:HB3    | 1:BE:147:HIS:CG   | 2.55                     | 0.42              |
| 1:BE:95:VAL:HG12  | 1:BE:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:BI:29:LEU:HD11  | 1:BI:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:BK:21:PHE:O     | 1:BK:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:BL:31:GLY:O     | 1:BL:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:BL:55:ALA:CB    | 1:BL:95:VAL:HG21  | 2.40                     | 0.42              |
| 1:BS:98:GLY:HA2   | 1:BS:102:LEU:HD23 | 2.02                     | 0.42              |
| 1:BT:6:HIS:HB3    | 1:BT:147:HIS:CG   | 2.55                     | 0.42              |
| 1:BV:88:TYR:CD2   | 1:BV:88:TYR:C     | 2.97                     | 0.42              |
| 1:BY:6:HIS:HB3    | 1:BY:147:HIS:CG   | 2.55                     | 0.42              |
| 1:BY:145:MET:O    | 1:BY:149:SER:HB3  | 2.20                     | 0.42              |
| 1:B1:31:GLY:O     | 1:B1:35:ASP:HB2   | 2.20                     | 0.42              |
| 1:B1:55:ALA:HA    | 1:B1:58:ILE:HG13  | 2.02                     | 0.42              |
| 1:B4:15:GLY:O     | 1:B4:74:VAL:HA    | 2.18                     | 0.42              |
| 1:CA:24:PHE:CD1   | 1:CN:28:LYS:HG3   | 2.54                     | 0.42              |
| 1:CE:95:VAL:HG12  | 1:CE:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:CF:18:VAL:HG22  | 1:CF:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:CJ:6:HIS:HB3    | 1:CJ:147:HIS:CG   | 2.55                     | 0.42              |
| 1:CL:52:VAL:O     | 1:CL:53:PRO:C     | 2.61                     | 0.42              |
| 1:CM:67:ASN:HD22  | 1:CM:67:ASN:HA    | 1.60                     | 0.42              |
| 1:CM:83:GLY:HA3   | 2:CM:2201:PO4:O3  | 2.20                     | 0.42              |
| 1:CO:21:PHE:O     | 1:CO:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:CP:20:ARG:HH12  | 1:CT:144:GLU:CD   | 2.26                     | 0.42              |
| 1:CP:90:TYR:O     | 1:CP:94:GLU:HG2   | 2.18                     | 0.42              |
| 1:CQ:97:LYS:HA    | 1:CQ:100:ALA:HB3  | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CZ:116:THR:O    | 1:C1:85:THR:HB    | 2.20                     | 0.42              |
| 1:C4:6:HIS:HB3    | 1:C4:147:HIS:CG   | 2.55                     | 0.42              |
| 1:AK:21:PHE:O     | 1:AK:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:AL:55:ALA:HA    | 1:AL:58:ILE:HG13  | 2.02                     | 0.42              |
| 1:AO:6:HIS:HB3    | 1:AO:147:HIS:CG   | 2.55                     | 0.42              |
| 1:AU:116:THR:O    | 1:AV:85:THR:HB    | 2.20                     | 0.42              |
| 1:AW:83:GLY:HA3   | 2:AW:201:PO4:O3   | 2.20                     | 0.42              |
| 1:AZ:116:THR:O    | 1:A1:85:THR:HB    | 2.20                     | 0.42              |
| 1:A2:30:LEU:C     | 1:A2:32:GLY:H     | 2.28                     | 0.42              |
| 1:A3:150:LYS:H    | 1:A3:150:LYS:HG3  | 1.33                     | 0.42              |
| 1:A4:95:VAL:HG12  | 1:A4:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:BN:29:LEU:HD11  | 1:BN:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:BQ:55:ALA:HA    | 1:BQ:58:ILE:HG13  | 2.02                     | 0.42              |
| 1:BT:21:PHE:O     | 1:BT:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:BV:55:ALA:HA    | 1:BV:58:ILE:HG13  | 2.02                     | 0.42              |
| 1:CB:88:TYR:CD2   | 1:CB:88:TYR:C     | 2.97                     | 0.42              |
| 1:CE:7:LEU:HD11   | 1:CE:140:VAL:HG22 | 2.01                     | 0.42              |
| 1:CE:15:GLY:O     | 1:CE:74:VAL:HA    | 2.18                     | 0.42              |
| 1:CE:145:MET:O    | 1:CE:149:SER:HB3  | 2.20                     | 0.42              |
| 1:CG:88:TYR:CD2   | 1:CG:88:TYR:C     | 2.97                     | 0.42              |
| 1:CH:30:LEU:C     | 1:CH:32:GLY:H     | 2.28                     | 0.42              |
| 1:CK:21:PHE:O     | 1:CK:22:ASN:HB2   | 2.20                     | 0.42              |
| 1:CM:91:VAL:O     | 1:CM:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:CN:6:HIS:HB3    | 1:CN:147:HIS:CG   | 2.55                     | 0.42              |
| 1:CV:88:TYR:CD2   | 1:CV:88:TYR:C     | 2.97                     | 0.42              |
| 1:CV:104:LEU:HD23 | 1:CW:60:LEU:HD13  | 2.00                     | 0.42              |
| 1:CX:29:LEU:HD11  | 1:CX:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:CY:95:VAL:HG12  | 1:CY:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:C1:129:THR:HG22 | 1:C1:130:LYS:N    | 2.33                     | 0.42              |
| 1:AD:88:TYR:CD2   | 1:AD:88:TYR:C     | 2.97                     | 0.42              |
| 1:AG:88:TYR:CD2   | 1:AG:88:TYR:C     | 2.97                     | 0.42              |
| 1:AI:98:GLY:HA2   | 1:AI:102:LEU:HD23 | 2.02                     | 0.42              |
| 1:AO:21:PHE:O     | 1:AO:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:AP:53:PRO:HD2   | 1:AP:57:GLU:CB    | 2.49                     | 0.42              |
| 1:AP:116:THR:O    | 1:AQ:85:THR:HB    | 2.20                     | 0.42              |
| 1:AQ:52:VAL:O     | 1:AQ:53:PRO:C     | 2.61                     | 0.42              |
| 1:AQ:55:ALA:HA    | 1:AQ:58:ILE:HG13  | 2.02                     | 0.42              |
| 1:AT:7:LEU:HD11   | 1:AT:140:VAL:HG22 | 2.01                     | 0.42              |
| 1:AU:18:VAL:HG22  | 1:AU:77:LEU:HB2   | 2.02                     | 0.42              |
| 1:AY:95:VAL:HG12  | 1:AY:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:A2:83:GLY:HA3   | 2:A2:1001:PO4:O3  | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A2:91:VAL:O    | 1:A2:95:VAL:HG23  | 2.19                     | 0.42              |
| 1:BC:129:THR:O   | 1:BC:131:ALA:N    | 2.53                     | 0.42              |
| 1:BD:98:GLY:HA2  | 1:BD:102:LEU:HD23 | 2.02                     | 0.42              |
| 1:BH:83:GLY:HA3  | 2:BH:1001:PO4:P   | 2.60                     | 0.42              |
| 1:BI:6:HIS:HB3   | 1:BI:147:HIS:CG   | 2.55                     | 0.42              |
| 1:BI:48:ASP:HB2  | 1:BI:71:TYR:CE1   | 2.50                     | 0.42              |
| 1:BJ:95:VAL:HG12 | 1:BJ:112:PHE:HE1  | 1.85                     | 0.42              |
| 1:BL:55:ALA:HA   | 1:BL:58:ILE:HG13  | 2.02                     | 0.42              |
| 1:BM:83:GLY:HA3  | 2:BM:1001:PO4:P   | 2.60                     | 0.42              |
| 1:BO:7:LEU:HD11  | 1:BO:140:VAL:HG22 | 2.01                     | 0.42              |
| 1:BO:21:PHE:O    | 1:BO:22:ASN:HB2   | 2.19                     | 0.42              |
| 1:BQ:88:TYR:CD2  | 1:BQ:88:TYR:C     | 2.97                     | 0.42              |
| 1:BR:63:LYS:O    | 1:BR:65:MET:N     | 2.53                     | 0.42              |
| 1:BR:83:GLY:HA3  | 2:BR:1001:PO4:O3  | 2.20                     | 0.42              |
| 1:BV:13:LYS:HG2  | 1:BV:70:LYS:O     | 2.18                     | 0.42              |
| 1:BV:100:ALA:O   | 1:BW:56:PHE:CE1   | 2.73                     | 0.42              |
| 1:BW:83:GLY:HA3  | 2:BW:1001:PO4:P   | 2.60                     | 0.42              |
| 1:BX:29:LEU:HD11 | 1:BX:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:B4:64:LYS:HD3  | 1:B4:64:LYS:HA    | 1.85                     | 0.42              |
| 1:CD:6:HIS:HB3   | 1:CD:147:HIS:CG   | 2.55                     | 0.42              |
| 1:CJ:7:LEU:HD11  | 1:CJ:140:VAL:HG22 | 2.01                     | 0.42              |
| 1:CJ:15:GLY:O    | 1:CJ:74:VAL:HA    | 2.19                     | 0.42              |
| 1:CR:34:LEU:C    | 1:CR:36:GLY:N     | 2.77                     | 0.42              |
| 1:CS:29:LEU:HD11 | 1:CS:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:CW:34:LEU:HD22 | 1:CW:38:LYS:CE    | 2.44                     | 0.42              |
| 1:CX:98:GLY:HA2  | 1:CX:102:LEU:HD23 | 2.02                     | 0.42              |
| 1:AB:95:VAL:C    | 1:AB:97:LYS:H     | 2.27                     | 0.42              |
| 1:AB:100:ALA:O   | 1:AC:56:PHE:CE1   | 2.73                     | 0.42              |
| 1:AF:34:LEU:C    | 1:AF:36:GLY:N     | 2.76                     | 0.42              |
| 1:AH:63:LYS:O    | 1:AH:65:MET:N     | 2.53                     | 0.42              |
| 1:AI:39:ARG:O    | 1:AO:7:LEU:CB     | 2.67                     | 0.42              |
| 1:AK:52:VAL:HB   | 1:AK:53:PRO:CD    | 2.50                     | 0.42              |
| 1:AP:65:MET:HE3  | 1:AP:71:TYR:CZ    | 2.54                     | 0.42              |
| 1:AR:129:THR:O   | 1:AR:131:ALA:N    | 2.53                     | 0.42              |
| 1:AY:15:GLY:O    | 1:AY:74:VAL:HA    | 2.19                     | 0.42              |
| 1:AZ:52:VAL:HB   | 1:AZ:53:PRO:CD    | 2.50                     | 0.42              |
| 1:A2:129:THR:O   | 1:A2:131:ALA:N    | 2.53                     | 0.42              |
| 1:A3:52:VAL:CG1  | 1:A3:61:ILE:HD12  | 2.35                     | 0.42              |
| 1:BA:52:VAL:HB   | 1:BA:53:PRO:CD    | 2.50                     | 0.42              |
| 1:BD:29:LEU:HD11 | 1:BD:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:BG:31:GLY:O    | 1:BG:35:ASP:HB2   | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BH:18:VAL:HA    | 1:BH:77:LEU:O     | 2.19                     | 0.42              |
| 1:BH:63:LYS:O     | 1:BH:65:MET:N     | 2.53                     | 0.42              |
| 1:BK:7:LEU:HD12   | 1:BK:7:LEU:HA     | 1.84                     | 0.42              |
| 1:BO:6:HIS:HB3    | 1:BO:147:HIS:CG   | 2.55                     | 0.42              |
| 1:BO:145:MET:O    | 1:BO:149:SER:HB3  | 2.20                     | 0.42              |
| 1:BQ:97:LYS:HA    | 1:BQ:100:ALA:HB3  | 2.00                     | 0.42              |
| 1:BR:83:GLY:HA3   | 2:BR:1001:PO4:P   | 2.60                     | 0.42              |
| 1:BU:53:PRO:HD2   | 1:BU:57:GLU:CB    | 2.49                     | 0.42              |
| 1:BX:6:HIS:HB3    | 1:BX:147:HIS:CG   | 2.55                     | 0.42              |
| 1:B2:34:LEU:C     | 1:B2:36:GLY:N     | 2.77                     | 0.42              |
| 1:B2:83:GLY:HA3   | 2:B2:1001:PO4:O3  | 2.20                     | 0.42              |
| 1:B3:29:LEU:HD11  | 1:B3:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:CB:55:ALA:CB    | 1:CB:95:VAL:HG21  | 2.40                     | 0.42              |
| 1:CB:100:ALA:O    | 1:CC:56:PHE:CE1   | 2.73                     | 0.42              |
| 1:CC:34:LEU:C     | 1:CC:36:GLY:N     | 2.77                     | 0.42              |
| 1:CE:52:VAL:CB    | 1:CE:53:PRO:CD    | 2.98                     | 0.42              |
| 1:CH:34:LEU:C     | 1:CH:36:GLY:N     | 2.77                     | 0.42              |
| 1:CJ:52:VAL:CB    | 1:CJ:53:PRO:CD    | 2.98                     | 0.42              |
| 1:CM:34:LEU:C     | 1:CM:36:GLY:N     | 2.77                     | 0.42              |
| 1:CP:116:THR:O    | 1:CQ:85:THR:HB    | 2.20                     | 0.42              |
| 1:C2:83:GLY:HA3   | 2:C2:2201:PO4:O3  | 2.20                     | 0.42              |
| 1:C3:29:LEU:HD11  | 1:C3:134:LYS:HB3  | 2.02                     | 0.42              |
| 1:AD:120:ILE:HG12 | 1:AR:129:THR:HG21 | 2.02                     | 0.41              |
| 1:AF:53:PRO:HD2   | 1:AF:57:GLU:CB    | 2.49                     | 0.41              |
| 1:AK:18:VAL:HG22  | 1:AK:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:AL:88:TYR:CD2   | 1:AL:88:TYR:C     | 2.97                     | 0.41              |
| 1:AM:18:VAL:HA    | 1:AM:77:LEU:O     | 2.19                     | 0.41              |
| 1:AS:148:LEU:HD23 | 1:AS:148:LEU:HA   | 1.82                     | 0.41              |
| 1:AU:21:PHE:O     | 1:AU:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:AU:52:VAL:HB    | 1:AU:53:PRO:CD    | 2.50                     | 0.41              |
| 1:AW:67:ASN:HD22  | 1:AW:67:ASN:HA    | 1.59                     | 0.41              |
| 1:AW:125:GLU:HA   | 1:AW:129:THR:HB   | 2.01                     | 0.41              |
| 1:A2:34:LEU:C     | 1:A2:36:GLY:N     | 2.77                     | 0.41              |
| 1:A4:145:MET:O    | 1:A4:149:SER:HB3  | 2.19                     | 0.41              |
| 1:BH:91:VAL:O     | 1:BH:95:VAL:HG23  | 2.19                     | 0.41              |
| 1:BJ:7:LEU:HD11   | 1:BJ:140:VAL:HG22 | 2.01                     | 0.41              |
| 1:BM:129:THR:O    | 1:BM:131:ALA:N    | 2.53                     | 0.41              |
| 1:BQ:71:TYR:O     | 1:BQ:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:BS:6:HIS:HB3    | 1:BS:147:HIS:CG   | 2.55                     | 0.41              |
| 1:B2:129:THR:O    | 1:B2:131:ALA:N    | 2.53                     | 0.41              |
| 1:CB:97:LYS:N     | 1:CB:100:ALA:HB2  | 2.31                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:CC:129:THR:O    | 1:CC:131:ALA:N   | 2.53                     | 0.41              |
| 1:CF:21:PHE:O     | 1:CF:22:ASN:HB2  | 2.20                     | 0.41              |
| 1:CH:91:VAL:O     | 1:CH:95:VAL:HG23 | 2.19                     | 0.41              |
| 1:CI:29:LEU:HD11  | 1:CI:134:LYS:HB3 | 2.02                     | 0.41              |
| 1:CI:88:TYR:CD2   | 1:CI:88:TYR:C    | 2.97                     | 0.41              |
| 1:CQ:31:GLY:O     | 1:CQ:35:ASP:HB2  | 2.20                     | 0.41              |
| 1:CR:83:GLY:HA3   | 2:CR:2201:PO4:O3 | 2.20                     | 0.41              |
| 1:CR:91:VAL:O     | 1:CR:95:VAL:HG23 | 2.19                     | 0.41              |
| 1:CS:75:ILE:HG22  | 1:CS:77:LEU:CD1  | 2.49                     | 0.41              |
| 1:CT:28:LYS:NZ    | 1:C4:28:LYS:NZ   | 2.67                     | 0.41              |
| 1:CT:95:VAL:HG12  | 1:CT:112:PHE:HE1 | 1.85                     | 0.41              |
| 1:CU:53:PRO:HD2   | 1:CU:57:GLU:CB   | 2.49                     | 0.41              |
| 1:CV:55:ALA:HA    | 1:CV:58:ILE:HG13 | 2.02                     | 0.41              |
| 1:CV:100:ALA:O    | 1:CW:56:PHE:CE1  | 2.73                     | 0.41              |
| 1:CW:30:LEU:C     | 1:CW:32:GLY:N    | 2.78                     | 0.41              |
| 1:CW:30:LEU:C     | 1:CW:32:GLY:H    | 2.28                     | 0.41              |
| 1:C4:30:LEU:HA    | 1:C4:77:LEU:HD23 | 2.02                     | 0.41              |
| 1:AA:53:PRO:HD2   | 1:AA:57:GLU:CB   | 2.49                     | 0.41              |
| 1:AC:83:GLY:HA3   | 2:AC:1001:PO4:O3 | 2.20                     | 0.41              |
| 1:AC:83:GLY:HA3   | 2:AC:1001:PO4:P  | 2.60                     | 0.41              |
| 1:AE:15:GLY:O     | 1:AE:74:VAL:HA   | 2.18                     | 0.41              |
| 1:AE:21:PHE:O     | 1:AE:22:ASN:HB2  | 2.19                     | 0.41              |
| 1:AT:30:LEU:HA    | 1:AT:77:LEU:HD23 | 2.02                     | 0.41              |
| 1:AT:145:MET:O    | 1:AT:149:SER:HB3 | 2.19                     | 0.41              |
| 1:AV:104:LEU:HD13 | 1:AW:102:LEU:CD2 | 2.46                     | 0.41              |
| 1:AX:88:TYR:CD2   | 1:AX:88:TYR:C    | 2.97                     | 0.41              |
| 1:A1:55:ALA:HA    | 1:A1:58:ILE:HG13 | 2.02                     | 0.41              |
| 1:A1:100:ALA:O    | 1:A2:56:PHE:CE1  | 2.73                     | 0.41              |
| 1:A2:63:LYS:O     | 1:A2:65:MET:N    | 2.53                     | 0.41              |
| 1:A2:83:GLY:HA3   | 2:A2:1001:PO4:P  | 2.60                     | 0.41              |
| 1:A4:65:MET:HE2   | 1:A4:65:MET:HB3  | 1.91                     | 0.41              |
| 1:BB:88:TYR:CD2   | 1:BB:88:TYR:C    | 2.97                     | 0.41              |
| 1:BF:53:PRO:HD2   | 1:BF:57:GLU:CB   | 2.49                     | 0.41              |
| 1:BK:52:VAL:HB    | 1:BK:53:PRO:CD   | 2.51                     | 0.41              |
| 1:BM:83:GLY:HA3   | 2:BM:1001:PO4:O3 | 2.20                     | 0.41              |
| 1:BN:6:HIS:HB3    | 1:BN:147:HIS:CG  | 2.55                     | 0.41              |
| 1:BP:116:THR:O    | 1:BQ:85:THR:HB   | 2.20                     | 0.41              |
| 1:BR:148:LEU:HD23 | 1:BR:148:LEU:HA  | 1.80                     | 0.41              |
| 1:BS:29:LEU:HD11  | 1:BS:134:LYS:HB3 | 2.02                     | 0.41              |
| 1:BS:88:TYR:CD2   | 1:BS:88:TYR:C    | 2.97                     | 0.41              |
| 1:B2:83:GLY:HA3   | 2:B2:1001:PO4:P  | 2.60                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B3:6:HIS:HB3    | 1:B3:147:HIS:CG   | 2.55                     | 0.41              |
| 1:B4:95:VAL:HG12  | 1:B4:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:CA:18:VAL:HG22  | 1:CA:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:CA:34:LEU:C     | 1:CA:36:GLY:N     | 2.76                     | 0.41              |
| 1:CA:65:MET:HE2   | 1:CA:65:MET:HB3   | 1.80                     | 0.41              |
| 1:CH:67:ASN:HD22  | 1:CH:67:ASN:HA    | 1.59                     | 0.41              |
| 1:CQ:55:ALA:HA    | 1:CQ:58:ILE:HG13  | 2.02                     | 0.41              |
| 1:CQ:88:TYR:CD2   | 1:CQ:88:TYR:C     | 2.97                     | 0.41              |
| 1:CW:83:GLY:HA3   | 2:CW:2201:PO4:P   | 2.60                     | 0.41              |
| 1:CW:83:GLY:HA3   | 2:CW:2201:PO4:O3  | 2.20                     | 0.41              |
| 1:CY:7:LEU:HD11   | 1:CY:140:VAL:HG22 | 2.01                     | 0.41              |
| 1:CY:64:LYS:HD3   | 1:CY:64:LYS:HA    | 1.85                     | 0.41              |
| 1:C1:58:ILE:O     | 1:C1:58:ILE:CG2   | 2.65                     | 0.41              |
| 1:C2:30:LEU:C     | 1:C2:32:GLY:N     | 2.78                     | 0.41              |
| 1:C2:63:LYS:O     | 1:C2:65:MET:N     | 2.53                     | 0.41              |
| 1:AC:30:LEU:C     | 1:AC:32:GLY:H     | 2.28                     | 0.41              |
| 1:AC:91:VAL:O     | 1:AC:95:VAL:HG23  | 2.19                     | 0.41              |
| 1:AL:31:GLY:O     | 1:AL:35:ASP:HB2   | 2.20                     | 0.41              |
| 1:AL:55:ALA:HB1   | 1:AL:95:VAL:CG2   | 2.40                     | 0.41              |
| 1:AM:83:GLY:HA3   | 2:AM:1001:PO4:O3  | 2.20                     | 0.41              |
| 1:AT:6:HIS:HB3    | 1:AT:147:HIS:CG   | 2.55                     | 0.41              |
| 1:AV:100:ALA:O    | 1:AW:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:A1:71:TYR:O     | 1:A1:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:A3:6:HIS:HB3    | 1:A3:147:HIS:CG   | 2.55                     | 0.41              |
| 1:BC:24:PHE:CE1   | 1:BU:28:LYS:HD2   | 2.53                     | 0.41              |
| 1:BC:30:LEU:C     | 1:BC:32:GLY:H     | 2.28                     | 0.41              |
| 1:BF:18:VAL:HG22  | 1:BF:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:BG:55:ALA:HA    | 1:BG:58:ILE:HG13  | 2.02                     | 0.41              |
| 1:BH:129:THR:O    | 1:BH:131:ALA:N    | 2.53                     | 0.41              |
| 1:BN:75:ILE:HG22  | 1:BN:77:LEU:CD1   | 2.49                     | 0.41              |
| 1:BQ:100:ALA:O    | 1:BR:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:BW:129:THR:O    | 1:BW:131:ALA:N    | 2.53                     | 0.41              |
| 1:BX:88:TYR:CD2   | 1:BX:88:TYR:C     | 2.97                     | 0.41              |
| 1:CB:55:ALA:HA    | 1:CB:58:ILE:HG13  | 2.02                     | 0.41              |
| 1:CC:39:ARG:CZ    | 1:CS:20:ARG:CZ    | 2.98                     | 0.41              |
| 1:CD:148:LEU:HD23 | 1:CD:148:LEU:HA   | 1.82                     | 0.41              |
| 1:CE:64:LYS:HA    | 1:CE:64:LYS:HD3   | 1.85                     | 0.41              |
| 1:CG:71:TYR:O     | 1:CG:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:CG:100:ALA:O    | 1:CH:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:CG:120:ILE:CD1  | 1:CQ:125:GLU:HG2  | 2.50                     | 0.41              |
| 1:CH:18:VAL:HA    | 1:CH:77:LEU:O     | 2.19                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CH:30:LEU:C    | 1:CH:32:GLY:N     | 2.78                     | 0.41              |
| 1:CJ:30:LEU:HA   | 1:CJ:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:CL:31:GLY:O    | 1:CL:35:ASP:HB2   | 2.20                     | 0.41              |
| 1:CO:95:VAL:HG12 | 1:CO:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:CT:39:ARG:O    | 1:C3:7:LEU:CB     | 2.68                     | 0.41              |
| 1:CU:21:PHE:O    | 1:CU:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:CU:52:VAL:HB   | 1:CU:53:PRO:CD    | 2.50                     | 0.41              |
| 1:CV:4:GLU:CG    | 1:CW:51:TRP:HD1   | 2.29                     | 0.41              |
| 1:CZ:18:VAL:HG22 | 1:CZ:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:C1:31:GLY:O    | 1:C1:35:ASP:HB2   | 2.20                     | 0.41              |
| 1:C1:71:TYR:O    | 1:C1:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:AD:6:HIS:HB3   | 1:AD:147:HIS:CG   | 2.55                     | 0.41              |
| 1:AE:64:LYS:HD3  | 1:AE:64:LYS:HA    | 1.85                     | 0.41              |
| 1:AF:18:VAL:HG22 | 1:AF:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:AG:24:PHE:CD1  | 1:AQ:28:LYS:HG3   | 2.55                     | 0.41              |
| 1:AG:25:ILE:HG23 | 1:AG:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:AG:55:ALA:HA   | 1:AG:58:ILE:HG13  | 2.02                     | 0.41              |
| 1:AI:48:ASP:HB2  | 1:AI:71:TYR:CE1   | 2.50                     | 0.41              |
| 1:AJ:30:LEU:HA   | 1:AJ:77:LEU:HD23  | 2.03                     | 0.41              |
| 1:AJ:52:VAL:CB   | 1:AJ:53:PRO:CD    | 2.98                     | 0.41              |
| 1:AM:63:LYS:O    | 1:AM:65:MET:N     | 2.53                     | 0.41              |
| 1:AN:150:LYS:H   | 1:AN:150:LYS:HG3  | 1.33                     | 0.41              |
| 1:AR:83:GLY:HA3  | 2:AR:1001:PO4:O3  | 2.20                     | 0.41              |
| 1:AX:29:LEU:HD11 | 1:AX:134:LYS:HB3  | 2.02                     | 0.41              |
| 1:A1:95:VAL:C    | 1:A1:97:LYS:H     | 2.27                     | 0.41              |
| 1:BC:30:LEU:C    | 1:BC:32:GLY:N     | 2.78                     | 0.41              |
| 1:BG:71:TYR:O    | 1:BG:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:BK:18:VAL:HG22 | 1:BK:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:BK:116:THR:O   | 1:BL:85:THR:HB    | 2.20                     | 0.41              |
| 1:BM:63:LYS:O    | 1:BM:65:MET:N     | 2.53                     | 0.41              |
| 1:BM:95:VAL:HG12 | 1:BM:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:BQ:97:LYS:N    | 1:BQ:100:ALA:HB2  | 2.31                     | 0.41              |
| 1:B2:30:LEU:C    | 1:B2:32:GLY:H     | 2.28                     | 0.41              |
| 1:B3:88:TYR:CD2  | 1:B3:88:TYR:C     | 2.97                     | 0.41              |
| 1:CC:63:LYS:O    | 1:CC:65:MET:N     | 2.53                     | 0.41              |
| 1:CH:83:GLY:HA3  | 2:CH:2201:PO4:O3  | 2.20                     | 0.41              |
| 1:CM:63:LYS:O    | 1:CM:65:MET:N     | 2.53                     | 0.41              |
| 1:CM:125:GLU:HA  | 1:CM:129:THR:HB   | 2.01                     | 0.41              |
| 1:CM:129:THR:O   | 1:CM:131:ALA:N    | 2.53                     | 0.41              |
| 1:CP:52:VAL:HB   | 1:CP:53:PRO:CD    | 2.50                     | 0.41              |
| 1:CP:65:MET:HE2  | 1:CP:65:MET:HB3   | 1.80                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CS:98:GLY:HA2   | 1:CS:102:LEU:HD23 | 2.02                     | 0.41              |
| 1:AB:31:GLY:O     | 1:AB:35:ASP:HB2   | 2.20                     | 0.41              |
| 1:AC:125:GLU:HA   | 1:AC:129:THR:HB   | 2.01                     | 0.41              |
| 1:AD:148:LEU:HD23 | 1:AD:148:LEU:HA   | 1.82                     | 0.41              |
| 1:AE:7:LEU:HD12   | 1:AE:7:LEU:HA     | 1.91                     | 0.41              |
| 1:AO:30:LEU:HA    | 1:AO:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:AP:21:PHE:O     | 1:AP:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:AP:52:VAL:HB    | 1:AP:53:PRO:CD    | 2.50                     | 0.41              |
| 1:AR:63:LYS:O     | 1:AR:65:MET:N     | 2.53                     | 0.41              |
| 1:AS:39:ARG:O     | 1:AY:7:LEU:HB3    | 2.21                     | 0.41              |
| 1:AT:64:LYS:HD3   | 1:AT:64:LYS:HA    | 1.85                     | 0.41              |
| 1:AV:55:ALA:HA    | 1:AV:58:ILE:HG13  | 2.02                     | 0.41              |
| 1:BA:18:VAL:HG22  | 1:BA:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:BA:116:THR:O    | 1:BB:85:THR:HB    | 2.20                     | 0.41              |
| 1:BC:148:LEU:HD23 | 1:BC:148:LEU:HA   | 1.80                     | 0.41              |
| 1:BL:88:TYR:CD2   | 1:BL:88:TYR:C     | 2.97                     | 0.41              |
| 1:BM:30:LEU:C     | 1:BM:32:GLY:N     | 2.78                     | 0.41              |
| 1:BR:129:THR:O    | 1:BR:131:ALA:N    | 2.53                     | 0.41              |
| 1:BU:52:VAL:HB    | 1:BU:53:PRO:CD    | 2.50                     | 0.41              |
| 1:BU:116:THR:O    | 1:BV:85:THR:HB    | 2.20                     | 0.41              |
| 1:BV:97:LYS:N     | 1:BV:100:ALA:HB2  | 2.31                     | 0.41              |
| 1:B2:65:MET:HE2   | 1:B2:65:MET:HB3   | 1.87                     | 0.41              |
| 1:B4:65:MET:HE2   | 1:B4:65:MET:HB3   | 1.91                     | 0.41              |
| 1:CD:28:LYS:HG3   | 1:CF:24:PHE:CD1   | 2.55                     | 0.41              |
| 1:CI:6:HIS:HB3    | 1:CI:147:HIS:CG   | 2.55                     | 0.41              |
| 1:CJ:7:LEU:HD12   | 1:CJ:7:LEU:HA     | 1.91                     | 0.41              |
| 1:CL:100:ALA:O    | 1:CM:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:CN:88:TYR:CD2   | 1:CN:88:TYR:C     | 2.97                     | 0.41              |
| 1:CU:116:THR:O    | 1:CV:85:THR:HB    | 2.20                     | 0.41              |
| 1:CW:34:LEU:C     | 1:CW:36:GLY:N     | 2.77                     | 0.41              |
| 1:CW:63:LYS:O     | 1:CW:65:MET:N     | 2.53                     | 0.41              |
| 1:CY:6:HIS:HB3    | 1:CY:147:HIS:CG   | 2.55                     | 0.41              |
| 1:CZ:52:VAL:HB    | 1:CZ:53:PRO:CD    | 2.50                     | 0.41              |
| 1:AB:55:ALA:HB1   | 1:AB:95:VAL:CG2   | 2.40                     | 0.41              |
| 1:AB:55:ALA:HA    | 1:AB:58:ILE:HG13  | 2.02                     | 0.41              |
| 1:AE:108:ILE:CG1  | 1:AE:150:LYS:HE3  | 2.42                     | 0.41              |
| 1:AF:65:MET:HE2   | 1:AF:65:MET:HB3   | 1.80                     | 0.41              |
| 1:AH:30:LEU:C     | 1:AH:32:GLY:H     | 2.28                     | 0.41              |
| 1:AH:129:THR:O    | 1:AH:131:ALA:N    | 2.53                     | 0.41              |
| 1:AI:6:HIS:HB3    | 1:AI:147:HIS:CG   | 2.55                     | 0.41              |
| 1:AN:6:HIS:HB3    | 1:AN:147:HIS:CG   | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AO:95:VAL:HG12  | 1:AO:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:AQ:97:LYS:N     | 1:AQ:100:ALA:HB2  | 2.31                     | 0.41              |
| 1:AQ:100:ALA:O    | 1:AR:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:AV:71:TYR:O     | 1:AV:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:AW:129:THR:O    | 1:AW:131:ALA:N    | 2.53                     | 0.41              |
| 1:BB:100:ALA:O    | 1:BC:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:BD:6:HIS:HB3    | 1:BD:147:HIS:CG   | 2.55                     | 0.41              |
| 1:BF:21:PHE:O     | 1:BF:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:BF:116:THR:O    | 1:BG:85:THR:HB    | 2.20                     | 0.41              |
| 1:BG:4:GLU:CG     | 1:BH:51:TRP:HD1   | 2.29                     | 0.41              |
| 1:BG:100:ALA:O    | 1:BH:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:BK:76:THR:CG2   | 1:BK:112:PHE:HA   | 2.51                     | 0.41              |
| 1:BL:25:ILE:HG23  | 1:BL:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:BP:52:VAL:HB    | 1:BP:53:PRO:CD    | 2.51                     | 0.41              |
| 1:BQ:25:ILE:HG23  | 1:BQ:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:BT:95:VAL:HG12  | 1:BT:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:BV:31:GLY:O     | 1:BV:35:ASP:HB2   | 2.20                     | 0.41              |
| 1:BW:63:LYS:O     | 1:BW:65:MET:N     | 2.53                     | 0.41              |
| 1:BY:14:VAL:HG21  | 1:BY:37:LEU:HD22  | 2.03                     | 0.41              |
| 1:BZ:116:THR:O    | 1:B1:85:THR:HB    | 2.20                     | 0.41              |
| 1:B1:71:TYR:O     | 1:B1:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:B2:30:LEU:C     | 1:B2:32:GLY:N     | 2.78                     | 0.41              |
| 1:B2:34:LEU:HD22  | 1:B2:38:LYS:CE    | 2.43                     | 0.41              |
| 1:B4:6:HIS:HB3    | 1:B4:147:HIS:CG   | 2.55                     | 0.41              |
| 1:CB:104:LEU:HD13 | 1:CC:102:LEU:CD2  | 2.46                     | 0.41              |
| 1:CE:6:HIS:HB3    | 1:CE:147:HIS:CG   | 2.55                     | 0.41              |
| 1:CK:52:VAL:HB    | 1:CK:53:PRO:CD    | 2.51                     | 0.41              |
| 1:CK:76:THR:CG2   | 1:CK:112:PHE:HA   | 2.51                     | 0.41              |
| 1:CL:71:TYR:O     | 1:CL:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:CM:30:LEU:C     | 1:CM:32:GLY:H     | 2.28                     | 0.41              |
| 1:CM:95:VAL:HG12  | 1:CM:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:CN:52:VAL:CG1   | 1:CN:61:ILE:HD12  | 2.35                     | 0.41              |
| 1:CO:64:LYS:HA    | 1:CO:64:LYS:HD3   | 1.85                     | 0.41              |
| 1:CQ:100:ALA:O    | 1:CR:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:CW:95:VAL:HG12  | 1:CW:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:CZ:21:PHE:O     | 1:CZ:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:C4:145:MET:O    | 1:C4:149:SER:HB3  | 2.20                     | 0.41              |
| 1:AA:52:VAL:HB    | 1:AA:53:PRO:CD    | 2.50                     | 0.41              |
| 1:AG:100:ALA:O    | 1:AH:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:AH:95:VAL:HG12  | 1:AH:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:AK:116:THR:O    | 1:AL:85:THR:HB    | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AM:30:LEU:C    | 1:AM:32:GLY:H     | 2.28                     | 0.41              |
| 1:AN:98:GLY:HA2  | 1:AN:102:LEU:HD23 | 2.02                     | 0.41              |
| 1:AR:95:VAL:HG12 | 1:AR:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:AS:6:HIS:HB3   | 1:AS:147:HIS:CG   | 2.55                     | 0.41              |
| 1:AT:65:MET:HE2  | 1:AT:65:MET:HB3   | 1.91                     | 0.41              |
| 1:BB:25:ILE:HG23 | 1:BB:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:BC:95:VAL:HG12 | 1:BC:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:BF:76:THR:CG2  | 1:BF:112:PHE:HA   | 2.51                     | 0.41              |
| 1:BL:100:ALA:O   | 1:BM:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:BT:30:LEU:HA   | 1:BT:77:LEU:HD23  | 2.03                     | 0.41              |
| 1:BT:52:VAL:CB   | 1:BT:53:PRO:CD    | 2.98                     | 0.41              |
| 1:BU:21:PHE:O    | 1:BU:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:BV:25:ILE:HG23 | 1:BV:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:BV:71:TYR:O    | 1:BV:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:BW:34:LEU:HD22 | 1:BW:38:LYS:CE    | 2.43                     | 0.41              |
| 1:BX:98:GLY:HA2  | 1:BX:102:LEU:HD23 | 2.02                     | 0.41              |
| 1:BY:95:VAL:HG12 | 1:BY:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:CC:30:LEU:C    | 1:CC:32:GLY:H     | 2.28                     | 0.41              |
| 1:CF:76:THR:CG2  | 1:CF:112:PHE:HA   | 2.51                     | 0.41              |
| 1:CG:25:ILE:HG23 | 1:CG:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:CH:45:ASN:HD22 | 1:CH:45:ASN:HA    | 1.64                     | 0.41              |
| 1:CH:95:VAL:HG12 | 1:CH:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:CI:98:GLY:HA2  | 1:CI:102:LEU:HD23 | 2.02                     | 0.41              |
| 1:CR:63:LYS:O    | 1:CR:65:MET:N     | 2.53                     | 0.41              |
| 1:CS:6:HIS:HB3   | 1:CS:147:HIS:CG   | 2.55                     | 0.41              |
| 1:CT:14:VAL:HG21 | 1:CT:37:LEU:HD22  | 2.03                     | 0.41              |
| 1:CU:18:VAL:HG22 | 1:CU:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:CU:76:THR:CG2  | 1:CU:112:PHE:HA   | 2.51                     | 0.41              |
| 1:C2:67:ASN:HD22 | 1:C2:67:ASN:HA    | 1.59                     | 0.41              |
| 1:C4:21:PHE:O    | 1:C4:22:ASN:HB2   | 2.19                     | 0.41              |
| 1:C4:95:VAL:HG12 | 1:C4:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:AB:88:TYR:CD2  | 1:AB:88:TYR:C     | 2.97                     | 0.41              |
| 1:AC:129:THR:O   | 1:AC:131:ALA:N    | 2.53                     | 0.41              |
| 1:AE:28:LYS:HG3  | 1:AO:24:PHE:CD1   | 2.56                     | 0.41              |
| 1:AF:21:PHE:O    | 1:AF:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:AF:116:THR:O   | 1:AG:85:THR:HB    | 2.20                     | 0.41              |
| 1:AJ:64:LYS:HA   | 1:AJ:64:LYS:HD3   | 1.85                     | 0.41              |
| 1:AM:129:THR:O   | 1:AM:131:ALA:N    | 2.53                     | 0.41              |
| 1:AP:34:LEU:C    | 1:AP:36:GLY:N     | 2.76                     | 0.41              |
| 1:AU:53:PRO:HD2  | 1:AU:57:GLU:CB    | 2.49                     | 0.41              |
| 1:AV:31:GLY:O    | 1:AV:35:ASP:HB2   | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AW:63:LYS:O     | 1:AW:65:MET:N     | 2.53                     | 0.41              |
| 1:A1:25:ILE:HG23  | 1:A1:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:A3:98:GLY:HA2   | 1:A3:102:LEU:HD23 | 2.02                     | 0.41              |
| 1:BO:30:LEU:HA    | 1:BO:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:BP:21:PHE:O     | 1:BP:22:ASN:HB2   | 2.20                     | 0.41              |
| 1:BR:34:LEU:HD22  | 1:BR:38:LYS:CE    | 2.43                     | 0.41              |
| 1:CB:65:MET:HE2   | 1:CB:65:MET:HB3   | 1.95                     | 0.41              |
| 1:CB:71:TYR:O     | 1:CB:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:CB:83:GLY:HA3   | 2:CB:1001:PO4:O1  | 2.21                     | 0.41              |
| 1:CE:30:LEU:HA    | 1:CE:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:CJ:14:VAL:HG21  | 1:CJ:37:LEU:HD22  | 2.03                     | 0.41              |
| 1:CK:116:THR:O    | 1:CL:85:THR:HB    | 2.20                     | 0.41              |
| 1:CU:34:LEU:C     | 1:CU:36:GLY:N     | 2.76                     | 0.41              |
| 1:CV:71:TYR:O     | 1:CV:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:CX:20:ARG:HD3   | 1:C2:39:ARG:NH2   | 2.35                     | 0.41              |
| 1:C1:100:ALA:O    | 1:C2:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:C2:30:LEU:C     | 1:C2:32:GLY:H     | 2.28                     | 0.41              |
| 1:AA:116:THR:O    | 1:AB:85:THR:HB    | 2.20                     | 0.41              |
| 1:AB:25:ILE:HG23  | 1:AB:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:AB:58:ILE:O     | 1:AB:62:ALA:CB    | 2.69                     | 0.41              |
| 1:AB:83:GLY:HA3   | 2:AB:1001:PO4:O1  | 2.21                     | 0.41              |
| 1:AC:63:LYS:O     | 1:AC:65:MET:N     | 2.53                     | 0.41              |
| 1:AC:95:VAL:HG12  | 1:AC:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:AD:29:LEU:HD11  | 1:AD:134:LYS:HB3  | 2.02                     | 0.41              |
| 1:AE:7:LEU:HD23   | 1:AN:40:HIS:CE1   | 2.56                     | 0.41              |
| 1:AE:30:LEU:HA    | 1:AE:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:AF:76:THR:CG2   | 1:AF:112:PHE:HA   | 2.51                     | 0.41              |
| 1:AG:71:TYR:O     | 1:AG:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:AH:30:LEU:C     | 1:AH:32:GLY:N     | 2.78                     | 0.41              |
| 1:AK:76:THR:CG2   | 1:AK:112:PHE:HA   | 2.51                     | 0.41              |
| 1:AL:100:ALA:O    | 1:AM:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:AL:111:ILE:HD12 | 1:AL:111:ILE:N    | 2.36                     | 0.41              |
| 1:AM:34:LEU:HD22  | 1:AM:38:LYS:CE    | 2.43                     | 0.41              |
| 1:AM:67:ASN:HD22  | 1:AM:67:ASN:HA    | 1.59                     | 0.41              |
| 1:AM:95:VAL:HG12  | 1:AM:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:AQ:25:ILE:HG23  | 1:AQ:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:AQ:70:LYS:HG3   | 1:BU:43:GLU:OE1   | 2.20                     | 0.41              |
| 1:AS:98:GLY:HA2   | 1:AS:102:LEU:HD23 | 2.02                     | 0.41              |
| 1:AT:108:ILE:CG1  | 1:AT:150:LYS:HE3  | 2.42                     | 0.41              |
| 1:AU:30:LEU:C     | 1:AU:32:GLY:H     | 2.29                     | 0.41              |
| 1:AY:14:VAL:HG12  | 1:AY:15:GLY:N     | 2.36                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BB:55:ALA:HA    | 1:BB:58:ILE:HG13  | 2.02                     | 0.41              |
| 1:BB:104:LEU:HD13 | 1:BC:102:LEU:CD2  | 2.46                     | 0.41              |
| 1:BC:45:ASN:HD22  | 1:BC:45:ASN:HA    | 1.64                     | 0.41              |
| 1:BC:63:LYS:O     | 1:BC:65:MET:N     | 2.53                     | 0.41              |
| 1:BF:40:HIS:CE1   | 1:BQ:7:LEU:HD23   | 2.56                     | 0.41              |
| 1:BF:52:VAL:HB    | 1:BF:53:PRO:CD    | 2.50                     | 0.41              |
| 1:BH:30:LEU:C     | 1:BH:32:GLY:H     | 2.28                     | 0.41              |
| 1:BI:88:TYR:CD2   | 1:BI:88:TYR:C     | 2.97                     | 0.41              |
| 1:BJ:30:LEU:HA    | 1:BJ:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:BL:71:TYR:O     | 1:BL:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:BO:65:MET:HE2   | 1:BO:65:MET:HB3   | 1.91                     | 0.41              |
| 1:BR:30:LEU:C     | 1:BR:32:GLY:N     | 2.78                     | 0.41              |
| 1:BU:76:THR:CG2   | 1:BU:112:PHE:HA   | 2.51                     | 0.41              |
| 1:BZ:34:LEU:C     | 1:BZ:36:GLY:N     | 2.76                     | 0.41              |
| 1:BZ:52:VAL:HB    | 1:BZ:53:PRO:CD    | 2.50                     | 0.41              |
| 1:BZ:76:THR:CG2   | 1:BZ:112:PHE:HA   | 2.51                     | 0.41              |
| 1:B1:55:ALA:HB1   | 1:B1:95:VAL:CG2   | 2.40                     | 0.41              |
| 1:B1:100:ALA:O    | 1:B2:56:PHE:CE1   | 2.73                     | 0.41              |
| 1:B2:97:LYS:HE3   | 1:B3:97:LYS:HZ3   | 1.85                     | 0.41              |
| 1:CA:26:THR:HA    | 1:CA:29:LEU:HB3   | 2.03                     | 0.41              |
| 1:CA:52:VAL:HB    | 1:CA:53:PRO:CD    | 2.50                     | 0.41              |
| 1:CA:76:THR:CG2   | 1:CA:112:PHE:HA   | 2.51                     | 0.41              |
| 1:CA:116:THR:O    | 1:CB:85:THR:HB    | 2.20                     | 0.41              |
| 1:CF:52:VAL:HB    | 1:CF:53:PRO:CD    | 2.51                     | 0.41              |
| 1:CH:63:LYS:O     | 1:CH:65:MET:N     | 2.53                     | 0.41              |
| 1:CJ:95:VAL:HG12  | 1:CJ:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:CL:25:ILE:HG23  | 1:CL:127:ALA:HB2  | 2.03                     | 0.41              |
| 1:CL:83:GLY:HA3   | 2:CL:1201:PO4:O1  | 2.21                     | 0.41              |
| 1:CL:129:THR:CG2  | 1:CL:130:LYS:H    | 2.28                     | 0.41              |
| 1:CN:29:LEU:HD11  | 1:CN:134:LYS:HB3  | 2.02                     | 0.41              |
| 1:CO:30:LEU:HA    | 1:CO:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:CP:76:THR:CG2   | 1:CP:112:PHE:HA   | 2.51                     | 0.41              |
| 1:CR:129:THR:O    | 1:CR:131:ALA:N    | 2.53                     | 0.41              |
| 1:CT:6:HIS:HB3    | 1:CT:147:HIS:CG   | 2.55                     | 0.41              |
| 1:CT:30:LEU:HA    | 1:CT:77:LEU:HD23  | 2.02                     | 0.41              |
| 1:CW:129:THR:O    | 1:CW:131:ALA:N    | 2.53                     | 0.41              |
| 1:C2:95:VAL:HG12  | 1:C2:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:C2:129:THR:O    | 1:C2:131:ALA:N    | 2.53                     | 0.41              |
| 1:C3:98:GLY:HA2   | 1:C3:102:LEU:HD23 | 2.02                     | 0.41              |
| 1:AA:58:ILE:N     | 1:AA:59:PRO:CD    | 2.84                     | 0.41              |
| 1:AB:71:TYR:O     | 1:AB:108:ILE:HD13 | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AE:14:VAL:HG21  | 1:AE:37:LEU:HD22  | 2.03                     | 0.41              |
| 1:AF:52:VAL:HB    | 1:AF:53:PRO:CD    | 2.50                     | 0.41              |
| 1:AI:29:LEU:HD11  | 1:AI:134:LYS:HB3  | 2.02                     | 0.41              |
| 1:AJ:14:VAL:HG12  | 1:AJ:15:GLY:N     | 2.36                     | 0.41              |
| 1:AJ:95:VAL:HG12  | 1:AJ:112:PHE:HE1  | 1.85                     | 0.41              |
| 1:AP:26:THR:HA    | 1:AP:29:LEU:HB3   | 2.03                     | 0.41              |
| 1:AQ:71:TYR:O     | 1:AQ:108:ILE:HD13 | 2.21                     | 0.41              |
| 1:AR:30:LEU:C     | 1:AR:32:GLY:N     | 2.78                     | 0.41              |
| 1:AW:83:GLY:HA3   | 2:AW:201:PO4:P    | 2.60                     | 0.41              |
| 1:AY:14:VAL:HG21  | 1:AY:37:LEU:HD22  | 2.03                     | 0.41              |
| 1:AZ:76:THR:CG2   | 1:AZ:112:PHE:HA   | 2.51                     | 0.41              |
| 1:A1:58:ILE:O     | 1:A1:62:ALA:CB    | 2.69                     | 0.41              |
| 1:A1:104:LEU:HD13 | 1:A2:102:LEU:CD2  | 2.46                     | 0.41              |
| 1:BB:83:GLY:HA3   | 2:BB:1001:PO4:O1  | 2.21                     | 0.41              |
| 1:BG:83:GLY:HA3   | 2:BG:1001:PO4:O1  | 2.21                     | 0.41              |
| 1:BG:111:ILE:HD12 | 1:BG:111:ILE:N    | 2.36                     | 0.41              |
| 1:BJ:64:LYS:HD3   | 1:BJ:64:LYS:HA    | 1.85                     | 0.41              |
| 1:BL:55:ALA:HB1   | 1:BL:95:VAL:CG2   | 2.40                     | 0.41              |
| 1:BO:14:VAL:HG12  | 1:BO:15:GLY:N     | 2.36                     | 0.41              |
| 1:BP:18:VAL:HG22  | 1:BP:77:LEU:HB2   | 2.02                     | 0.41              |
| 1:BP:65:MET:HE2   | 1:BP:65:MET:HB3   | 1.80                     | 0.41              |
| 1:BQ:83:GLY:HA3   | 2:BQ:1001:PO4:O1  | 2.21                     | 0.41              |
| 1:BW:83:GLY:HA3   | 2:BW:1001:PO4:O3  | 2.20                     | 0.41              |
| 1:BY:14:VAL:HG12  | 1:BY:15:GLY:N     | 2.36                     | 0.41              |
| 1:B2:95:VAL:HG12  | 1:B2:112:PHE:HE1  | 1.86                     | 0.41              |
| 1:B3:7:LEU:HD12   | 1:B3:7:LEU:HA     | 1.96                     | 0.41              |
| 1:CB:31:GLY:O     | 1:CB:35:ASP:HB2   | 2.20                     | 0.41              |
| 1:CC:39:ARG:NE    | 1:CS:20:ARG:CZ    | 2.84                     | 0.41              |
| 1:CF:26:THR:HA    | 1:CF:29:LEU:HB3   | 2.03                     | 0.41              |
| 1:CF:30:LEU:C     | 1:CF:32:GLY:H     | 2.29                     | 0.41              |
| 1:CG:58:ILE:O     | 1:CG:62:ALA:CB    | 2.69                     | 0.41              |
| 1:CG:129:THR:CG2  | 1:CG:130:LYS:H    | 2.28                     | 0.41              |
| 1:CH:34:LEU:HD22  | 1:CH:38:LYS:CE    | 2.43                     | 0.41              |
| 1:CH:129:THR:O    | 1:CH:131:ALA:N    | 2.53                     | 0.41              |
| 1:CL:55:ALA:CB    | 1:CL:95:VAL:HG21  | 2.40                     | 0.41              |
| 1:CV:31:GLY:O     | 1:CV:35:ASP:HB2   | 2.20                     | 0.41              |
| 1:C1:83:GLY:HA3   | 2:C1:1201:PO4:O1  | 2.21                     | 0.41              |
| 1:C1:129:THR:CG2  | 1:C1:130:LYS:H    | 2.28                     | 0.41              |
| 1:C4:14:VAL:HG12  | 1:C4:15:GLY:N     | 2.36                     | 0.41              |
| 1:AE:14:VAL:HG12  | 1:AE:15:GLY:N     | 2.36                     | 0.40              |
| 1:AK:26:THR:HA    | 1:AK:29:LEU:HB3   | 2.04                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:65:MET:HB3   | 1:AK:65:MET:HE2   | 1.79                     | 0.40              |
| 1:AL:23:GLU:HA    | 1:AL:26:THR:OG1   | 2.21                     | 0.40              |
| 1:AP:76:THR:CG2   | 1:AP:112:PHE:HA   | 2.51                     | 0.40              |
| 1:AQ:83:GLY:HA3   | 2:AQ:1001:PO4:O1  | 2.21                     | 0.40              |
| 1:AV:25:ILE:HG23  | 1:AV:127:ALA:HB2  | 2.03                     | 0.40              |
| 1:AY:30:LEU:HA    | 1:AY:77:LEU:HD23  | 2.02                     | 0.40              |
| 1:A1:23:GLU:HA    | 1:A1:26:THR:OG1   | 2.22                     | 0.40              |
| 1:BB:129:THR:O    | 1:BB:130:LYS:C    | 2.65                     | 0.40              |
| 1:BD:11:GLY:C     | 1:CM:11:GLY:HA3   | 2.46                     | 0.40              |
| 1:BJ:14:VAL:HG12  | 1:BJ:15:GLY:N     | 2.36                     | 0.40              |
| 1:BK:30:LEU:C     | 1:BK:32:GLY:H     | 2.29                     | 0.40              |
| 1:BP:30:LEU:C     | 1:BP:32:GLY:H     | 2.29                     | 0.40              |
| 1:BQ:58:ILE:O     | 1:BQ:62:ALA:CB    | 2.69                     | 0.40              |
| 1:BQ:111:ILE:N    | 1:BQ:111:ILE:HD12 | 2.36                     | 0.40              |
| 1:BW:30:LEU:C     | 1:BW:32:GLY:H     | 2.28                     | 0.40              |
| 1:B1:25:ILE:HG23  | 1:B1:127:ALA:HB2  | 2.03                     | 0.40              |
| 1:B1:83:GLY:HA3   | 2:B1:1001:PO4:O1  | 2.21                     | 0.40              |
| 1:CB:25:ILE:HG23  | 1:CB:127:ALA:HB2  | 2.03                     | 0.40              |
| 1:CD:29:LEU:HD11  | 1:CD:134:LYS:HB3  | 2.02                     | 0.40              |
| 1:CD:98:GLY:HA2   | 1:CD:102:LEU:HD23 | 2.02                     | 0.40              |
| 1:CG:111:ILE:N    | 1:CG:111:ILE:HD12 | 2.37                     | 0.40              |
| 1:CH:28:LYS:HZ3   | 1:CU:28:LYS:CE    | 2.34                     | 0.40              |
| 1:CK:18:VAL:HG22  | 1:CK:77:LEU:HB2   | 2.02                     | 0.40              |
| 1:CL:65:MET:HE2   | 1:CL:65:MET:HB3   | 1.95                     | 0.40              |
| 1:CQ:71:TYR:O     | 1:CQ:108:ILE:HD13 | 2.21                     | 0.40              |
| 1:CZ:7:LEU:HD12   | 1:CZ:7:LEU:HA     | 1.84                     | 0.40              |
| 1:AC:30:LEU:C     | 1:AC:32:GLY:N     | 2.78                     | 0.40              |
| 1:AG:83:GLY:HA3   | 2:AG:1001:PO4:O1  | 2.21                     | 0.40              |
| 1:AO:14:VAL:HG21  | 1:AO:37:LEU:HD22  | 2.03                     | 0.40              |
| 1:AQ:111:ILE:N    | 1:AQ:111:ILE:HD12 | 2.36                     | 0.40              |
| 1:A4:14:VAL:HG12  | 1:A4:15:GLY:N     | 2.36                     | 0.40              |
| 1:BG:58:ILE:O     | 1:BG:62:ALA:CB    | 2.69                     | 0.40              |
| 1:BM:20:ARG:HB3   | 1:BM:20:ARG:HH11  | 1.87                     | 0.40              |
| 1:BR:30:LEU:C     | 1:BR:32:GLY:H     | 2.28                     | 0.40              |
| 1:BW:95:VAL:HG12  | 1:BW:112:PHE:HE1  | 1.86                     | 0.40              |
| 1:BW:148:LEU:HD23 | 1:BW:148:LEU:HA   | 1.80                     | 0.40              |
| 1:B2:63:LYS:O     | 1:B2:65:MET:N     | 2.53                     | 0.40              |
| 1:CF:116:THR:O    | 1:CG:85:THR:HB    | 2.20                     | 0.40              |
| 1:CG:55:ALA:HA    | 1:CG:58:ILE:HG13  | 2.02                     | 0.40              |
| 1:CR:30:LEU:C     | 1:CR:32:GLY:H     | 2.28                     | 0.40              |
| 1:CR:95:VAL:HG12  | 1:CR:112:PHE:HE1  | 1.86                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CV:25:ILE:HG23  | 1:CV:127:ALA:HB2  | 2.03                     | 0.40              |
| 1:CY:14:VAL:HG21  | 1:CY:37:LEU:HD22  | 2.03                     | 0.40              |
| 1:CY:108:ILE:CG1  | 1:CY:150:LYS:HE3  | 2.42                     | 0.40              |
| 1:CZ:76:THR:CG2   | 1:CZ:112:PHE:HA   | 2.51                     | 0.40              |
| 1:C2:34:LEU:C     | 1:C2:36:GLY:N     | 2.77                     | 0.40              |
| 1:AA:30:LEU:C     | 1:AA:32:GLY:H     | 2.29                     | 0.40              |
| 1:AG:58:ILE:O     | 1:AG:62:ALA:CB    | 2.69                     | 0.40              |
| 1:AH:106:THR:HG23 | 1:AH:107:ASP:N    | 2.37                     | 0.40              |
| 1:AK:30:LEU:C     | 1:AK:32:GLY:H     | 2.29                     | 0.40              |
| 1:AK:53:PRO:HD2   | 1:AK:57:GLU:CB    | 2.49                     | 0.40              |
| 1:AL:58:ILE:O     | 1:AL:62:ALA:CB    | 2.69                     | 0.40              |
| 1:AL:71:TYR:O     | 1:AL:108:ILE:HD13 | 2.21                     | 0.40              |
| 1:AM:30:LEU:C     | 1:AM:32:GLY:N     | 2.78                     | 0.40              |
| 1:AO:14:VAL:HG12  | 1:AO:15:GLY:N     | 2.36                     | 0.40              |
| 1:AP:67:ASN:HD22  | 1:AP:67:ASN:HA    | 1.69                     | 0.40              |
| 1:AT:53:PRO:HD2   | 1:AT:57:GLU:CB    | 2.52                     | 0.40              |
| 1:AV:83:GLY:HA3   | 2:AV:1001:PO4:O1  | 2.21                     | 0.40              |
| 1:BB:71:TYR:O     | 1:BB:108:ILE:HD13 | 2.21                     | 0.40              |
| 1:BE:14:VAL:HG12  | 1:BE:15:GLY:N     | 2.36                     | 0.40              |
| 1:BF:28:LYS:HE3   | 1:BR:28:LYS:NZ    | 2.37                     | 0.40              |
| 1:BH:106:THR:HG23 | 1:BH:107:ASP:N    | 2.37                     | 0.40              |
| 1:BL:23:GLU:HA    | 1:BL:26:THR:OG1   | 2.22                     | 0.40              |
| 1:BN:98:GLY:HA2   | 1:BN:102:LEU:HD23 | 2.02                     | 0.40              |
| 1:BV:23:GLU:HA    | 1:BV:26:THR:OG1   | 2.22                     | 0.40              |
| 1:BW:121:GLU:O    | 1:BW:125:GLU:HB2  | 2.22                     | 0.40              |
| 1:B1:58:ILE:O     | 1:B1:62:ALA:CB    | 2.69                     | 0.40              |
| 1:CG:23:GLU:HA    | 1:CG:26:THR:OG1   | 2.22                     | 0.40              |
| 1:CI:7:LEU:HD12   | 1:CI:7:LEU:HA     | 1.96                     | 0.40              |
| 1:CJ:14:VAL:HG12  | 1:CJ:15:GLY:N     | 2.36                     | 0.40              |
| 1:CL:55:ALA:HA    | 1:CL:58:ILE:HG13  | 2.02                     | 0.40              |
| 1:CM:106:THR:HG23 | 1:CM:107:ASP:N    | 2.37                     | 0.40              |
| 1:CO:14:VAL:HG12  | 1:CO:15:GLY:N     | 2.36                     | 0.40              |
| 1:CO:14:VAL:HG21  | 1:CO:37:LEU:HD22  | 2.03                     | 0.40              |
| 1:CP:58:ILE:O     | 1:CP:58:ILE:HG22  | 2.11                     | 0.40              |
| 1:CQ:122:GLN:O    | 1:CQ:126:ARG:HD2  | 2.22                     | 0.40              |
| 1:CZ:58:ILE:N     | 1:CZ:59:PRO:CD    | 2.84                     | 0.40              |
| 1:C1:122:GLN:O    | 1:C1:126:ARG:HD2  | 2.22                     | 0.40              |
| 1:AA:58:ILE:O     | 1:AA:58:ILE:HG22  | 2.11                     | 0.40              |
| 1:AA:76:THR:CG2   | 1:AA:112:PHE:HA   | 2.51                     | 0.40              |
| 1:AB:98:GLY:C     | 1:AB:100:ALA:H    | 2.30                     | 0.40              |
| 1:AB:122:GLN:O    | 1:AB:126:ARG:HD2  | 2.22                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AE:52:VAL:CB    | 1:AE:53:PRO:CD    | 2.98                     | 0.40              |
| 1:AF:58:ILE:N     | 1:AF:59:PRO:CD    | 2.84                     | 0.40              |
| 1:AJ:14:VAL:HG21  | 1:AJ:37:LEU:HD22  | 2.03                     | 0.40              |
| 1:AJ:53:PRO:HD2   | 1:AJ:57:GLU:CB    | 2.52                     | 0.40              |
| 1:AP:30:LEU:C     | 1:AP:32:GLY:H     | 2.29                     | 0.40              |
| 1:AU:151:HIS:CD2  | 1:AU:151:HIS:O    | 2.75                     | 0.40              |
| 1:AW:95:VAL:HG12  | 1:AW:112:PHE:HE1  | 1.86                     | 0.40              |
| 1:AW:106:THR:HG23 | 1:AW:107:ASP:N    | 2.37                     | 0.40              |
| 1:BB:58:ILE:O     | 1:BB:62:ALA:CB    | 2.69                     | 0.40              |
| 1:BF:151:HIS:CD2  | 1:BF:151:HIS:O    | 2.75                     | 0.40              |
| 1:BL:83:GLY:HA3   | 2:BL:1001:PO4:O1  | 2.21                     | 0.40              |
| 1:BN:17:VAL:CG2   | 1:BN:76:THR:HG22  | 2.52                     | 0.40              |
| 1:BQ:98:GLY:C     | 1:BQ:100:ALA:H    | 2.30                     | 0.40              |
| 1:BS:65:MET:C     | 1:BS:67:ASN:H     | 2.30                     | 0.40              |
| 1:BU:26:THR:HA    | 1:BU:29:LEU:HB3   | 2.04                     | 0.40              |
| 1:BY:30:LEU:HA    | 1:BY:77:LEU:HD23  | 2.02                     | 0.40              |
| 1:BY:53:PRO:HD2   | 1:BY:57:GLU:CB    | 2.52                     | 0.40              |
| 1:B1:129:THR:O    | 1:B1:130:LYS:C    | 2.65                     | 0.40              |
| 1:CA:97:LYS:NZ    | 1:CE:97:LYS:HG3   | 2.37                     | 0.40              |
| 1:CB:23:GLU:HA    | 1:CB:26:THR:OG1   | 2.21                     | 0.40              |
| 1:CF:151:HIS:O    | 1:CF:151:HIS:CD2  | 2.75                     | 0.40              |
| 1:CG:83:GLY:HA3   | 2:CG:1201:PO4:O1  | 2.21                     | 0.40              |
| 1:CL:23:GLU:HA    | 1:CL:26:THR:OG1   | 2.21                     | 0.40              |
| 1:CM:34:LEU:HD22  | 1:CM:38:LYS:CE    | 2.43                     | 0.40              |
| 1:CN:98:GLY:HA2   | 1:CN:102:LEU:HD23 | 2.02                     | 0.40              |
| 1:CO:71:TYR:O     | 1:CO:150:LYS:NZ   | 2.44                     | 0.40              |
| 1:CQ:25:ILE:HG23  | 1:CQ:127:ALA:HB2  | 2.03                     | 0.40              |
| 1:C2:121:GLU:O    | 1:C2:125:GLU:HB2  | 2.22                     | 0.40              |
| 1:C3:17:VAL:CG2   | 1:C3:76:THR:HG22  | 2.52                     | 0.40              |
| 1:C4:14:VAL:HG21  | 1:C4:37:LEU:HD22  | 2.03                     | 0.40              |
| 1:AB:104:LEU:HD23 | 1:AC:60:LEU:CD1   | 2.52                     | 0.40              |
| 1:AC:106:THR:HG23 | 1:AC:107:ASP:N    | 2.37                     | 0.40              |
| 1:AE:53:PRO:HD2   | 1:AE:57:GLU:CB    | 2.52                     | 0.40              |
| 1:AF:97:LYS:NZ    | 1:AJ:97:LYS:HG3   | 2.37                     | 0.40              |
| 1:AF:151:HIS:O    | 1:AF:151:HIS:CD2  | 2.75                     | 0.40              |
| 1:AG:122:GLN:O    | 1:AG:126:ARG:HD2  | 2.22                     | 0.40              |
| 1:AP:151:HIS:CD2  | 1:AP:151:HIS:O    | 2.75                     | 0.40              |
| 1:AR:106:THR:HG23 | 1:AR:107:ASP:N    | 2.37                     | 0.40              |
| 1:AT:14:VAL:HG21  | 1:AT:37:LEU:HD22  | 2.03                     | 0.40              |
| 1:AU:26:THR:HA    | 1:AU:29:LEU:HB3   | 2.03                     | 0.40              |
| 1:AU:76:THR:CG2   | 1:AU:112:PHE:HA   | 2.51                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AV:111:ILE:HD12 | 1:AV:111:ILE:N   | 2.36                     | 0.40              |
| 1:AY:53:PRO:HD2   | 1:AY:57:GLU:CB   | 2.52                     | 0.40              |
| 1:BB:23:GLU:HA    | 1:BB:26:THR:OG1  | 2.22                     | 0.40              |
| 1:BF:26:THR:HA    | 1:BF:29:LEU:HB3  | 2.03                     | 0.40              |
| 1:BH:80:VAL:HG12  | 1:BH:88:TYR:CD1  | 2.57                     | 0.40              |
| 1:BK:26:THR:HA    | 1:BK:29:LEU:HB3  | 2.04                     | 0.40              |
| 1:BM:30:LEU:C     | 1:BM:32:GLY:H    | 2.28                     | 0.40              |
| 1:BO:53:PRO:HD2   | 1:BO:57:GLU:CB   | 2.52                     | 0.40              |
| 1:BP:76:THR:CG2   | 1:BP:112:PHE:HA  | 2.51                     | 0.40              |
| 1:BQ:104:LEU:HD23 | 1:BR:60:LEU:CD1  | 2.52                     | 0.40              |
| 1:BS:40:HIS:CE1   | 1:BY:7:LEU:HD23  | 2.57                     | 0.40              |
| 1:BT:64:LYS:HD3   | 1:BT:64:LYS:HA   | 1.85                     | 0.40              |
| 1:BU:58:ILE:N     | 1:BU:59:PRO:CD   | 2.84                     | 0.40              |
| 1:BW:80:VAL:HG12  | 1:BW:88:TYR:CD1  | 2.57                     | 0.40              |
| 1:B2:106:THR:HG23 | 1:B2:107:ASP:N   | 2.37                     | 0.40              |
| 1:B4:30:LEU:HA    | 1:B4:77:LEU:HD23 | 2.02                     | 0.40              |
| 1:CA:28:LYS:NZ    | 1:CN:28:LYS:HZ1  | 2.20                     | 0.40              |
| 1:CB:98:GLY:C     | 1:CB:100:ALA:H   | 2.30                     | 0.40              |
| 1:CD:17:VAL:CG2   | 1:CD:76:THR:HG22 | 2.52                     | 0.40              |
| 1:CE:53:PRO:HD2   | 1:CE:57:GLU:CB   | 2.52                     | 0.40              |
| 1:CH:121:GLU:O    | 1:CH:125:GLU:HB2 | 2.22                     | 0.40              |
| 1:CM:80:VAL:HG12  | 1:CM:88:TYR:CD1  | 2.57                     | 0.40              |
| 1:CN:17:VAL:CG2   | 1:CN:76:THR:HG22 | 2.52                     | 0.40              |
| 1:CT:8:VAL:HG22   | 1:C3:8:VAL:HG13  | 2.01                     | 0.40              |
| 1:CU:129:THR:HB   | 1:CU:130:LYS:H   | 1.75                     | 0.40              |
| 1:CW:121:GLU:O    | 1:CW:125:GLU:HB2 | 2.22                     | 0.40              |
| 1:CX:17:VAL:CG2   | 1:CX:76:THR:HG22 | 2.52                     | 0.40              |
| 1:CY:14:VAL:HG12  | 1:CY:15:GLY:N    | 2.36                     | 0.40              |
| 1:CZ:151:HIS:O    | 1:CZ:151:HIS:CG  | 2.75                     | 0.40              |
| 1:C1:25:ILE:HG23  | 1:C1:127:ALA:HB2 | 2.03                     | 0.40              |
| 1:C2:106:THR:HG23 | 1:C2:107:ASP:N   | 2.37                     | 0.40              |

All (13) 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:AG:153:ALA:O   | 1:AH:46:ASP:OD1[2_565] | 1.84                     | 0.36              |
| 1:AH:69:GLY:O    | 1:AH:69:GLY:O[2_565]   | 1.90                     | 0.30              |
| 1:BJ:151:HIS:CE1 | 1:CY:13:LYS:CE[2_665]  | 1.91                     | 0.29              |
| 1:CB:153:ALA:O   | 1:CC:69:GLY:CA[2_565]  | 1.94                     | 0.26              |

*Continued on next page...*

Continued from previous page...

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:CH:39:ARG:NH2 | 1:CM:20:ARG:NH1[2_665] | 1.96                     | 0.24              |
| 1:BL:11:GLY:O   | 1:CG:153:ALA:C[1_545]  | 1.99                     | 0.21              |
| 1:BL:72:ASP:OD2 | 1:CG:153:ALA:O[1_545]  | 2.03                     | 0.17              |
| 1:CB:153:ALA:O  | 1:CC:69:GLY:N[2_565]   | 2.10                     | 0.10              |
| 1:CZ:24:PHE:CB  | 1:C4:128:GLY:O[2_665]  | 2.12                     | 0.08              |
| 1:BL:72:ASP:OD2 | 1:CG:153:ALA:CB[1_545] | 2.13                     | 0.07              |
| 1:CH:39:ARG:NH2 | 1:CM:20:ARG:NH2[2_665] | 2.17                     | 0.03              |
| 1:AG:153:ALA:CB | 1:AH:46:ASP:OD1[2_565] | 2.18                     | 0.02              |
| 1:CH:39:ARG:NH2 | 1:CM:20:ARG:CZ[2_665]  | 2.19                     | 0.01              |

## 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   | A1    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | A2    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | A3    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | A4    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | AA    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | AB    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | AC    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | AD    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | AE    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | AF    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | AG    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | AH    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | AI    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | AJ    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | AK    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | AL    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | AM    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | AN    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | AO    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | AP    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | AQ    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | AR    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | AS    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | AT    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | AU    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | AV    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | AW    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | AX    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | AY    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | AZ    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | B1    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | B2    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | B3    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | B4    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | BA    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | BB    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | BC    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | BD    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | BE    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | BF    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | BG    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | BH    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | BI    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | BJ    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | BK    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | BL    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | BM    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | BN    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | BO    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | BP    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | BQ    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | BR    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | BS    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | BT    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | BU    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | BV    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | BW    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | BX    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | BY    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | BZ    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | C1    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | C2    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | C3    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | C4    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | CA    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | CB    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | CC    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | CD    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | CE    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | CF    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | CG    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |
| 1   | CH    | 150/153 (98%) | 126 (84%) | 19 (13%) | 5 (3%)   | 3           | 23  |
| 1   | CI    | 150/153 (98%) | 137 (91%) | 11 (7%)  | 2 (1%)   | 9           | 39  |
| 1   | CJ    | 150/153 (98%) | 133 (89%) | 17 (11%) | 0        | 100         | 100 |
| 1   | CK    | 150/153 (98%) | 129 (86%) | 19 (13%) | 2 (1%)   | 9           | 39  |
| 1   | CL    | 150/153 (98%) | 132 (88%) | 18 (12%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 1   | CM    | 150/153 (98%)     | 126 (84%)   | 19 (13%)   | 5 (3%)   | 3           | 23  |
| 1   | CN    | 150/153 (98%)     | 137 (91%)   | 11 (7%)    | 2 (1%)   | 9           | 39  |
| 1   | CO    | 150/153 (98%)     | 133 (89%)   | 17 (11%)   | 0        | 100         | 100 |
| 1   | CP    | 150/153 (98%)     | 129 (86%)   | 19 (13%)   | 2 (1%)   | 9           | 39  |
| 1   | CQ    | 150/153 (98%)     | 132 (88%)   | 18 (12%)   | 0        | 100         | 100 |
| 1   | CR    | 150/153 (98%)     | 126 (84%)   | 19 (13%)   | 5 (3%)   | 3           | 23  |
| 1   | CS    | 150/153 (98%)     | 137 (91%)   | 11 (7%)    | 2 (1%)   | 9           | 39  |
| 1   | CT    | 150/153 (98%)     | 133 (89%)   | 17 (11%)   | 0        | 100         | 100 |
| 1   | CU    | 150/153 (98%)     | 129 (86%)   | 19 (13%)   | 2 (1%)   | 9           | 39  |
| 1   | CV    | 150/153 (98%)     | 132 (88%)   | 18 (12%)   | 0        | 100         | 100 |
| 1   | CW    | 150/153 (98%)     | 126 (84%)   | 19 (13%)   | 5 (3%)   | 3           | 23  |
| 1   | CX    | 150/153 (98%)     | 137 (91%)   | 11 (7%)    | 2 (1%)   | 9           | 39  |
| 1   | CY    | 150/153 (98%)     | 133 (89%)   | 17 (11%)   | 0        | 100         | 100 |
| 1   | CZ    | 150/153 (98%)     | 129 (86%)   | 19 (13%)   | 2 (1%)   | 9           | 39  |
| All | All   | 13500/13770 (98%) | 11826 (88%) | 1512 (11%) | 162 (1%) | 10          | 41  |

All (162) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AC    | 130 | LYS  |
| 1   | AH    | 130 | LYS  |
| 1   | AM    | 130 | LYS  |
| 1   | AR    | 130 | LYS  |
| 1   | AW    | 130 | LYS  |
| 1   | A2    | 130 | LYS  |
| 1   | BC    | 130 | LYS  |
| 1   | BH    | 130 | LYS  |
| 1   | BM    | 130 | LYS  |
| 1   | BR    | 130 | LYS  |
| 1   | BW    | 130 | LYS  |
| 1   | B2    | 130 | LYS  |
| 1   | CC    | 130 | LYS  |
| 1   | CH    | 130 | LYS  |
| 1   | CM    | 130 | LYS  |
| 1   | CR    | 130 | LYS  |
| 1   | CW    | 130 | LYS  |
| 1   | C2    | 130 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 33  | ALA  |
| 1   | AA    | 36  | GLY  |
| 1   | AC    | 64  | LYS  |
| 1   | AF    | 33  | ALA  |
| 1   | AF    | 36  | GLY  |
| 1   | AH    | 64  | LYS  |
| 1   | AK    | 33  | ALA  |
| 1   | AK    | 36  | GLY  |
| 1   | AM    | 64  | LYS  |
| 1   | AP    | 33  | ALA  |
| 1   | AP    | 36  | GLY  |
| 1   | AR    | 64  | LYS  |
| 1   | AU    | 33  | ALA  |
| 1   | AU    | 36  | GLY  |
| 1   | AW    | 64  | LYS  |
| 1   | AZ    | 33  | ALA  |
| 1   | AZ    | 36  | GLY  |
| 1   | A2    | 64  | LYS  |
| 1   | BA    | 33  | ALA  |
| 1   | BA    | 36  | GLY  |
| 1   | BC    | 64  | LYS  |
| 1   | BF    | 33  | ALA  |
| 1   | BF    | 36  | GLY  |
| 1   | BH    | 64  | LYS  |
| 1   | BK    | 33  | ALA  |
| 1   | BK    | 36  | GLY  |
| 1   | BM    | 64  | LYS  |
| 1   | BP    | 33  | ALA  |
| 1   | BP    | 36  | GLY  |
| 1   | BR    | 64  | LYS  |
| 1   | BU    | 33  | ALA  |
| 1   | BU    | 36  | GLY  |
| 1   | BW    | 64  | LYS  |
| 1   | BZ    | 33  | ALA  |
| 1   | BZ    | 36  | GLY  |
| 1   | B2    | 64  | LYS  |
| 1   | CA    | 33  | ALA  |
| 1   | CA    | 36  | GLY  |
| 1   | CC    | 64  | LYS  |
| 1   | CF    | 33  | ALA  |
| 1   | CF    | 36  | GLY  |
| 1   | CH    | 64  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CK    | 33  | ALA  |
| 1   | CK    | 36  | GLY  |
| 1   | CM    | 64  | LYS  |
| 1   | CP    | 33  | ALA  |
| 1   | CP    | 36  | GLY  |
| 1   | CR    | 64  | LYS  |
| 1   | CU    | 33  | ALA  |
| 1   | CU    | 36  | GLY  |
| 1   | CW    | 64  | LYS  |
| 1   | CZ    | 33  | ALA  |
| 1   | CZ    | 36  | GLY  |
| 1   | C2    | 64  | LYS  |
| 1   | AD    | 53  | PRO  |
| 1   | AI    | 53  | PRO  |
| 1   | AN    | 53  | PRO  |
| 1   | AS    | 53  | PRO  |
| 1   | AX    | 53  | PRO  |
| 1   | A3    | 53  | PRO  |
| 1   | BD    | 53  | PRO  |
| 1   | BI    | 53  | PRO  |
| 1   | BN    | 53  | PRO  |
| 1   | BS    | 53  | PRO  |
| 1   | BX    | 53  | PRO  |
| 1   | B3    | 53  | PRO  |
| 1   | CD    | 53  | PRO  |
| 1   | CI    | 53  | PRO  |
| 1   | CN    | 53  | PRO  |
| 1   | CS    | 53  | PRO  |
| 1   | CX    | 53  | PRO  |
| 1   | C3    | 53  | PRO  |
| 1   | AC    | 36  | GLY  |
| 1   | AC    | 53  | PRO  |
| 1   | AH    | 36  | GLY  |
| 1   | AH    | 53  | PRO  |
| 1   | AM    | 36  | GLY  |
| 1   | AM    | 53  | PRO  |
| 1   | AR    | 36  | GLY  |
| 1   | AR    | 53  | PRO  |
| 1   | AW    | 36  | GLY  |
| 1   | AW    | 53  | PRO  |
| 1   | A2    | 36  | GLY  |
| 1   | A2    | 53  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BC    | 36  | GLY  |
| 1   | BC    | 53  | PRO  |
| 1   | BH    | 36  | GLY  |
| 1   | BH    | 53  | PRO  |
| 1   | BM    | 36  | GLY  |
| 1   | BM    | 53  | PRO  |
| 1   | BR    | 36  | GLY  |
| 1   | BR    | 53  | PRO  |
| 1   | BW    | 36  | GLY  |
| 1   | BW    | 53  | PRO  |
| 1   | B2    | 36  | GLY  |
| 1   | B2    | 53  | PRO  |
| 1   | CC    | 36  | GLY  |
| 1   | CC    | 53  | PRO  |
| 1   | CH    | 36  | GLY  |
| 1   | CH    | 53  | PRO  |
| 1   | CM    | 36  | GLY  |
| 1   | CM    | 53  | PRO  |
| 1   | CR    | 36  | GLY  |
| 1   | CR    | 53  | PRO  |
| 1   | CW    | 36  | GLY  |
| 1   | CW    | 53  | PRO  |
| 1   | C2    | 36  | GLY  |
| 1   | C2    | 53  | PRO  |
| 1   | AD    | 130 | LYS  |
| 1   | AI    | 130 | LYS  |
| 1   | AN    | 130 | LYS  |
| 1   | AS    | 130 | LYS  |
| 1   | AX    | 130 | LYS  |
| 1   | A3    | 130 | LYS  |
| 1   | BD    | 130 | LYS  |
| 1   | BI    | 130 | LYS  |
| 1   | BN    | 130 | LYS  |
| 1   | BS    | 130 | LYS  |
| 1   | BX    | 130 | LYS  |
| 1   | B3    | 130 | LYS  |
| 1   | CD    | 130 | LYS  |
| 1   | CI    | 130 | LYS  |
| 1   | CN    | 130 | LYS  |
| 1   | CS    | 130 | LYS  |
| 1   | CX    | 130 | LYS  |
| 1   | C3    | 130 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AC    | 69  | GLY  |
| 1   | AH    | 69  | GLY  |
| 1   | AM    | 69  | GLY  |
| 1   | AR    | 69  | GLY  |
| 1   | AW    | 69  | GLY  |
| 1   | A2    | 69  | GLY  |
| 1   | BC    | 69  | GLY  |
| 1   | BH    | 69  | GLY  |
| 1   | BM    | 69  | GLY  |
| 1   | BR    | 69  | GLY  |
| 1   | BW    | 69  | GLY  |
| 1   | B2    | 69  | GLY  |
| 1   | CC    | 69  | GLY  |
| 1   | CH    | 69  | GLY  |
| 1   | CM    | 69  | GLY  |
| 1   | CR    | 69  | GLY  |
| 1   | CW    | 69  | GLY  |
| 1   | C2    | 69  | 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   | A1    | 115/118 (98%) | 102 (89%) | 13 (11%) | 5           | 25 |
| 1   | A2    | 116/118 (98%) | 112 (97%) | 4 (3%)   | 32          | 57 |
| 1   | A3    | 116/118 (98%) | 108 (93%) | 8 (7%)   | 14          | 39 |
| 1   | A4    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 17          | 44 |
| 1   | AA    | 115/118 (98%) | 111 (96%) | 4 (4%)   | 32          | 57 |
| 1   | AB    | 115/118 (98%) | 102 (89%) | 13 (11%) | 5           | 25 |
| 1   | AC    | 116/118 (98%) | 112 (97%) | 4 (3%)   | 32          | 57 |
| 1   | AD    | 116/118 (98%) | 108 (93%) | 8 (7%)   | 14          | 39 |
| 1   | AE    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 17          | 44 |
| 1   | AF    | 115/118 (98%) | 111 (96%) | 4 (4%)   | 32          | 57 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | AG    | 115/118 (98%) | 102 (89%) | 13 (11%) | 5           | 25 |
| 1   | AH    | 116/118 (98%) | 112 (97%) | 4 (3%)   | 32          | 57 |
| 1   | AI    | 116/118 (98%) | 108 (93%) | 8 (7%)   | 14          | 39 |
| 1   | AJ    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 17          | 44 |
| 1   | AK    | 115/118 (98%) | 111 (96%) | 4 (4%)   | 32          | 57 |
| 1   | AL    | 115/118 (98%) | 102 (89%) | 13 (11%) | 5           | 25 |
| 1   | AM    | 116/118 (98%) | 112 (97%) | 4 (3%)   | 32          | 57 |
| 1   | AN    | 116/118 (98%) | 108 (93%) | 8 (7%)   | 14          | 39 |
| 1   | AO    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 17          | 44 |
| 1   | AP    | 115/118 (98%) | 111 (96%) | 4 (4%)   | 32          | 57 |
| 1   | AQ    | 115/118 (98%) | 102 (89%) | 13 (11%) | 5           | 25 |
| 1   | AR    | 116/118 (98%) | 112 (97%) | 4 (3%)   | 32          | 57 |
| 1   | AS    | 116/118 (98%) | 108 (93%) | 8 (7%)   | 14          | 39 |
| 1   | AT    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 17          | 44 |
| 1   | AU    | 115/118 (98%) | 111 (96%) | 4 (4%)   | 32          | 57 |
| 1   | AV    | 115/118 (98%) | 102 (89%) | 13 (11%) | 5           | 25 |
| 1   | AW    | 116/118 (98%) | 112 (97%) | 4 (3%)   | 32          | 57 |
| 1   | AX    | 116/118 (98%) | 108 (93%) | 8 (7%)   | 14          | 39 |
| 1   | AY    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 17          | 44 |
| 1   | AZ    | 115/118 (98%) | 111 (96%) | 4 (4%)   | 32          | 57 |
| 1   | B1    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | B2    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | B3    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | B4    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | BA    | 117/118 (99%) | 112 (96%) | 5 (4%)   | 26          | 51 |
| 1   | BB    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | BC    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BD    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | BE    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | BF    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BG    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | BH    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BI    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | BJ    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | BK    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BL    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | BM    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BN    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | BO    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | BP    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BQ    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | BR    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BS    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | BT    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | BU    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BV    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | BW    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | BX    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | BY    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | BZ    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | C1    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | C2    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | C3    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | C4    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | CA    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | CB    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | CC    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | CD    | 117/118 (99%) | 109 (93%) | 8 (7%)   | 14          | 40 |
| 1   | CE    | 117/118 (99%) | 110 (94%) | 7 (6%)   | 17          | 44 |
| 1   | CF    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |
| 1   | CG    | 117/118 (99%) | 104 (89%) | 13 (11%) | 6           | 25 |
| 1   | CH    | 117/118 (99%) | 113 (97%) | 4 (3%)   | 32          | 57 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-------------------|------------|----------|-------------|----|
| 1   | CI    | 117/118 (99%)     | 109 (93%)  | 8 (7%)   | 14          | 40 |
| 1   | CJ    | 117/118 (99%)     | 110 (94%)  | 7 (6%)   | 17          | 44 |
| 1   | CK    | 117/118 (99%)     | 113 (97%)  | 4 (3%)   | 32          | 57 |
| 1   | CL    | 117/118 (99%)     | 104 (89%)  | 13 (11%) | 6           | 25 |
| 1   | CM    | 117/118 (99%)     | 113 (97%)  | 4 (3%)   | 32          | 57 |
| 1   | CN    | 117/118 (99%)     | 109 (93%)  | 8 (7%)   | 14          | 40 |
| 1   | CO    | 117/118 (99%)     | 110 (94%)  | 7 (6%)   | 17          | 44 |
| 1   | CP    | 117/118 (99%)     | 113 (97%)  | 4 (3%)   | 32          | 57 |
| 1   | CQ    | 117/118 (99%)     | 104 (89%)  | 13 (11%) | 6           | 25 |
| 1   | CR    | 117/118 (99%)     | 113 (97%)  | 4 (3%)   | 32          | 57 |
| 1   | CS    | 117/118 (99%)     | 109 (93%)  | 8 (7%)   | 14          | 40 |
| 1   | CT    | 117/118 (99%)     | 110 (94%)  | 7 (6%)   | 17          | 44 |
| 1   | CU    | 117/118 (99%)     | 113 (97%)  | 4 (3%)   | 32          | 57 |
| 1   | CV    | 117/118 (99%)     | 104 (89%)  | 13 (11%) | 6           | 25 |
| 1   | CW    | 117/118 (99%)     | 113 (97%)  | 4 (3%)   | 32          | 57 |
| 1   | CX    | 117/118 (99%)     | 109 (93%)  | 8 (7%)   | 14          | 40 |
| 1   | CY    | 117/118 (99%)     | 110 (94%)  | 7 (6%)   | 17          | 44 |
| 1   | CZ    | 117/118 (99%)     | 113 (97%)  | 4 (3%)   | 32          | 57 |
| All | All   | 10488/10620 (99%) | 9839 (94%) | 649 (6%) | 16          | 43 |

All (649) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 116 | THR  |
| 1   | AA    | 130 | LYS  |
| 1   | AA    | 147 | HIS  |
| 1   | AA    | 150 | LYS  |
| 1   | AB    | 13  | LYS  |
| 1   | AB    | 34  | LEU  |
| 1   | AB    | 42  | VAL  |
| 1   | AB    | 43  | GLU  |
| 1   | AB    | 77  | LEU  |
| 1   | AB    | 102 | LEU  |
| 1   | AB    | 103 | SER  |
| 1   | AB    | 104 | LEU  |
| 1   | AB    | 106 | THR  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 108 | ILE  |
| 1   | AB    | 109 | PRO  |
| 1   | AB    | 116 | THR  |
| 1   | AB    | 152 | TRP  |
| 1   | AC    | 45  | ASN  |
| 1   | AC    | 67  | ASN  |
| 1   | AC    | 82  | ARG  |
| 1   | AC    | 109 | PRO  |
| 1   | AD    | 67  | ASN  |
| 1   | AD    | 77  | LEU  |
| 1   | AD    | 106 | THR  |
| 1   | AD    | 109 | PRO  |
| 1   | AD    | 116 | THR  |
| 1   | AD    | 129 | THR  |
| 1   | AD    | 130 | LYS  |
| 1   | AD    | 152 | TRP  |
| 1   | AE    | 77  | LEU  |
| 1   | AE    | 88  | TYR  |
| 1   | AE    | 107 | ASP  |
| 1   | AE    | 116 | THR  |
| 1   | AE    | 129 | THR  |
| 1   | AE    | 149 | SER  |
| 1   | AE    | 152 | TRP  |
| 1   | AF    | 116 | THR  |
| 1   | AF    | 130 | LYS  |
| 1   | AF    | 147 | HIS  |
| 1   | AF    | 150 | LYS  |
| 1   | AG    | 13  | LYS  |
| 1   | AG    | 34  | LEU  |
| 1   | AG    | 42  | VAL  |
| 1   | AG    | 43  | GLU  |
| 1   | AG    | 77  | LEU  |
| 1   | AG    | 102 | LEU  |
| 1   | AG    | 103 | SER  |
| 1   | AG    | 104 | LEU  |
| 1   | AG    | 106 | THR  |
| 1   | AG    | 108 | ILE  |
| 1   | AG    | 109 | PRO  |
| 1   | AG    | 116 | THR  |
| 1   | AG    | 152 | TRP  |
| 1   | AH    | 45  | ASN  |
| 1   | AH    | 67  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AH    | 82  | ARG  |
| 1   | AH    | 109 | PRO  |
| 1   | AI    | 67  | ASN  |
| 1   | AI    | 77  | LEU  |
| 1   | AI    | 106 | THR  |
| 1   | AI    | 109 | PRO  |
| 1   | AI    | 116 | THR  |
| 1   | AI    | 129 | THR  |
| 1   | AI    | 130 | LYS  |
| 1   | AI    | 152 | TRP  |
| 1   | AJ    | 77  | LEU  |
| 1   | AJ    | 88  | TYR  |
| 1   | AJ    | 107 | ASP  |
| 1   | AJ    | 116 | THR  |
| 1   | AJ    | 129 | THR  |
| 1   | AJ    | 149 | SER  |
| 1   | AJ    | 152 | TRP  |
| 1   | AK    | 116 | THR  |
| 1   | AK    | 130 | LYS  |
| 1   | AK    | 147 | HIS  |
| 1   | AK    | 150 | LYS  |
| 1   | AL    | 13  | LYS  |
| 1   | AL    | 34  | LEU  |
| 1   | AL    | 42  | VAL  |
| 1   | AL    | 43  | GLU  |
| 1   | AL    | 77  | LEU  |
| 1   | AL    | 102 | LEU  |
| 1   | AL    | 103 | SER  |
| 1   | AL    | 104 | LEU  |
| 1   | AL    | 106 | THR  |
| 1   | AL    | 108 | ILE  |
| 1   | AL    | 109 | PRO  |
| 1   | AL    | 116 | THR  |
| 1   | AL    | 152 | TRP  |
| 1   | AM    | 45  | ASN  |
| 1   | AM    | 67  | ASN  |
| 1   | AM    | 82  | ARG  |
| 1   | AM    | 109 | PRO  |
| 1   | AN    | 67  | ASN  |
| 1   | AN    | 77  | LEU  |
| 1   | AN    | 106 | THR  |
| 1   | AN    | 109 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AN    | 116 | THR  |
| 1   | AN    | 129 | THR  |
| 1   | AN    | 130 | LYS  |
| 1   | AN    | 152 | TRP  |
| 1   | AO    | 77  | LEU  |
| 1   | AO    | 88  | TYR  |
| 1   | AO    | 107 | ASP  |
| 1   | AO    | 116 | THR  |
| 1   | AO    | 129 | THR  |
| 1   | AO    | 149 | SER  |
| 1   | AO    | 152 | TRP  |
| 1   | AP    | 116 | THR  |
| 1   | AP    | 130 | LYS  |
| 1   | AP    | 147 | HIS  |
| 1   | AP    | 150 | LYS  |
| 1   | AQ    | 13  | LYS  |
| 1   | AQ    | 34  | LEU  |
| 1   | AQ    | 42  | VAL  |
| 1   | AQ    | 43  | GLU  |
| 1   | AQ    | 77  | LEU  |
| 1   | AQ    | 102 | LEU  |
| 1   | AQ    | 103 | SER  |
| 1   | AQ    | 104 | LEU  |
| 1   | AQ    | 106 | THR  |
| 1   | AQ    | 108 | ILE  |
| 1   | AQ    | 109 | PRO  |
| 1   | AQ    | 116 | THR  |
| 1   | AQ    | 152 | TRP  |
| 1   | AR    | 45  | ASN  |
| 1   | AR    | 67  | ASN  |
| 1   | AR    | 82  | ARG  |
| 1   | AR    | 109 | PRO  |
| 1   | AS    | 67  | ASN  |
| 1   | AS    | 77  | LEU  |
| 1   | AS    | 106 | THR  |
| 1   | AS    | 109 | PRO  |
| 1   | AS    | 116 | THR  |
| 1   | AS    | 129 | THR  |
| 1   | AS    | 130 | LYS  |
| 1   | AS    | 152 | TRP  |
| 1   | AT    | 77  | LEU  |
| 1   | AT    | 88  | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AT    | 107 | ASP  |
| 1   | AT    | 116 | THR  |
| 1   | AT    | 129 | THR  |
| 1   | AT    | 149 | SER  |
| 1   | AT    | 152 | TRP  |
| 1   | AU    | 116 | THR  |
| 1   | AU    | 130 | LYS  |
| 1   | AU    | 147 | HIS  |
| 1   | AU    | 150 | LYS  |
| 1   | AV    | 13  | LYS  |
| 1   | AV    | 34  | LEU  |
| 1   | AV    | 42  | VAL  |
| 1   | AV    | 43  | GLU  |
| 1   | AV    | 77  | LEU  |
| 1   | AV    | 102 | LEU  |
| 1   | AV    | 103 | SER  |
| 1   | AV    | 104 | LEU  |
| 1   | AV    | 106 | THR  |
| 1   | AV    | 108 | ILE  |
| 1   | AV    | 109 | PRO  |
| 1   | AV    | 116 | THR  |
| 1   | AV    | 152 | TRP  |
| 1   | AW    | 45  | ASN  |
| 1   | AW    | 67  | ASN  |
| 1   | AW    | 82  | ARG  |
| 1   | AW    | 109 | PRO  |
| 1   | AX    | 67  | ASN  |
| 1   | AX    | 77  | LEU  |
| 1   | AX    | 106 | THR  |
| 1   | AX    | 109 | PRO  |
| 1   | AX    | 116 | THR  |
| 1   | AX    | 129 | THR  |
| 1   | AX    | 130 | LYS  |
| 1   | AX    | 152 | TRP  |
| 1   | AY    | 77  | LEU  |
| 1   | AY    | 88  | TYR  |
| 1   | AY    | 107 | ASP  |
| 1   | AY    | 116 | THR  |
| 1   | AY    | 129 | THR  |
| 1   | AY    | 149 | SER  |
| 1   | AY    | 152 | TRP  |
| 1   | AZ    | 116 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AZ    | 130 | LYS  |
| 1   | AZ    | 147 | HIS  |
| 1   | AZ    | 150 | LYS  |
| 1   | A1    | 13  | LYS  |
| 1   | A1    | 34  | LEU  |
| 1   | A1    | 42  | VAL  |
| 1   | A1    | 43  | GLU  |
| 1   | A1    | 77  | LEU  |
| 1   | A1    | 102 | LEU  |
| 1   | A1    | 103 | SER  |
| 1   | A1    | 104 | LEU  |
| 1   | A1    | 106 | THR  |
| 1   | A1    | 108 | ILE  |
| 1   | A1    | 109 | PRO  |
| 1   | A1    | 116 | THR  |
| 1   | A1    | 152 | TRP  |
| 1   | A2    | 45  | ASN  |
| 1   | A2    | 67  | ASN  |
| 1   | A2    | 82  | ARG  |
| 1   | A2    | 109 | PRO  |
| 1   | A3    | 67  | ASN  |
| 1   | A3    | 77  | LEU  |
| 1   | A3    | 106 | THR  |
| 1   | A3    | 109 | PRO  |
| 1   | A3    | 116 | THR  |
| 1   | A3    | 129 | THR  |
| 1   | A3    | 130 | LYS  |
| 1   | A3    | 152 | TRP  |
| 1   | A4    | 77  | LEU  |
| 1   | A4    | 88  | TYR  |
| 1   | A4    | 107 | ASP  |
| 1   | A4    | 116 | THR  |
| 1   | A4    | 129 | THR  |
| 1   | A4    | 149 | SER  |
| 1   | A4    | 152 | TRP  |
| 1   | BA    | 6   | HIS  |
| 1   | BA    | 116 | THR  |
| 1   | BA    | 130 | LYS  |
| 1   | BA    | 147 | HIS  |
| 1   | BA    | 150 | LYS  |
| 1   | BB    | 13  | LYS  |
| 1   | BB    | 34  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BB    | 42  | VAL  |
| 1   | BB    | 43  | GLU  |
| 1   | BB    | 77  | LEU  |
| 1   | BB    | 102 | LEU  |
| 1   | BB    | 103 | SER  |
| 1   | BB    | 104 | LEU  |
| 1   | BB    | 106 | THR  |
| 1   | BB    | 108 | ILE  |
| 1   | BB    | 109 | PRO  |
| 1   | BB    | 116 | THR  |
| 1   | BB    | 152 | TRP  |
| 1   | BC    | 45  | ASN  |
| 1   | BC    | 67  | ASN  |
| 1   | BC    | 82  | ARG  |
| 1   | BC    | 109 | PRO  |
| 1   | BD    | 67  | ASN  |
| 1   | BD    | 77  | LEU  |
| 1   | BD    | 106 | THR  |
| 1   | BD    | 109 | PRO  |
| 1   | BD    | 116 | THR  |
| 1   | BD    | 129 | THR  |
| 1   | BD    | 130 | LYS  |
| 1   | BD    | 152 | TRP  |
| 1   | BE    | 77  | LEU  |
| 1   | BE    | 88  | TYR  |
| 1   | BE    | 107 | ASP  |
| 1   | BE    | 116 | THR  |
| 1   | BE    | 129 | THR  |
| 1   | BE    | 149 | SER  |
| 1   | BE    | 152 | TRP  |
| 1   | BF    | 116 | THR  |
| 1   | BF    | 130 | LYS  |
| 1   | BF    | 147 | HIS  |
| 1   | BF    | 150 | LYS  |
| 1   | BG    | 13  | LYS  |
| 1   | BG    | 34  | LEU  |
| 1   | BG    | 42  | VAL  |
| 1   | BG    | 43  | GLU  |
| 1   | BG    | 77  | LEU  |
| 1   | BG    | 102 | LEU  |
| 1   | BG    | 103 | SER  |
| 1   | BG    | 104 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BG    | 106 | THR  |
| 1   | BG    | 108 | ILE  |
| 1   | BG    | 109 | PRO  |
| 1   | BG    | 116 | THR  |
| 1   | BG    | 152 | TRP  |
| 1   | BH    | 45  | ASN  |
| 1   | BH    | 67  | ASN  |
| 1   | BH    | 82  | ARG  |
| 1   | BH    | 109 | PRO  |
| 1   | BI    | 67  | ASN  |
| 1   | BI    | 77  | LEU  |
| 1   | BI    | 106 | THR  |
| 1   | BI    | 109 | PRO  |
| 1   | BI    | 116 | THR  |
| 1   | BI    | 129 | THR  |
| 1   | BI    | 130 | LYS  |
| 1   | BI    | 152 | TRP  |
| 1   | BJ    | 77  | LEU  |
| 1   | BJ    | 88  | TYR  |
| 1   | BJ    | 107 | ASP  |
| 1   | BJ    | 116 | THR  |
| 1   | BJ    | 129 | THR  |
| 1   | BJ    | 149 | SER  |
| 1   | BJ    | 152 | TRP  |
| 1   | BK    | 116 | THR  |
| 1   | BK    | 130 | LYS  |
| 1   | BK    | 147 | HIS  |
| 1   | BK    | 150 | LYS  |
| 1   | BL    | 13  | LYS  |
| 1   | BL    | 34  | LEU  |
| 1   | BL    | 42  | VAL  |
| 1   | BL    | 43  | GLU  |
| 1   | BL    | 77  | LEU  |
| 1   | BL    | 102 | LEU  |
| 1   | BL    | 103 | SER  |
| 1   | BL    | 104 | LEU  |
| 1   | BL    | 106 | THR  |
| 1   | BL    | 108 | ILE  |
| 1   | BL    | 109 | PRO  |
| 1   | BL    | 116 | THR  |
| 1   | BL    | 152 | TRP  |
| 1   | BM    | 45  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BM    | 67  | ASN  |
| 1   | BM    | 82  | ARG  |
| 1   | BM    | 109 | PRO  |
| 1   | BN    | 67  | ASN  |
| 1   | BN    | 77  | LEU  |
| 1   | BN    | 106 | THR  |
| 1   | BN    | 109 | PRO  |
| 1   | BN    | 116 | THR  |
| 1   | BN    | 129 | THR  |
| 1   | BN    | 130 | LYS  |
| 1   | BN    | 152 | TRP  |
| 1   | BO    | 77  | LEU  |
| 1   | BO    | 88  | TYR  |
| 1   | BO    | 107 | ASP  |
| 1   | BO    | 116 | THR  |
| 1   | BO    | 129 | THR  |
| 1   | BO    | 149 | SER  |
| 1   | BO    | 152 | TRP  |
| 1   | BP    | 116 | THR  |
| 1   | BP    | 130 | LYS  |
| 1   | BP    | 147 | HIS  |
| 1   | BP    | 150 | LYS  |
| 1   | BQ    | 13  | LYS  |
| 1   | BQ    | 34  | LEU  |
| 1   | BQ    | 42  | VAL  |
| 1   | BQ    | 43  | GLU  |
| 1   | BQ    | 77  | LEU  |
| 1   | BQ    | 102 | LEU  |
| 1   | BQ    | 103 | SER  |
| 1   | BQ    | 104 | LEU  |
| 1   | BQ    | 106 | THR  |
| 1   | BQ    | 108 | ILE  |
| 1   | BQ    | 109 | PRO  |
| 1   | BQ    | 116 | THR  |
| 1   | BQ    | 152 | TRP  |
| 1   | BR    | 45  | ASN  |
| 1   | BR    | 67  | ASN  |
| 1   | BR    | 82  | ARG  |
| 1   | BR    | 109 | PRO  |
| 1   | BS    | 67  | ASN  |
| 1   | BS    | 77  | LEU  |
| 1   | BS    | 106 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BS    | 109 | PRO  |
| 1   | BS    | 116 | THR  |
| 1   | BS    | 129 | THR  |
| 1   | BS    | 130 | LYS  |
| 1   | BS    | 152 | TRP  |
| 1   | BT    | 77  | LEU  |
| 1   | BT    | 88  | TYR  |
| 1   | BT    | 107 | ASP  |
| 1   | BT    | 116 | THR  |
| 1   | BT    | 129 | THR  |
| 1   | BT    | 149 | SER  |
| 1   | BT    | 152 | TRP  |
| 1   | BU    | 116 | THR  |
| 1   | BU    | 130 | LYS  |
| 1   | BU    | 147 | HIS  |
| 1   | BU    | 150 | LYS  |
| 1   | BV    | 13  | LYS  |
| 1   | BV    | 34  | LEU  |
| 1   | BV    | 42  | VAL  |
| 1   | BV    | 43  | GLU  |
| 1   | BV    | 77  | LEU  |
| 1   | BV    | 102 | LEU  |
| 1   | BV    | 103 | SER  |
| 1   | BV    | 104 | LEU  |
| 1   | BV    | 106 | THR  |
| 1   | BV    | 108 | ILE  |
| 1   | BV    | 109 | PRO  |
| 1   | BV    | 116 | THR  |
| 1   | BV    | 152 | TRP  |
| 1   | BW    | 45  | ASN  |
| 1   | BW    | 67  | ASN  |
| 1   | BW    | 82  | ARG  |
| 1   | BW    | 109 | PRO  |
| 1   | BX    | 67  | ASN  |
| 1   | BX    | 77  | LEU  |
| 1   | BX    | 106 | THR  |
| 1   | BX    | 109 | PRO  |
| 1   | BX    | 116 | THR  |
| 1   | BX    | 129 | THR  |
| 1   | BX    | 130 | LYS  |
| 1   | BX    | 152 | TRP  |
| 1   | BY    | 77  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BY    | 88  | TYR  |
| 1   | BY    | 107 | ASP  |
| 1   | BY    | 116 | THR  |
| 1   | BY    | 129 | THR  |
| 1   | BY    | 149 | SER  |
| 1   | BY    | 152 | TRP  |
| 1   | BZ    | 116 | THR  |
| 1   | BZ    | 130 | LYS  |
| 1   | BZ    | 147 | HIS  |
| 1   | BZ    | 150 | LYS  |
| 1   | B1    | 13  | LYS  |
| 1   | B1    | 34  | LEU  |
| 1   | B1    | 42  | VAL  |
| 1   | B1    | 43  | GLU  |
| 1   | B1    | 77  | LEU  |
| 1   | B1    | 102 | LEU  |
| 1   | B1    | 103 | SER  |
| 1   | B1    | 104 | LEU  |
| 1   | B1    | 106 | THR  |
| 1   | B1    | 108 | ILE  |
| 1   | B1    | 109 | PRO  |
| 1   | B1    | 116 | THR  |
| 1   | B1    | 152 | TRP  |
| 1   | B2    | 45  | ASN  |
| 1   | B2    | 67  | ASN  |
| 1   | B2    | 82  | ARG  |
| 1   | B2    | 109 | PRO  |
| 1   | B3    | 67  | ASN  |
| 1   | B3    | 77  | LEU  |
| 1   | B3    | 106 | THR  |
| 1   | B3    | 109 | PRO  |
| 1   | B3    | 116 | THR  |
| 1   | B3    | 129 | THR  |
| 1   | B3    | 130 | LYS  |
| 1   | B3    | 152 | TRP  |
| 1   | B4    | 77  | LEU  |
| 1   | B4    | 88  | TYR  |
| 1   | B4    | 107 | ASP  |
| 1   | B4    | 116 | THR  |
| 1   | B4    | 129 | THR  |
| 1   | B4    | 149 | SER  |
| 1   | B4    | 152 | TRP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 116 | THR  |
| 1   | CA    | 130 | LYS  |
| 1   | CA    | 147 | HIS  |
| 1   | CA    | 150 | LYS  |
| 1   | CB    | 13  | LYS  |
| 1   | CB    | 34  | LEU  |
| 1   | CB    | 42  | VAL  |
| 1   | CB    | 43  | GLU  |
| 1   | CB    | 77  | LEU  |
| 1   | CB    | 102 | LEU  |
| 1   | CB    | 103 | SER  |
| 1   | CB    | 104 | LEU  |
| 1   | CB    | 106 | THR  |
| 1   | CB    | 108 | ILE  |
| 1   | CB    | 109 | PRO  |
| 1   | CB    | 116 | THR  |
| 1   | CB    | 152 | TRP  |
| 1   | CC    | 45  | ASN  |
| 1   | CC    | 67  | ASN  |
| 1   | CC    | 82  | ARG  |
| 1   | CC    | 109 | PRO  |
| 1   | CD    | 67  | ASN  |
| 1   | CD    | 77  | LEU  |
| 1   | CD    | 106 | THR  |
| 1   | CD    | 109 | PRO  |
| 1   | CD    | 116 | THR  |
| 1   | CD    | 129 | THR  |
| 1   | CD    | 130 | LYS  |
| 1   | CD    | 152 | TRP  |
| 1   | CE    | 77  | LEU  |
| 1   | CE    | 88  | TYR  |
| 1   | CE    | 107 | ASP  |
| 1   | CE    | 116 | THR  |
| 1   | CE    | 129 | THR  |
| 1   | CE    | 149 | SER  |
| 1   | CE    | 152 | TRP  |
| 1   | CF    | 116 | THR  |
| 1   | CF    | 130 | LYS  |
| 1   | CF    | 147 | HIS  |
| 1   | CF    | 150 | LYS  |
| 1   | CG    | 13  | LYS  |
| 1   | CG    | 34  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CG    | 42  | VAL  |
| 1   | CG    | 43  | GLU  |
| 1   | CG    | 77  | LEU  |
| 1   | CG    | 102 | LEU  |
| 1   | CG    | 103 | SER  |
| 1   | CG    | 104 | LEU  |
| 1   | CG    | 106 | THR  |
| 1   | CG    | 108 | ILE  |
| 1   | CG    | 109 | PRO  |
| 1   | CG    | 116 | THR  |
| 1   | CG    | 152 | TRP  |
| 1   | CH    | 45  | ASN  |
| 1   | CH    | 67  | ASN  |
| 1   | CH    | 82  | ARG  |
| 1   | CH    | 109 | PRO  |
| 1   | CI    | 67  | ASN  |
| 1   | CI    | 77  | LEU  |
| 1   | CI    | 106 | THR  |
| 1   | CI    | 109 | PRO  |
| 1   | CI    | 116 | THR  |
| 1   | CI    | 129 | THR  |
| 1   | CI    | 130 | LYS  |
| 1   | CI    | 152 | TRP  |
| 1   | CJ    | 77  | LEU  |
| 1   | CJ    | 88  | TYR  |
| 1   | CJ    | 107 | ASP  |
| 1   | CJ    | 116 | THR  |
| 1   | CJ    | 129 | THR  |
| 1   | CJ    | 149 | SER  |
| 1   | CJ    | 152 | TRP  |
| 1   | CK    | 116 | THR  |
| 1   | CK    | 130 | LYS  |
| 1   | CK    | 147 | HIS  |
| 1   | CK    | 150 | LYS  |
| 1   | CL    | 13  | LYS  |
| 1   | CL    | 34  | LEU  |
| 1   | CL    | 42  | VAL  |
| 1   | CL    | 43  | GLU  |
| 1   | CL    | 77  | LEU  |
| 1   | CL    | 102 | LEU  |
| 1   | CL    | 103 | SER  |
| 1   | CL    | 104 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CL    | 106 | THR  |
| 1   | CL    | 108 | ILE  |
| 1   | CL    | 109 | PRO  |
| 1   | CL    | 116 | THR  |
| 1   | CL    | 152 | TRP  |
| 1   | CM    | 45  | ASN  |
| 1   | CM    | 67  | ASN  |
| 1   | CM    | 82  | ARG  |
| 1   | CM    | 109 | PRO  |
| 1   | CN    | 67  | ASN  |
| 1   | CN    | 77  | LEU  |
| 1   | CN    | 106 | THR  |
| 1   | CN    | 109 | PRO  |
| 1   | CN    | 116 | THR  |
| 1   | CN    | 129 | THR  |
| 1   | CN    | 130 | LYS  |
| 1   | CN    | 152 | TRP  |
| 1   | CO    | 77  | LEU  |
| 1   | CO    | 88  | TYR  |
| 1   | CO    | 107 | ASP  |
| 1   | CO    | 116 | THR  |
| 1   | CO    | 129 | THR  |
| 1   | CO    | 149 | SER  |
| 1   | CO    | 152 | TRP  |
| 1   | CP    | 116 | THR  |
| 1   | CP    | 130 | LYS  |
| 1   | CP    | 147 | HIS  |
| 1   | CP    | 150 | LYS  |
| 1   | CQ    | 13  | LYS  |
| 1   | CQ    | 34  | LEU  |
| 1   | CQ    | 42  | VAL  |
| 1   | CQ    | 43  | GLU  |
| 1   | CQ    | 77  | LEU  |
| 1   | CQ    | 102 | LEU  |
| 1   | CQ    | 103 | SER  |
| 1   | CQ    | 104 | LEU  |
| 1   | CQ    | 106 | THR  |
| 1   | CQ    | 108 | ILE  |
| 1   | CQ    | 109 | PRO  |
| 1   | CQ    | 116 | THR  |
| 1   | CQ    | 152 | TRP  |
| 1   | CR    | 45  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CR    | 67  | ASN  |
| 1   | CR    | 82  | ARG  |
| 1   | CR    | 109 | PRO  |
| 1   | CS    | 67  | ASN  |
| 1   | CS    | 77  | LEU  |
| 1   | CS    | 106 | THR  |
| 1   | CS    | 109 | PRO  |
| 1   | CS    | 116 | THR  |
| 1   | CS    | 129 | THR  |
| 1   | CS    | 130 | LYS  |
| 1   | CS    | 152 | TRP  |
| 1   | CT    | 77  | LEU  |
| 1   | CT    | 88  | TYR  |
| 1   | CT    | 107 | ASP  |
| 1   | CT    | 116 | THR  |
| 1   | CT    | 129 | THR  |
| 1   | CT    | 149 | SER  |
| 1   | CT    | 152 | TRP  |
| 1   | CU    | 116 | THR  |
| 1   | CU    | 130 | LYS  |
| 1   | CU    | 147 | HIS  |
| 1   | CU    | 150 | LYS  |
| 1   | CV    | 13  | LYS  |
| 1   | CV    | 34  | LEU  |
| 1   | CV    | 42  | VAL  |
| 1   | CV    | 43  | GLU  |
| 1   | CV    | 77  | LEU  |
| 1   | CV    | 102 | LEU  |
| 1   | CV    | 103 | SER  |
| 1   | CV    | 104 | LEU  |
| 1   | CV    | 106 | THR  |
| 1   | CV    | 108 | ILE  |
| 1   | CV    | 109 | PRO  |
| 1   | CV    | 116 | THR  |
| 1   | CV    | 152 | TRP  |
| 1   | CW    | 45  | ASN  |
| 1   | CW    | 67  | ASN  |
| 1   | CW    | 82  | ARG  |
| 1   | CW    | 109 | PRO  |
| 1   | CX    | 67  | ASN  |
| 1   | CX    | 77  | LEU  |
| 1   | CX    | 106 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CX    | 109 | PRO  |
| 1   | CX    | 116 | THR  |
| 1   | CX    | 129 | THR  |
| 1   | CX    | 130 | LYS  |
| 1   | CX    | 152 | TRP  |
| 1   | CY    | 77  | LEU  |
| 1   | CY    | 88  | TYR  |
| 1   | CY    | 107 | ASP  |
| 1   | CY    | 116 | THR  |
| 1   | CY    | 129 | THR  |
| 1   | CY    | 149 | SER  |
| 1   | CY    | 152 | TRP  |
| 1   | CZ    | 116 | THR  |
| 1   | CZ    | 130 | LYS  |
| 1   | CZ    | 147 | HIS  |
| 1   | CZ    | 150 | LYS  |
| 1   | C1    | 13  | LYS  |
| 1   | C1    | 34  | LEU  |
| 1   | C1    | 42  | VAL  |
| 1   | C1    | 43  | GLU  |
| 1   | C1    | 77  | LEU  |
| 1   | C1    | 102 | LEU  |
| 1   | C1    | 103 | SER  |
| 1   | C1    | 104 | LEU  |
| 1   | C1    | 106 | THR  |
| 1   | C1    | 108 | ILE  |
| 1   | C1    | 109 | PRO  |
| 1   | C1    | 116 | THR  |
| 1   | C1    | 152 | TRP  |
| 1   | C2    | 45  | ASN  |
| 1   | C2    | 67  | ASN  |
| 1   | C2    | 82  | ARG  |
| 1   | C2    | 109 | PRO  |
| 1   | C3    | 67  | ASN  |
| 1   | C3    | 77  | LEU  |
| 1   | C3    | 106 | THR  |
| 1   | C3    | 109 | PRO  |
| 1   | C3    | 116 | THR  |
| 1   | C3    | 129 | THR  |
| 1   | C3    | 130 | LYS  |
| 1   | C3    | 152 | TRP  |
| 1   | C4    | 77  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C4    | 88  | TYR  |
| 1   | C4    | 107 | ASP  |
| 1   | C4    | 116 | THR  |
| 1   | C4    | 129 | THR  |
| 1   | C4    | 149 | SER  |
| 1   | C4    | 152 | TRP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (299) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 45  | ASN  |
| 1   | AA    | 67  | ASN  |
| 1   | AA    | 87  | HIS  |
| 1   | AA    | 151 | HIS  |
| 1   | AB    | 45  | ASN  |
| 1   | AB    | 67  | ASN  |
| 1   | AB    | 93  | ASN  |
| 1   | AC    | 6   | HIS  |
| 1   | AC    | 45  | ASN  |
| 1   | AC    | 67  | ASN  |
| 1   | AC    | 93  | ASN  |
| 1   | AD    | 67  | ASN  |
| 1   | AD    | 93  | ASN  |
| 1   | AD    | 147 | HIS  |
| 1   | AE    | 6   | HIS  |
| 1   | AE    | 67  | ASN  |
| 1   | AE    | 93  | ASN  |
| 1   | AF    | 45  | ASN  |
| 1   | AF    | 67  | ASN  |
| 1   | AF    | 87  | HIS  |
| 1   | AF    | 151 | HIS  |
| 1   | AG    | 45  | ASN  |
| 1   | AG    | 67  | ASN  |
| 1   | AG    | 93  | ASN  |
| 1   | AH    | 6   | HIS  |
| 1   | AH    | 45  | ASN  |
| 1   | AH    | 67  | ASN  |
| 1   | AH    | 147 | HIS  |
| 1   | AI    | 67  | ASN  |
| 1   | AI    | 93  | ASN  |
| 1   | AI    | 147 | HIS  |
| 1   | AJ    | 6   | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AJ    | 67  | ASN  |
| 1   | AJ    | 93  | ASN  |
| 1   | AK    | 45  | ASN  |
| 1   | AK    | 67  | ASN  |
| 1   | AK    | 87  | HIS  |
| 1   | AK    | 151 | HIS  |
| 1   | AL    | 45  | ASN  |
| 1   | AL    | 67  | ASN  |
| 1   | AL    | 93  | ASN  |
| 1   | AM    | 6   | HIS  |
| 1   | AM    | 45  | ASN  |
| 1   | AM    | 67  | ASN  |
| 1   | AM    | 93  | ASN  |
| 1   | AM    | 147 | HIS  |
| 1   | AN    | 67  | ASN  |
| 1   | AN    | 93  | ASN  |
| 1   | AN    | 147 | HIS  |
| 1   | AO    | 6   | HIS  |
| 1   | AO    | 67  | ASN  |
| 1   | AO    | 93  | ASN  |
| 1   | AP    | 45  | ASN  |
| 1   | AP    | 67  | ASN  |
| 1   | AP    | 87  | HIS  |
| 1   | AP    | 151 | HIS  |
| 1   | AQ    | 45  | ASN  |
| 1   | AQ    | 67  | ASN  |
| 1   | AQ    | 93  | ASN  |
| 1   | AR    | 6   | HIS  |
| 1   | AR    | 45  | ASN  |
| 1   | AR    | 67  | ASN  |
| 1   | AS    | 6   | HIS  |
| 1   | AS    | 67  | ASN  |
| 1   | AS    | 93  | ASN  |
| 1   | AS    | 147 | HIS  |
| 1   | AT    | 6   | HIS  |
| 1   | AT    | 67  | ASN  |
| 1   | AT    | 93  | ASN  |
| 1   | AU    | 45  | ASN  |
| 1   | AU    | 67  | ASN  |
| 1   | AU    | 87  | HIS  |
| 1   | AU    | 151 | HIS  |
| 1   | AV    | 45  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AV    | 67  | ASN  |
| 1   | AV    | 93  | ASN  |
| 1   | AW    | 6   | HIS  |
| 1   | AW    | 67  | ASN  |
| 1   | AW    | 93  | ASN  |
| 1   | AX    | 6   | HIS  |
| 1   | AX    | 67  | ASN  |
| 1   | AX    | 93  | ASN  |
| 1   | AX    | 147 | HIS  |
| 1   | AY    | 6   | HIS  |
| 1   | AY    | 67  | ASN  |
| 1   | AY    | 93  | ASN  |
| 1   | AZ    | 45  | ASN  |
| 1   | AZ    | 67  | ASN  |
| 1   | AZ    | 87  | HIS  |
| 1   | AZ    | 151 | HIS  |
| 1   | A1    | 45  | ASN  |
| 1   | A1    | 67  | ASN  |
| 1   | A1    | 93  | ASN  |
| 1   | A2    | 6   | HIS  |
| 1   | A2    | 45  | ASN  |
| 1   | A2    | 67  | ASN  |
| 1   | A2    | 93  | ASN  |
| 1   | A2    | 147 | HIS  |
| 1   | A3    | 6   | HIS  |
| 1   | A3    | 67  | ASN  |
| 1   | A3    | 93  | ASN  |
| 1   | A3    | 147 | HIS  |
| 1   | A4    | 6   | HIS  |
| 1   | A4    | 67  | ASN  |
| 1   | BA    | 45  | ASN  |
| 1   | BA    | 67  | ASN  |
| 1   | BA    | 87  | HIS  |
| 1   | BA    | 151 | HIS  |
| 1   | BB    | 45  | ASN  |
| 1   | BB    | 67  | ASN  |
| 1   | BB    | 93  | ASN  |
| 1   | BC    | 6   | HIS  |
| 1   | BC    | 45  | ASN  |
| 1   | BC    | 67  | ASN  |
| 1   | BC    | 93  | ASN  |
| 1   | BC    | 147 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BD    | 67  | ASN  |
| 1   | BD    | 93  | ASN  |
| 1   | BD    | 147 | HIS  |
| 1   | BE    | 6   | HIS  |
| 1   | BE    | 67  | ASN  |
| 1   | BE    | 93  | ASN  |
| 1   | BF    | 45  | ASN  |
| 1   | BF    | 67  | ASN  |
| 1   | BF    | 87  | HIS  |
| 1   | BF    | 151 | HIS  |
| 1   | BG    | 45  | ASN  |
| 1   | BG    | 67  | ASN  |
| 1   | BG    | 93  | ASN  |
| 1   | BH    | 6   | HIS  |
| 1   | BH    | 67  | ASN  |
| 1   | BI    | 67  | ASN  |
| 1   | BI    | 93  | ASN  |
| 1   | BI    | 147 | HIS  |
| 1   | BJ    | 6   | HIS  |
| 1   | BJ    | 67  | ASN  |
| 1   | BK    | 45  | ASN  |
| 1   | BK    | 67  | ASN  |
| 1   | BK    | 87  | HIS  |
| 1   | BK    | 151 | HIS  |
| 1   | BL    | 45  | ASN  |
| 1   | BL    | 67  | ASN  |
| 1   | BL    | 93  | ASN  |
| 1   | BM    | 6   | HIS  |
| 1   | BM    | 45  | ASN  |
| 1   | BM    | 67  | ASN  |
| 1   | BM    | 93  | ASN  |
| 1   | BN    | 67  | ASN  |
| 1   | BN    | 93  | ASN  |
| 1   | BN    | 147 | HIS  |
| 1   | BO    | 6   | HIS  |
| 1   | BO    | 67  | ASN  |
| 1   | BP    | 45  | ASN  |
| 1   | BP    | 67  | ASN  |
| 1   | BP    | 87  | HIS  |
| 1   | BP    | 151 | HIS  |
| 1   | BQ    | 45  | ASN  |
| 1   | BQ    | 67  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BQ    | 93  | ASN  |
| 1   | BR    | 6   | HIS  |
| 1   | BR    | 67  | ASN  |
| 1   | BR    | 93  | ASN  |
| 1   | BR    | 147 | HIS  |
| 1   | BS    | 6   | HIS  |
| 1   | BS    | 67  | ASN  |
| 1   | BS    | 93  | ASN  |
| 1   | BS    | 147 | HIS  |
| 1   | BT    | 6   | HIS  |
| 1   | BT    | 67  | ASN  |
| 1   | BT    | 93  | ASN  |
| 1   | BU    | 45  | ASN  |
| 1   | BU    | 67  | ASN  |
| 1   | BU    | 87  | HIS  |
| 1   | BU    | 151 | HIS  |
| 1   | BV    | 67  | ASN  |
| 1   | BV    | 93  | ASN  |
| 1   | BW    | 6   | HIS  |
| 1   | BW    | 45  | ASN  |
| 1   | BW    | 67  | ASN  |
| 1   | BW    | 93  | ASN  |
| 1   | BW    | 147 | HIS  |
| 1   | BX    | 67  | ASN  |
| 1   | BX    | 93  | ASN  |
| 1   | BX    | 147 | HIS  |
| 1   | BY    | 6   | HIS  |
| 1   | BY    | 67  | ASN  |
| 1   | BZ    | 45  | ASN  |
| 1   | BZ    | 67  | ASN  |
| 1   | BZ    | 87  | HIS  |
| 1   | BZ    | 151 | HIS  |
| 1   | B1    | 45  | ASN  |
| 1   | B1    | 67  | ASN  |
| 1   | B1    | 93  | ASN  |
| 1   | B2    | 6   | HIS  |
| 1   | B2    | 45  | ASN  |
| 1   | B2    | 67  | ASN  |
| 1   | B2    | 147 | HIS  |
| 1   | B3    | 67  | ASN  |
| 1   | B3    | 147 | HIS  |
| 1   | B4    | 6   | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B4    | 67  | ASN  |
| 1   | B4    | 93  | ASN  |
| 1   | CA    | 45  | ASN  |
| 1   | CA    | 67  | ASN  |
| 1   | CA    | 87  | HIS  |
| 1   | CA    | 151 | HIS  |
| 1   | CB    | 67  | ASN  |
| 1   | CB    | 93  | ASN  |
| 1   | CC    | 6   | HIS  |
| 1   | CC    | 45  | ASN  |
| 1   | CC    | 67  | ASN  |
| 1   | CC    | 93  | ASN  |
| 1   | CD    | 67  | ASN  |
| 1   | CD    | 93  | ASN  |
| 1   | CD    | 147 | HIS  |
| 1   | CE    | 6   | HIS  |
| 1   | CE    | 67  | ASN  |
| 1   | CE    | 93  | ASN  |
| 1   | CF    | 45  | ASN  |
| 1   | CF    | 67  | ASN  |
| 1   | CF    | 87  | HIS  |
| 1   | CF    | 151 | HIS  |
| 1   | CG    | 45  | ASN  |
| 1   | CG    | 67  | ASN  |
| 1   | CG    | 93  | ASN  |
| 1   | CH    | 6   | HIS  |
| 1   | CH    | 45  | ASN  |
| 1   | CH    | 67  | ASN  |
| 1   | CH    | 93  | ASN  |
| 1   | CI    | 67  | ASN  |
| 1   | CI    | 93  | ASN  |
| 1   | CI    | 147 | HIS  |
| 1   | CJ    | 6   | HIS  |
| 1   | CJ    | 40  | HIS  |
| 1   | CJ    | 67  | ASN  |
| 1   | CJ    | 93  | ASN  |
| 1   | CK    | 45  | ASN  |
| 1   | CK    | 67  | ASN  |
| 1   | CK    | 87  | HIS  |
| 1   | CK    | 151 | HIS  |
| 1   | CL    | 67  | ASN  |
| 1   | CL    | 93  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CM    | 6   | HIS  |
| 1   | CM    | 45  | ASN  |
| 1   | CM    | 67  | ASN  |
| 1   | CM    | 93  | ASN  |
| 1   | CN    | 67  | ASN  |
| 1   | CN    | 93  | ASN  |
| 1   | CN    | 147 | HIS  |
| 1   | CO    | 67  | ASN  |
| 1   | CO    | 93  | ASN  |
| 1   | CP    | 45  | ASN  |
| 1   | CP    | 67  | ASN  |
| 1   | CP    | 87  | HIS  |
| 1   | CP    | 151 | HIS  |
| 1   | CQ    | 45  | ASN  |
| 1   | CQ    | 67  | ASN  |
| 1   | CQ    | 93  | ASN  |
| 1   | CR    | 6   | HIS  |
| 1   | CR    | 45  | ASN  |
| 1   | CR    | 67  | ASN  |
| 1   | CR    | 93  | ASN  |
| 1   | CS    | 67  | ASN  |
| 1   | CS    | 93  | ASN  |
| 1   | CS    | 147 | HIS  |
| 1   | CT    | 6   | HIS  |
| 1   | CT    | 67  | ASN  |
| 1   | CT    | 93  | ASN  |
| 1   | CU    | 45  | ASN  |
| 1   | CU    | 67  | ASN  |
| 1   | CU    | 87  | HIS  |
| 1   | CU    | 151 | HIS  |
| 1   | CV    | 67  | ASN  |
| 1   | CV    | 93  | ASN  |
| 1   | CW    | 6   | HIS  |
| 1   | CW    | 67  | ASN  |
| 1   | CX    | 67  | ASN  |
| 1   | CX    | 93  | ASN  |
| 1   | CX    | 147 | HIS  |
| 1   | CY    | 6   | HIS  |
| 1   | CY    | 67  | ASN  |
| 1   | CY    | 93  | ASN  |
| 1   | CZ    | 45  | ASN  |
| 1   | CZ    | 67  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CZ    | 87  | HIS  |
| 1   | CZ    | 151 | HIS  |
| 1   | C1    | 45  | ASN  |
| 1   | C1    | 67  | ASN  |
| 1   | C1    | 93  | ASN  |
| 1   | C2    | 6   | HIS  |
| 1   | C2    | 67  | ASN  |
| 1   | C2    | 93  | ASN  |
| 1   | C3    | 6   | HIS  |
| 1   | C3    | 67  | ASN  |
| 1   | C3    | 93  | ASN  |
| 1   | C3    | 147 | HIS  |
| 1   | C4    | 6   | HIS  |
| 1   | C4    | 67  | ASN  |
| 1   | C4    | 93  | 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 ⓘ

90 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PO4  | BQ    | 1001 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | CE    | 1001 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | AG    | 1001 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | BD    | 1001 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.43 | 0        |
| 2   | PO4  | BN    | 1001 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | CZ    | 201  | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | AP    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | CS    | 3201 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | CV    | 1201 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | B2    | 1001 | -    | 4,4,4        | 1.06 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | AK    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | AU    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | CG    | 1201 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | A2    | 1001 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | BM    | 1001 | -    | 4,4,4        | 1.04 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | CO    | 4201 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | BP    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | AY    | 1001 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | AH    | 1001 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | CA    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | CR    | 2201 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | BG    | 1001 | -    | 4,4,4        | 0.94 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | AS    | 1001 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | A4    | 1001 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | BT    | 1001 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | AO    | 1001 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | CK    | 201  | -    | 4,4,4        | 0.93 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | C2    | 2201 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | BZ    | 1001 | -    | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | BU    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | CU    | 201  | -    | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | AD    | 1001 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | BI    | 1001 | -    | 4,4,4        | 1.03 | 0        | 6,6,6       | 0.43 | 0        |
| 2   | PO4  | CQ    | 1201 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.39 | 0        |
| 2   | PO4  | AN    | 1001 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.43 | 0        |
| 2   | PO4  | AE    | 1001 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | CH    | 2201 | -    | 4,4,4        | 1.06 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | AZ    | 1001 | -    | 4,4,4        | 0.93 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | AR    | 1001 | -    | 4,4,4        | 1.04 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | CP    | 201  | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | BY    | 1001 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | BK    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | B4    | 1001 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PO4  | BW    | 1001 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | AC    | 1001 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | CY    | 4201 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | BA    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | CC    | 1001 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | BL    | 1001 | -    | 4,4,4        | 0.96 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | BE    | 1001 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | CF    | 201  | -    | 4,4,4        | 0.90 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | BV    | 1001 | -    | 4,4,4        | 0.94 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | CM    | 2201 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | CN    | 3201 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | AV    | 1001 | -    | 4,4,4        | 0.94 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | AW    | 201  | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | BO    | 1001 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | B3    | 1001 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.43 | 0        |
| 2   | PO4  | C1    | 1201 | -    | 4,4,4        | 0.96 | 0        | 6,6,6       | 0.39 | 0        |
| 2   | PO4  | BC    | 1001 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | BX    | 1001 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.43 | 0        |
| 2   | PO4  | CJ    | 4201 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | CX    | 3201 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | C3    | 3201 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | A3    | 1001 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | AT    | 1001 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | CW    | 2201 | -    | 4,4,4        | 1.06 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | BR    | 1001 | -    | 4,4,4        | 1.06 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | AB    | 1001 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | CI    | 3201 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.43 | 0        |
| 2   | PO4  | AM    | 1001 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | CT    | 4201 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | CB    | 1001 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | CD    | 1001 | -    | 4,4,4        | 1.03 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | BB    | 1001 | -    | 4,4,4        | 0.96 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | AA    | 1001 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | PO4  | BS    | 1001 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | AI    | 1001 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | AQ    | 1001 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.39 | 0        |
| 2   | PO4  | AL    | 1001 | -    | 4,4,4        | 0.94 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | BH    | 1001 | -    | 4,4,4        | 1.06 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | A1    | 1001 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.39 | 0        |
| 2   | PO4  | C4    | 4201 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.61 | 0        |
| 2   | PO4  | AX    | 1001 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | BJ    | 1001 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | BF    | 1001 | -    | 4,4,4        | 0.93 | 0        | 6,6,6       | 0.56 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PO4  | B1    | 1001 | -    | 4,4,4        | 0.96 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | CL    | 1201 | -    | 4,4,4        | 0.96 | 0        | 6,6,6       | 0.39 | 0        |
| 2   | PO4  | AF    | 1001 | -    | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.54 | 0        |
| 2   | PO4  | AJ    | 1001 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.61 | 0        |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

67 monomers are involved in 121 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | BQ    | 1001 | PO4  | 1       | 0            |
| 2   | CE    | 1001 | PO4  | 2       | 0            |
| 2   | AG    | 1001 | PO4  | 1       | 0            |
| 2   | CZ    | 201  | PO4  | 1       | 0            |
| 2   | AP    | 1001 | PO4  | 1       | 0            |
| 2   | B2    | 1001 | PO4  | 3       | 0            |
| 2   | AK    | 1001 | PO4  | 1       | 0            |
| 2   | AU    | 1001 | PO4  | 1       | 0            |
| 2   | CG    | 1201 | PO4  | 1       | 0            |
| 2   | A2    | 1001 | PO4  | 3       | 0            |
| 2   | BM    | 1001 | PO4  | 3       | 0            |
| 2   | CO    | 4201 | PO4  | 2       | 0            |
| 2   | BP    | 1001 | PO4  | 1       | 0            |
| 2   | AY    | 1001 | PO4  | 2       | 0            |
| 2   | AH    | 1001 | PO4  | 3       | 0            |
| 2   | CA    | 1001 | PO4  | 1       | 0            |
| 2   | CR    | 2201 | PO4  | 3       | 0            |
| 2   | BG    | 1001 | PO4  | 1       | 0            |
| 2   | A4    | 1001 | PO4  | 2       | 0            |
| 2   | BT    | 1001 | PO4  | 2       | 0            |
| 2   | AO    | 1001 | PO4  | 2       | 0            |
| 2   | CK    | 201  | PO4  | 1       | 0            |
| 2   | C2    | 2201 | PO4  | 3       | 0            |
| 2   | BZ    | 1001 | PO4  | 1       | 0            |
| 2   | BU    | 1001 | PO4  | 1       | 0            |
| 2   | CU    | 201  | PO4  | 1       | 0            |
| 2   | AE    | 1001 | PO4  | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | CH    | 2201 | PO4  | 3       | 0            |
| 2   | AZ    | 1001 | PO4  | 1       | 0            |
| 2   | AR    | 1001 | PO4  | 3       | 0            |
| 2   | CP    | 201  | PO4  | 1       | 0            |
| 2   | BY    | 1001 | PO4  | 2       | 0            |
| 2   | BK    | 1001 | PO4  | 1       | 0            |
| 2   | B4    | 1001 | PO4  | 2       | 0            |
| 2   | BW    | 1001 | PO4  | 3       | 0            |
| 2   | AC    | 1001 | PO4  | 3       | 0            |
| 2   | CY    | 4201 | PO4  | 2       | 0            |
| 2   | BA    | 1001 | PO4  | 1       | 0            |
| 2   | CC    | 1001 | PO4  | 3       | 0            |
| 2   | BL    | 1001 | PO4  | 1       | 0            |
| 2   | BE    | 1001 | PO4  | 2       | 0            |
| 2   | CF    | 201  | PO4  | 1       | 0            |
| 2   | CM    | 2201 | PO4  | 3       | 0            |
| 2   | AV    | 1001 | PO4  | 1       | 0            |
| 2   | AW    | 201  | PO4  | 3       | 0            |
| 2   | BO    | 1001 | PO4  | 2       | 0            |
| 2   | C1    | 1201 | PO4  | 1       | 0            |
| 2   | BC    | 1001 | PO4  | 3       | 0            |
| 2   | CJ    | 4201 | PO4  | 2       | 0            |
| 2   | AT    | 1001 | PO4  | 2       | 0            |
| 2   | CW    | 2201 | PO4  | 3       | 0            |
| 2   | BR    | 1001 | PO4  | 3       | 0            |
| 2   | AB    | 1001 | PO4  | 1       | 0            |
| 2   | AM    | 1001 | PO4  | 3       | 0            |
| 2   | CT    | 4201 | PO4  | 2       | 0            |
| 2   | CB    | 1001 | PO4  | 1       | 0            |
| 2   | BB    | 1001 | PO4  | 1       | 0            |
| 2   | AA    | 1001 | PO4  | 1       | 0            |
| 2   | AQ    | 1001 | PO4  | 1       | 0            |
| 2   | BH    | 1001 | PO4  | 3       | 0            |
| 2   | C4    | 4201 | PO4  | 2       | 0            |
| 2   | BJ    | 1001 | PO4  | 2       | 0            |
| 2   | BF    | 1001 | PO4  | 1       | 0            |
| 2   | B1    | 1001 | PO4  | 1       | 0            |
| 2   | CL    | 1201 | PO4  | 1       | 0            |
| 2   | AF    | 1001 | PO4  | 1       | 0            |
| 2   | AJ    | 1001 | PO4  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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   | A1    | 152/153 (99%) | 1.00   | 16 (10%) 11 8 | 65, 95, 151, 347      | 0     |
| 1   | A2    | 152/153 (99%) | 1.09   | 18 (11%) 9 6  | 56, 97, 184, 226      | 0     |
| 1   | A3    | 152/153 (99%) | 0.93   | 14 (9%) 14 9  | 57, 96, 147, 259      | 0     |
| 1   | A4    | 152/153 (99%) | 0.95   | 13 (8%) 16 11 | 56, 94, 153, 393      | 0     |
| 1   | AA    | 152/153 (99%) | 0.99   | 15 (9%) 13 8  | 55, 97, 150, 271      | 0     |
| 1   | AB    | 152/153 (99%) | 1.01   | 20 (13%) 7 6  | 65, 95, 151, 347      | 0     |
| 1   | AC    | 152/153 (99%) | 1.05   | 20 (13%) 7 6  | 56, 97, 184, 226      | 0     |
| 1   | AD    | 152/153 (99%) | 1.02   | 15 (9%) 13 8  | 57, 96, 147, 259      | 0     |
| 1   | AE    | 152/153 (99%) | 0.99   | 15 (9%) 13 8  | 56, 94, 153, 393      | 0     |
| 1   | AF    | 152/153 (99%) | 1.25   | 23 (15%) 5 5  | 55, 97, 150, 271      | 0     |
| 1   | AG    | 152/153 (99%) | 1.44   | 31 (20%) 3 3  | 65, 95, 151, 347      | 0     |
| 1   | AH    | 152/153 (99%) | 1.76   | 50 (32%) 1 1  | 56, 97, 184, 226      | 0     |
| 1   | AI    | 152/153 (99%) | 1.51   | 39 (25%) 1 2  | 57, 96, 147, 259      | 0     |
| 1   | AJ    | 152/153 (99%) | 1.42   | 29 (19%) 3 3  | 56, 94, 153, 393      | 0     |
| 1   | AK    | 152/153 (99%) | 1.42   | 34 (22%) 2 2  | 55, 97, 150, 271      | 0     |
| 1   | AL    | 152/153 (99%) | 1.36   | 30 (19%) 3 3  | 65, 95, 151, 347      | 0     |
| 1   | AM    | 152/153 (99%) | 1.33   | 26 (17%) 4 4  | 56, 97, 184, 226      | 0     |
| 1   | AN    | 152/153 (99%) | 1.10   | 15 (9%) 13 8  | 57, 96, 147, 259      | 0     |
| 1   | AO    | 152/153 (99%) | 1.25   | 25 (16%) 4 4  | 56, 94, 153, 393      | 0     |
| 1   | AP    | 152/153 (99%) | 0.87   | 10 (6%) 24 15 | 55, 97, 150, 271      | 0     |
| 1   | AQ    | 152/153 (99%) | 1.01   | 16 (10%) 11 8 | 65, 95, 151, 347      | 0     |
| 1   | AR    | 152/153 (99%) | 1.18   | 23 (15%) 5 5  | 56, 97, 184, 226      | 0     |
| 1   | AS    | 152/153 (99%) | 0.83   | 11 (7%) 21 14 | 57, 96, 147, 259      | 0     |
| 1   | AT    | 152/153 (99%) | 0.79   | 11 (7%) 21 14 | 56, 94, 153, 393      | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|----------|-------|-----------------------|-------|
| 1   | AU    | 152/153 (99%) | 1.08   | 16 (10%) | 11 8  | 55, 97, 150, 271      | 0     |
| 1   | AV    | 152/153 (99%) | 1.39   | 31 (20%) | 3 3   | 65, 95, 151, 347      | 0     |
| 1   | AW    | 152/153 (99%) | 1.65   | 38 (25%) | 2 2   | 56, 97, 184, 226      | 0     |
| 1   | AX    | 152/153 (99%) | 1.26   | 30 (19%) | 3 3   | 57, 96, 147, 259      | 0     |
| 1   | AY    | 152/153 (99%) | 1.11   | 18 (11%) | 9 6   | 56, 94, 153, 393      | 0     |
| 1   | AZ    | 152/153 (99%) | 1.01   | 15 (9%)  | 13 8  | 55, 97, 150, 271      | 0     |
| 1   | B1    | 152/153 (99%) | 0.71   | 8 (5%)   | 32 18 | 60, 95, 151, 347      | 0     |
| 1   | B2    | 152/153 (99%) | 0.73   | 8 (5%)   | 32 18 | 56, 97, 184, 226      | 0     |
| 1   | B3    | 152/153 (99%) | 0.48   | 5 (3%)   | 49 28 | 57, 96, 147, 259      | 0     |
| 1   | B4    | 152/153 (99%) | 0.73   | 8 (5%)   | 32 18 | 55, 93, 153, 393      | 0     |
| 1   | BA    | 152/153 (99%) | 0.48   | 3 (1%)   | 65 39 | 55, 97, 147, 271      | 0     |
| 1   | BB    | 152/153 (99%) | 0.81   | 9 (5%)   | 28 16 | 60, 95, 151, 347      | 0     |
| 1   | BC    | 152/153 (99%) | 0.75   | 9 (5%)   | 28 16 | 56, 97, 184, 226      | 0     |
| 1   | BD    | 152/153 (99%) | 0.61   | 5 (3%)   | 49 28 | 57, 96, 147, 259      | 0     |
| 1   | BE    | 152/153 (99%) | 0.61   | 3 (1%)   | 65 39 | 55, 93, 153, 393      | 0     |
| 1   | BF    | 152/153 (99%) | 0.54   | 5 (3%)   | 49 28 | 55, 97, 147, 271      | 0     |
| 1   | BG    | 152/153 (99%) | 0.65   | 8 (5%)   | 32 18 | 60, 95, 151, 347      | 0     |
| 1   | BH    | 152/153 (99%) | 0.67   | 9 (5%)   | 28 16 | 56, 97, 184, 226      | 0     |
| 1   | BI    | 152/153 (99%) | 0.56   | 4 (2%)   | 57 33 | 57, 96, 147, 259      | 0     |
| 1   | BJ    | 152/153 (99%) | 0.65   | 6 (3%)   | 43 23 | 55, 93, 153, 393      | 0     |
| 1   | BK    | 152/153 (99%) | 0.49   | 3 (1%)   | 65 39 | 55, 97, 147, 271      | 0     |
| 1   | BL    | 152/153 (99%) | 0.62   | 9 (5%)   | 28 16 | 60, 95, 151, 347      | 0     |
| 1   | BM    | 152/153 (99%) | 0.62   | 6 (3%)   | 43 23 | 56, 97, 184, 226      | 0     |
| 1   | BN    | 152/153 (99%) | 0.51   | 4 (2%)   | 57 33 | 57, 96, 147, 259      | 0     |
| 1   | BO    | 152/153 (99%) | 0.59   | 6 (3%)   | 43 23 | 55, 93, 153, 393      | 0     |
| 1   | BP    | 152/153 (99%) | 0.49   | 5 (3%)   | 49 28 | 55, 97, 147, 271      | 0     |
| 1   | BQ    | 152/153 (99%) | 0.63   | 7 (4%)   | 37 20 | 60, 95, 151, 347      | 0     |
| 1   | BR    | 152/153 (99%) | 0.69   | 7 (4%)   | 37 20 | 56, 97, 184, 226      | 0     |
| 1   | BS    | 152/153 (99%) | 0.57   | 4 (2%)   | 57 33 | 57, 96, 147, 259      | 0     |
| 1   | BT    | 152/153 (99%) | 0.63   | 6 (3%)   | 43 23 | 55, 93, 153, 393      | 0     |
| 1   | BU    | 152/153 (99%) | 0.77   | 11 (7%)  | 21 14 | 55, 97, 147, 271      | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|----------|-------|-----------------------|-------|
| 1   | BV    | 152/153 (99%) | 0.82   | 10 (6%)  | 24 15 | 60, 95, 151, 347      | 0     |
| 1   | BW    | 152/153 (99%) | 0.88   | 12 (7%)  | 18 12 | 56, 97, 184, 226      | 0     |
| 1   | BX    | 152/153 (99%) | 0.63   | 3 (1%)   | 65 39 | 57, 96, 147, 259      | 0     |
| 1   | BY    | 152/153 (99%) | 0.67   | 5 (3%)   | 49 28 | 55, 93, 153, 393      | 0     |
| 1   | BZ    | 152/153 (99%) | 0.65   | 5 (3%)   | 49 28 | 55, 97, 147, 271      | 0     |
| 1   | C1    | 152/153 (99%) | 1.46   | 35 (23%) | 2 2   | 60, 95, 151, 347      | 0     |
| 1   | C2    | 152/153 (99%) | 1.40   | 29 (19%) | 3 3   | 56, 97, 184, 226      | 0     |
| 1   | C3    | 152/153 (99%) | 1.51   | 40 (26%) | 1 2   | 57, 96, 147, 259      | 0     |
| 1   | C4    | 152/153 (99%) | 1.67   | 48 (31%) | 1 1   | 55, 93, 153, 393      | 0     |
| 1   | CA    | 152/153 (99%) | 0.84   | 9 (5%)   | 28 16 | 55, 97, 147, 271      | 0     |
| 1   | CB    | 152/153 (99%) | 1.06   | 17 (11%) | 10 7  | 60, 95, 151, 347      | 0     |
| 1   | CC    | 152/153 (99%) | 1.21   | 23 (15%) | 5 5   | 56, 97, 184, 226      | 0     |
| 1   | CD    | 152/153 (99%) | 1.04   | 20 (13%) | 7 6   | 57, 96, 147, 259      | 0     |
| 1   | CE    | 152/153 (99%) | 0.72   | 8 (5%)   | 32 18 | 55, 93, 153, 393      | 0     |
| 1   | CF    | 152/153 (99%) | 1.27   | 27 (17%) | 4 4   | 55, 97, 147, 271      | 0     |
| 1   | CG    | 152/153 (99%) | 1.03   | 15 (9%)  | 13 8  | 60, 95, 151, 347      | 0     |
| 1   | CH    | 152/153 (99%) | 0.54   | 3 (1%)   | 65 39 | 56, 97, 184, 226      | 0     |
| 1   | CI    | 152/153 (99%) | 0.49   | 4 (2%)   | 57 33 | 57, 96, 147, 259      | 0     |
| 1   | CJ    | 152/153 (99%) | 0.88   | 12 (7%)  | 18 12 | 55, 93, 153, 393      | 0     |
| 1   | CK    | 152/153 (99%) | 0.79   | 13 (8%)  | 16 11 | 55, 97, 147, 271      | 0     |
| 1   | CL    | 152/153 (99%) | 0.75   | 12 (7%)  | 18 12 | 60, 95, 151, 347      | 0     |
| 1   | CM    | 152/153 (99%) | 0.73   | 6 (3%)   | 43 23 | 56, 97, 184, 226      | 0     |
| 1   | CN    | 152/153 (99%) | 0.68   | 4 (2%)   | 57 33 | 57, 96, 147, 259      | 0     |
| 1   | CO    | 152/153 (99%) | 0.61   | 8 (5%)   | 32 18 | 55, 93, 153, 393      | 0     |
| 1   | CP    | 152/153 (99%) | 1.30   | 25 (16%) | 4 4   | 55, 97, 147, 271      | 0     |
| 1   | CQ    | 152/153 (99%) | 1.34   | 31 (20%) | 3 3   | 60, 95, 151, 347      | 0     |
| 1   | CR    | 152/153 (99%) | 1.60   | 42 (27%) | 1 1   | 56, 97, 184, 226      | 0     |
| 1   | CS    | 152/153 (99%) | 1.95   | 67 (44%) | 0 1   | 57, 96, 147, 259      | 0     |
| 1   | CT    | 152/153 (99%) | 1.77   | 50 (32%) | 1 1   | 55, 93, 153, 393      | 0     |
| 1   | CU    | 152/153 (99%) | 0.73   | 7 (4%)   | 37 20 | 55, 97, 147, 271      | 0     |
| 1   | CV    | 152/153 (99%) | 1.01   | 12 (7%)  | 18 12 | 60, 95, 151, 347      | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 1   | CW    | 152/153 (99%)     | 1.17   | 20 (13%) 7 6    | 56, 97, 184, 226      | 0     |
| 1   | CX    | 152/153 (99%)     | 0.89   | 14 (9%) 14 9    | 57, 96, 147, 259      | 0     |
| 1   | CY    | 152/153 (99%)     | 0.78   | 7 (4%) 37 20    | 55, 93, 153, 393      | 0     |
| 1   | CZ    | 152/153 (99%)     | 1.68   | 46 (30%) 1 1    | 55, 97, 147, 271      | 0     |
| All | All   | 13680/13770 (99%) | 0.97   | 1514 (11%) 10 7 | 55, 96, 157, 393      | 0     |

All (1514) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AW    | 152 | TRP  | 9.5  |
| 1   | CS    | 66  | ALA  | 8.9  |
| 1   | AH    | 152 | TRP  | 8.4  |
| 1   | AD    | 153 | ALA  | 8.2  |
| 1   | CY    | 149 | SER  | 8.0  |
| 1   | AE    | 149 | SER  | 7.5  |
| 1   | AJ    | 150 | LYS  | 6.7  |
| 1   | A2    | 152 | TRP  | 6.6  |
| 1   | A4    | 149 | SER  | 6.5  |
| 1   | AV    | 101 | SER  | 6.5  |
| 1   | CV    | 101 | SER  | 6.3  |
| 1   | AL    | 101 | SER  | 6.3  |
| 1   | AH    | 107 | ASP  | 6.1  |
| 1   | AM    | 152 | TRP  | 6.1  |
| 1   | AW    | 153 | ALA  | 6.0  |
| 1   | CZ    | 145 | MET  | 5.7  |
| 1   | CL    | 101 | SER  | 5.6  |
| 1   | AO    | 150 | LYS  | 5.6  |
| 1   | CZ    | 113 | GLY  | 5.6  |
| 1   | CZ    | 78  | GLY  | 5.5  |
| 1   | BV    | 101 | SER  | 5.3  |
| 1   | CS    | 109 | PRO  | 5.2  |
| 1   | C4    | 145 | MET  | 5.2  |
| 1   | AR    | 153 | ALA  | 5.2  |
| 1   | CZ    | 73  | ALA  | 5.1  |
| 1   | CT    | 50  | ALA  | 5.1  |
| 1   | CS    | 62  | ALA  | 5.0  |
| 1   | AB    | 133 | ASN  | 5.0  |
| 1   | C4    | 92  | CYS  | 5.0  |
| 1   | CG    | 101 | SER  | 4.9  |
| 1   | AY    | 149 | SER  | 4.9  |
| 1   | CQ    | 74  | VAL  | 4.9  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C2    | 92  | CYS  | 4.9  |
| 1   | AW    | 44  | GLU  | 4.8  |
| 1   | AL    | 100 | ALA  | 4.8  |
| 1   | C1    | 50  | ALA  | 4.8  |
| 1   | A1    | 101 | SER  | 4.8  |
| 1   | AE    | 6   | HIS  | 4.8  |
| 1   | CS    | 102 | LEU  | 4.8  |
| 1   | A1    | 152 | TRP  | 4.7  |
| 1   | AB    | 101 | SER  | 4.7  |
| 1   | AH    | 5   | GLY  | 4.7  |
| 1   | AG    | 101 | SER  | 4.7  |
| 1   | BJ    | 151 | HIS  | 4.7  |
| 1   | AW    | 70  | LYS  | 4.6  |
| 1   | B2    | 152 | TRP  | 4.6  |
| 1   | AO    | 149 | SER  | 4.6  |
| 1   | AW    | 34  | LEU  | 4.6  |
| 1   | B1    | 100 | ALA  | 4.5  |
| 1   | CR    | 142 | ALA  | 4.5  |
| 1   | CQ    | 101 | SER  | 4.5  |
| 1   | C2    | 145 | MET  | 4.5  |
| 1   | AH    | 153 | ALA  | 4.5  |
| 1   | AG    | 35  | ASP  | 4.5  |
| 1   | CW    | 73  | ALA  | 4.5  |
| 1   | AW    | 132 | GLY  | 4.4  |
| 1   | CT    | 19  | GLY  | 4.4  |
| 1   | BC    | 69  | GLY  | 4.4  |
| 1   | AR    | 152 | TRP  | 4.4  |
| 1   | BO    | 149 | SER  | 4.4  |
| 1   | AH    | 35  | ASP  | 4.4  |
| 1   | AW    | 151 | HIS  | 4.4  |
| 1   | CS    | 117 | THR  | 4.4  |
| 1   | AW    | 133 | ASN  | 4.4  |
| 1   | AH    | 70  | LYS  | 4.4  |
| 1   | C3    | 78  | GLY  | 4.4  |
| 1   | AM    | 153 | ALA  | 4.4  |
| 1   | CS    | 74  | VAL  | 4.3  |
| 1   | CD    | 66  | ALA  | 4.3  |
| 1   | CS    | 73  | ALA  | 4.3  |
| 1   | AB    | 152 | TRP  | 4.3  |
| 1   | BB    | 101 | SER  | 4.3  |
| 1   | C3    | 139 | ALA  | 4.3  |
| 1   | AH    | 6   | HIS  | 4.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AJ    | 149 | SER  | 4.3  |
| 1   | AL    | 62  | ALA  | 4.3  |
| 1   | AN    | 153 | ALA  | 4.3  |
| 1   | C3    | 17  | VAL  | 4.2  |
| 1   | AE    | 151 | HIS  | 4.2  |
| 1   | CT    | 78  | GLY  | 4.1  |
| 1   | AI    | 45  | ASN  | 4.1  |
| 1   | AJ    | 151 | HIS  | 4.1  |
| 1   | AO    | 151 | HIS  | 4.1  |
| 1   | BJ    | 149 | SER  | 4.1  |
| 1   | C1    | 101 | SER  | 4.1  |
| 1   | AI    | 66  | ALA  | 4.1  |
| 1   | CM    | 152 | TRP  | 4.1  |
| 1   | AW    | 6   | HIS  | 4.1  |
| 1   | AX    | 152 | TRP  | 4.1  |
| 1   | AV    | 45  | ASN  | 4.1  |
| 1   | CS    | 33  | ALA  | 4.1  |
| 1   | AT    | 149 | SER  | 4.1  |
| 1   | AW    | 8   | VAL  | 4.0  |
| 1   | CT    | 102 | LEU  | 4.0  |
| 1   | AR    | 129 | THR  | 4.0  |
| 1   | AV    | 100 | ALA  | 4.0  |
| 1   | AJ    | 128 | GLY  | 4.0  |
| 1   | AH    | 50  | ALA  | 4.0  |
| 1   | AT    | 6   | HIS  | 4.0  |
| 1   | AM    | 57  | GLU  | 4.0  |
| 1   | BM    | 152 | TRP  | 4.0  |
| 1   | AX    | 66  | ALA  | 4.0  |
| 1   | BY    | 96  | ALA  | 4.0  |
| 1   | AG    | 152 | TRP  | 4.0  |
| 1   | AK    | 152 | TRP  | 4.0  |
| 1   | CF    | 18  | VAL  | 3.9  |
| 1   | AD    | 152 | TRP  | 3.9  |
| 1   | CY    | 151 | HIS  | 3.9  |
| 1   | AG    | 34  | LEU  | 3.9  |
| 1   | BM    | 153 | ALA  | 3.9  |
| 1   | CC    | 73  | ALA  | 3.9  |
| 1   | CP    | 133 | ASN  | 3.9  |
| 1   | CS    | 18  | VAL  | 3.9  |
| 1   | C1    | 40  | HIS  | 3.9  |
| 1   | AW    | 69  | GLY  | 3.9  |
| 1   | A3    | 66  | ALA  | 3.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AI    | 6   | HIS  | 3.9  |
| 1   | CT    | 9   | GLY  | 3.9  |
| 1   | CT    | 15  | GLY  | 3.9  |
| 1   | CV    | 50  | ALA  | 3.9  |
| 1   | CX    | 66  | ALA  | 3.9  |
| 1   | AF    | 45  | ASN  | 3.9  |
| 1   | AW    | 35  | ASP  | 3.9  |
| 1   | CZ    | 74  | VAL  | 3.9  |
| 1   | CF    | 109 | PRO  | 3.9  |
| 1   | CS    | 99  | VAL  | 3.9  |
| 1   | B1    | 101 | SER  | 3.9  |
| 1   | AR    | 35  | ASP  | 3.8  |
| 1   | AH    | 34  | LEU  | 3.8  |
| 1   | B2    | 153 | ALA  | 3.8  |
| 1   | CL    | 127 | ALA  | 3.8  |
| 1   | C4    | 151 | HIS  | 3.8  |
| 1   | CE    | 14  | VAL  | 3.8  |
| 1   | AM    | 45  | ASN  | 3.8  |
| 1   | CG    | 152 | TRP  | 3.8  |
| 1   | CS    | 153 | ALA  | 3.8  |
| 1   | BG    | 101 | SER  | 3.8  |
| 1   | AI    | 131 | ALA  | 3.8  |
| 1   | AO    | 5   | GLY  | 3.8  |
| 1   | AC    | 152 | TRP  | 3.8  |
| 1   | AF    | 57  | GLU  | 3.8  |
| 1   | BW    | 73  | ALA  | 3.7  |
| 1   | CS    | 55  | ALA  | 3.7  |
| 1   | AD    | 66  | ALA  | 3.7  |
| 1   | AG    | 100 | ALA  | 3.7  |
| 1   | AK    | 153 | ALA  | 3.7  |
| 1   | AU    | 146 | ALA  | 3.7  |
| 1   | BL    | 96  | ALA  | 3.7  |
| 1   | BO    | 73  | ALA  | 3.7  |
| 1   | CT    | 17  | VAL  | 3.7  |
| 1   | AC    | 68  | SER  | 3.7  |
| 1   | BY    | 149 | SER  | 3.7  |
| 1   | CN    | 66  | ALA  | 3.7  |
| 1   | AW    | 42  | VAL  | 3.7  |
| 1   | AJ    | 44  | GLU  | 3.7  |
| 1   | CK    | 45  | ASN  | 3.7  |
| 1   | BV    | 5   | GLY  | 3.7  |
| 1   | BV    | 44  | GLU  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AS    | 62  | ALA  | 3.7  |
| 1   | A1    | 100 | ALA  | 3.7  |
| 1   | AG    | 3   | PHE  | 3.7  |
| 1   | AH    | 12  | LEU  | 3.7  |
| 1   | BC    | 153 | ALA  | 3.6  |
| 1   | AM    | 133 | ASN  | 3.6  |
| 1   | AH    | 151 | HIS  | 3.6  |
| 1   | BL    | 100 | ALA  | 3.6  |
| 1   | AA    | 45  | ASN  | 3.6  |
| 1   | AL    | 44  | GLU  | 3.6  |
| 1   | AW    | 23  | GLU  | 3.6  |
| 1   | CT    | 33  | ALA  | 3.6  |
| 1   | CZ    | 14  | VAL  | 3.6  |
| 1   | AQ    | 100 | ALA  | 3.6  |
| 1   | AK    | 6   | HIS  | 3.6  |
| 1   | AN    | 151 | HIS  | 3.6  |
| 1   | AZ    | 35  | ASP  | 3.6  |
| 1   | AY    | 45  | ASN  | 3.6  |
| 1   | BL    | 101 | SER  | 3.6  |
| 1   | CK    | 101 | SER  | 3.6  |
| 1   | CF    | 19  | GLY  | 3.6  |
| 1   | AY    | 151 | HIS  | 3.6  |
| 1   | CT    | 52  | VAL  | 3.6  |
| 1   | CF    | 143 | ILE  | 3.5  |
| 1   | AH    | 57  | GLU  | 3.5  |
| 1   | CB    | 73  | ALA  | 3.5  |
| 1   | AW    | 68  | SER  | 3.5  |
| 1   | AW    | 102 | LEU  | 3.5  |
| 1   | A2    | 73  | ALA  | 3.5  |
| 1   | AM    | 23  | GLU  | 3.5  |
| 1   | CB    | 50  | ALA  | 3.5  |
| 1   | CQ    | 62  | ALA  | 3.5  |
| 1   | C3    | 18  | VAL  | 3.5  |
| 1   | CO    | 149 | SER  | 3.5  |
| 1   | AF    | 4   | GLU  | 3.5  |
| 1   | B2    | 88  | TYR  | 3.5  |
| 1   | AI    | 152 | TRP  | 3.5  |
| 1   | CS    | 61  | ILE  | 3.5  |
| 1   | CS    | 111 | ILE  | 3.5  |
| 1   | CT    | 5   | GLY  | 3.5  |
| 1   | A4    | 151 | HIS  | 3.5  |
| 1   | BB    | 107 | ASP  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A1    | 44  | GLU  | 3.5  |
| 1   | AG    | 45  | ASN  | 3.5  |
| 1   | C1    | 18  | VAL  | 3.4  |
| 1   | BQ    | 133 | ASN  | 3.4  |
| 1   | AN    | 6   | HIS  | 3.4  |
| 1   | CZ    | 61  | ILE  | 3.4  |
| 1   | BR    | 153 | ALA  | 3.4  |
| 1   | BX    | 66  | ALA  | 3.4  |
| 1   | C3    | 33  | ALA  | 3.4  |
| 1   | AG    | 23  | GLU  | 3.4  |
| 1   | C3    | 35  | ASP  | 3.4  |
| 1   | AK    | 133 | ASN  | 3.4  |
| 1   | AZ    | 133 | ASN  | 3.4  |
| 1   | CR    | 62  | ALA  | 3.4  |
| 1   | AG    | 6   | HIS  | 3.4  |
| 1   | C2    | 99  | VAL  | 3.4  |
| 1   | CS    | 35  | ASP  | 3.4  |
| 1   | AK    | 105 | GLN  | 3.4  |
| 1   | AR    | 34  | LEU  | 3.4  |
| 1   | AN    | 66  | ALA  | 3.4  |
| 1   | CT    | 49  | VAL  | 3.4  |
| 1   | AI    | 132 | GLY  | 3.4  |
| 1   | AB    | 34  | LEU  | 3.4  |
| 1   | AF    | 102 | LEU  | 3.4  |
| 1   | CV    | 115 | LEU  | 3.4  |
| 1   | AS    | 153 | ALA  | 3.4  |
| 1   | CJ    | 73  | ALA  | 3.4  |
| 1   | B4    | 149 | SER  | 3.4  |
| 1   | AI    | 151 | HIS  | 3.4  |
| 1   | AO    | 6   | HIS  | 3.4  |
| 1   | C2    | 19  | GLY  | 3.3  |
| 1   | AX    | 153 | ALA  | 3.3  |
| 1   | CT    | 16  | VAL  | 3.3  |
| 1   | CW    | 14  | VAL  | 3.3  |
| 1   | AV    | 3   | PHE  | 3.3  |
| 1   | BT    | 150 | LYS  | 3.3  |
| 1   | AM    | 151 | HIS  | 3.3  |
| 1   | CJ    | 5   | GLY  | 3.3  |
| 1   | AW    | 107 | ASP  | 3.3  |
| 1   | CJ    | 72  | ASP  | 3.3  |
| 1   | AB    | 142 | ALA  | 3.3  |
| 1   | AC    | 153 | ALA  | 3.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AI    | 33  | ALA  | 3.3  |
| 1   | CR    | 153 | ALA  | 3.3  |
| 1   | BK    | 45  | ASN  | 3.3  |
| 1   | AZ    | 4   | GLU  | 3.3  |
| 1   | AF    | 66  | ALA  | 3.3  |
| 1   | CT    | 99  | VAL  | 3.3  |
| 1   | AG    | 102 | LEU  | 3.3  |
| 1   | AM    | 43  | GLU  | 3.3  |
| 1   | AL    | 66  | ALA  | 3.3  |
| 1   | BH    | 59  | PRO  | 3.3  |
| 1   | CK    | 107 | ASP  | 3.3  |
| 1   | CP    | 78  | GLY  | 3.3  |
| 1   | CR    | 26  | THR  | 3.3  |
| 1   | AQ    | 137 | GLU  | 3.3  |
| 1   | AQ    | 3   | PHE  | 3.3  |
| 1   | CP    | 123 | ALA  | 3.3  |
| 1   | AH    | 68  | SER  | 3.3  |
| 1   | BL    | 152 | TRP  | 3.3  |
| 1   | AL    | 35  | ASP  | 3.3  |
| 1   | B4    | 45  | ASN  | 3.3  |
| 1   | AL    | 23  | GLU  | 3.3  |
| 1   | BF    | 4   | GLU  | 3.3  |
| 1   | AU    | 6   | HIS  | 3.3  |
| 1   | AH    | 66  | ALA  | 3.2  |
| 1   | CV    | 127 | ALA  | 3.2  |
| 1   | B3    | 35  | ASP  | 3.2  |
| 1   | CR    | 107 | ASP  | 3.2  |
| 1   | AX    | 45  | ASN  | 3.2  |
| 1   | AZ    | 45  | ASN  | 3.2  |
| 1   | AX    | 43  | GLU  | 3.2  |
| 1   | BV    | 100 | ALA  | 3.2  |
| 1   | CZ    | 18  | VAL  | 3.2  |
| 1   | AN    | 152 | TRP  | 3.2  |
| 1   | C1    | 19  | GLY  | 3.2  |
| 1   | AI    | 129 | THR  | 3.2  |
| 1   | AQ    | 43  | GLU  | 3.2  |
| 1   | A3    | 23  | GLU  | 3.2  |
| 1   | CT    | 66  | ALA  | 3.2  |
| 1   | AM    | 34  | LEU  | 3.2  |
| 1   | AX    | 35  | ASP  | 3.2  |
| 1   | C3    | 9   | GLY  | 3.2  |
| 1   | AA    | 47  | ILE  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CS    | 94  | GLU  | 3.2  |
| 1   | AC    | 151 | HIS  | 3.2  |
| 1   | BC    | 29  | LEU  | 3.2  |
| 1   | CQ    | 152 | TRP  | 3.2  |
| 1   | CW    | 152 | TRP  | 3.2  |
| 1   | CS    | 15  | GLY  | 3.2  |
| 1   | C4    | 133 | ASN  | 3.2  |
| 1   | C3    | 42  | VAL  | 3.2  |
| 1   | C3    | 50  | ALA  | 3.2  |
| 1   | C4    | 146 | ALA  | 3.2  |
| 1   | AI    | 128 | GLY  | 3.2  |
| 1   | BV    | 152 | TRP  | 3.2  |
| 1   | CV    | 128 | GLY  | 3.2  |
| 1   | AS    | 133 | ASN  | 3.2  |
| 1   | C3    | 101 | SER  | 3.2  |
| 1   | CD    | 29  | LEU  | 3.2  |
| 1   | AX    | 69  | GLY  | 3.1  |
| 1   | CC    | 152 | TRP  | 3.1  |
| 1   | C4    | 20  | ARG  | 3.1  |
| 1   | AH    | 88  | TYR  | 3.1  |
| 1   | A4    | 150 | LYS  | 3.1  |
| 1   | CS    | 65  | MET  | 3.1  |
| 1   | AP    | 146 | ALA  | 3.1  |
| 1   | AR    | 68  | SER  | 3.1  |
| 1   | BB    | 100 | ALA  | 3.1  |
| 1   | CF    | 14  | VAL  | 3.1  |
| 1   | CT    | 100 | ALA  | 3.1  |
| 1   | CS    | 152 | TRP  | 3.1  |
| 1   | AJ    | 102 | LEU  | 3.1  |
| 1   | AN    | 101 | SER  | 3.1  |
| 1   | CT    | 40  | HIS  | 3.1  |
| 1   | A4    | 5   | GLY  | 3.1  |
| 1   | CU    | 45  | ASN  | 3.1  |
| 1   | BY    | 4   | GLU  | 3.1  |
| 1   | CS    | 123 | ALA  | 3.1  |
| 1   | CR    | 92  | CYS  | 3.1  |
| 1   | AR    | 6   | HIS  | 3.1  |
| 1   | BT    | 151 | HIS  | 3.1  |
| 1   | AJ    | 14  | VAL  | 3.1  |
| 1   | AR    | 107 | ASP  | 3.1  |
| 1   | CL    | 107 | ASP  | 3.1  |
| 1   | CP    | 9   | GLY  | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CX    | 132 | GLY  | 3.1  |
| 1   | AB    | 84  | ALA  | 3.1  |
| 1   | AK    | 45  | ASN  | 3.1  |
| 1   | CC    | 123 | ALA  | 3.1  |
| 1   | C4    | 144 | GLU  | 3.1  |
| 1   | C4    | 37  | LEU  | 3.1  |
| 1   | BT    | 128 | GLY  | 3.1  |
| 1   | C3    | 40  | HIS  | 3.1  |
| 1   | AE    | 140 | VAL  | 3.0  |
| 1   | BW    | 153 | ALA  | 3.0  |
| 1   | AH    | 71  | TYR  | 3.0  |
| 1   | AY    | 150 | LYS  | 3.0  |
| 1   | BC    | 152 | TRP  | 3.0  |
| 1   | BW    | 152 | TRP  | 3.0  |
| 1   | AI    | 36  | GLY  | 3.0  |
| 1   | CQ    | 9   | GLY  | 3.0  |
| 1   | AK    | 101 | SER  | 3.0  |
| 1   | AN    | 67  | ASN  | 3.0  |
| 1   | AL    | 152 | TRP  | 3.0  |
| 1   | AG    | 86  | THR  | 3.0  |
| 1   | CZ    | 76  | THR  | 3.0  |
| 1   | AY    | 101 | SER  | 3.0  |
| 1   | CG    | 91  | VAL  | 3.0  |
| 1   | AY    | 33  | ALA  | 3.0  |
| 1   | AY    | 55  | ALA  | 3.0  |
| 1   | AP    | 4   | GLU  | 3.0  |
| 1   | AN    | 128 | GLY  | 3.0  |
| 1   | AO    | 9   | GLY  | 3.0  |
| 1   | CW    | 69  | GLY  | 3.0  |
| 1   | AW    | 119 | THR  | 3.0  |
| 1   | AZ    | 6   | HIS  | 3.0  |
| 1   | BD    | 66  | ALA  | 3.0  |
| 1   | CR    | 66  | ALA  | 3.0  |
| 1   | CR    | 90  | TYR  | 3.0  |
| 1   | C3    | 133 | ASN  | 3.0  |
| 1   | AI    | 43  | GLU  | 3.0  |
| 1   | AX    | 57  | GLU  | 3.0  |
| 1   | C4    | 61  | ILE  | 3.0  |
| 1   | AR    | 69  | GLY  | 3.0  |
| 1   | CD    | 128 | GLY  | 3.0  |
| 1   | AZ    | 8   | VAL  | 3.0  |
| 1   | BM    | 68  | SER  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AF    | 35  | ASP  | 3.0  |
| 1   | AQ    | 46  | ASP  | 3.0  |
| 1   | CF    | 73  | ALA  | 3.0  |
| 1   | CG    | 127 | ALA  | 3.0  |
| 1   | C4    | 142 | ALA  | 3.0  |
| 1   | AC    | 23  | GLU  | 3.0  |
| 1   | AD    | 4   | GLU  | 3.0  |
| 1   | CK    | 4   | GLU  | 3.0  |
| 1   | CZ    | 117 | THR  | 3.0  |
| 1   | C1    | 86  | THR  | 3.0  |
| 1   | C4    | 99  | VAL  | 3.0  |
| 1   | CK    | 73  | ALA  | 3.0  |
| 1   | AE    | 45  | ASN  | 2.9  |
| 1   | AS    | 4   | GLU  | 2.9  |
| 1   | CV    | 4   | GLU  | 2.9  |
| 1   | CF    | 5   | GLY  | 2.9  |
| 1   | CC    | 50  | ALA  | 2.9  |
| 1   | AJ    | 35  | ASP  | 2.9  |
| 1   | AQ    | 35  | ASP  | 2.9  |
| 1   | AV    | 35  | ASP  | 2.9  |
| 1   | A3    | 89  | ASP  | 2.9  |
| 1   | AB    | 6   | HIS  | 2.9  |
| 1   | AW    | 67  | ASN  | 2.9  |
| 1   | AJ    | 56  | PHE  | 2.9  |
| 1   | AV    | 152 | TRP  | 2.9  |
| 1   | C3    | 41  | GLY  | 2.9  |
| 1   | AI    | 105 | GLN  | 2.9  |
| 1   | CZ    | 62  | ALA  | 2.9  |
| 1   | AD    | 35  | ASP  | 2.9  |
| 1   | AX    | 6   | HIS  | 2.9  |
| 1   | AY    | 6   | HIS  | 2.9  |
| 1   | AI    | 44  | GLU  | 2.9  |
| 1   | AU    | 45  | ASN  | 2.9  |
| 1   | CZ    | 93  | ASN  | 2.9  |
| 1   | AH    | 132 | GLY  | 2.9  |
| 1   | C4    | 123 | ALA  | 2.9  |
| 1   | AI    | 12  | LEU  | 2.9  |
| 1   | BA    | 107 | ASP  | 2.9  |
| 1   | AJ    | 45  | ASN  | 2.9  |
| 1   | AR    | 67  | ASN  | 2.9  |
| 1   | AX    | 67  | ASN  | 2.9  |
| 1   | CF    | 6   | HIS  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CQ    | 40  | HIS  | 2.9  |
| 1   | C2    | 85  | THR  | 2.9  |
| 1   | BT    | 146 | ALA  | 2.9  |
| 1   | CQ    | 73  | ALA  | 2.9  |
| 1   | CZ    | 146 | ALA  | 2.9  |
| 1   | CQ    | 108 | ILE  | 2.9  |
| 1   | C4    | 29  | LEU  | 2.9  |
| 1   | AQ    | 45  | ASN  | 2.9  |
| 1   | CS    | 40  | HIS  | 2.9  |
| 1   | CT    | 72  | ASP  | 2.9  |
| 1   | CW    | 72  | ASP  | 2.9  |
| 1   | AG    | 52  | VAL  | 2.9  |
| 1   | A1    | 41  | GLY  | 2.9  |
| 1   | C3    | 135 | GLY  | 2.9  |
| 1   | CT    | 116 | THR  | 2.9  |
| 1   | AB    | 127 | ALA  | 2.9  |
| 1   | BX    | 153 | ALA  | 2.9  |
| 1   | C4    | 33  | ALA  | 2.9  |
| 1   | AL    | 46  | ASP  | 2.8  |
| 1   | BQ    | 101 | SER  | 2.8  |
| 1   | CK    | 128 | GLY  | 2.8  |
| 1   | CX    | 19  | GLY  | 2.8  |
| 1   | AI    | 153 | ALA  | 2.8  |
| 1   | BN    | 153 | ALA  | 2.8  |
| 1   | CH    | 152 | TRP  | 2.8  |
| 1   | CR    | 148 | LEU  | 2.8  |
| 1   | C1    | 34  | LEU  | 2.8  |
| 1   | C4    | 116 | THR  | 2.8  |
| 1   | AO    | 14  | VAL  | 2.8  |
| 1   | BW    | 4   | GLU  | 2.8  |
| 1   | AK    | 9   | GLY  | 2.8  |
| 1   | AQ    | 9   | GLY  | 2.8  |
| 1   | AX    | 151 | HIS  | 2.8  |
| 1   | CT    | 14  | VAL  | 2.8  |
| 1   | C1    | 17  | VAL  | 2.8  |
| 1   | CZ    | 9   | GLY  | 2.8  |
| 1   | C4    | 102 | LEU  | 2.8  |
| 1   | AS    | 55  | ALA  | 2.8  |
| 1   | C1    | 55  | ALA  | 2.8  |
| 1   | C2    | 62  | ALA  | 2.8  |
| 1   | C1    | 51  | TRP  | 2.8  |
| 1   | BW    | 65  | MET  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AI    | 99  | VAL  | 2.8  |
| 1   | AK    | 43  | GLU  | 2.8  |
| 1   | C3    | 143 | ILE  | 2.8  |
| 1   | A3    | 45  | ASN  | 2.8  |
| 1   | B1    | 133 | ASN  | 2.8  |
| 1   | C4    | 95  | VAL  | 2.8  |
| 1   | AJ    | 40  | HIS  | 2.8  |
| 1   | BI    | 5   | GLY  | 2.8  |
| 1   | CS    | 113 | GLY  | 2.8  |
| 1   | AC    | 106 | THR  | 2.8  |
| 1   | AW    | 129 | THR  | 2.8  |
| 1   | CC    | 153 | ALA  | 2.8  |
| 1   | CF    | 33  | ALA  | 2.8  |
| 1   | AK    | 65  | MET  | 2.8  |
| 1   | CB    | 152 | TRP  | 2.8  |
| 1   | CZ    | 59  | PRO  | 2.8  |
| 1   | CP    | 14  | VAL  | 2.8  |
| 1   | CS    | 52  | VAL  | 2.8  |
| 1   | C4    | 101 | SER  | 2.8  |
| 1   | AB    | 23  | GLU  | 2.8  |
| 1   | AB    | 45  | ASN  | 2.8  |
| 1   | AX    | 22  | ASN  | 2.8  |
| 1   | B2    | 69  | GLY  | 2.8  |
| 1   | C3    | 19  | GLY  | 2.8  |
| 1   | AV    | 6   | HIS  | 2.8  |
| 1   | A3    | 151 | HIS  | 2.8  |
| 1   | BO    | 151 | HIS  | 2.8  |
| 1   | CX    | 40  | HIS  | 2.8  |
| 1   | B3    | 72  | ASP  | 2.8  |
| 1   | AW    | 12  | LEU  | 2.8  |
| 1   | CD    | 7   | LEU  | 2.8  |
| 1   | AP    | 101 | SER  | 2.8  |
| 1   | CS    | 14  | VAL  | 2.8  |
| 1   | CZ    | 52  | VAL  | 2.8  |
| 1   | BC    | 15  | GLY  | 2.8  |
| 1   | CF    | 31  | GLY  | 2.8  |
| 1   | CL    | 44  | GLU  | 2.8  |
| 1   | C3    | 128 | GLY  | 2.8  |
| 1   | AK    | 142 | ALA  | 2.8  |
| 1   | AV    | 146 | ALA  | 2.8  |
| 1   | CC    | 66  | ALA  | 2.8  |
| 1   | CR    | 50  | ALA  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CU    | 146 | ALA  | 2.8  |
| 1   | AF    | 6   | HIS  | 2.8  |
| 1   | CZ    | 6   | HIS  | 2.8  |
| 1   | CF    | 92  | CYS  | 2.8  |
| 1   | A3    | 152 | TRP  | 2.8  |
| 1   | CT    | 30  | LEU  | 2.8  |
| 1   | CV    | 152 | TRP  | 2.8  |
| 1   | C4    | 115 | LEU  | 2.8  |
| 1   | AH    | 128 | GLY  | 2.8  |
| 1   | AV    | 9   | GLY  | 2.8  |
| 1   | CH    | 69  | GLY  | 2.8  |
| 1   | AI    | 50  | ALA  | 2.8  |
| 1   | AO    | 133 | ASN  | 2.8  |
| 1   | B3    | 142 | ALA  | 2.8  |
| 1   | C1    | 133 | ASN  | 2.8  |
| 1   | B4    | 151 | HIS  | 2.7  |
| 1   | AJ    | 29  | LEU  | 2.7  |
| 1   | CR    | 110 | VAL  | 2.7  |
| 1   | C1    | 99  | VAL  | 2.7  |
| 1   | AT    | 150 | LYS  | 2.7  |
| 1   | CQ    | 90  | TYR  | 2.7  |
| 1   | AE    | 57  | GLU  | 2.7  |
| 1   | AO    | 57  | GLU  | 2.7  |
| 1   | CT    | 36  | GLY  | 2.7  |
| 1   | AL    | 45  | ASN  | 2.7  |
| 1   | C2    | 153 | ALA  | 2.7  |
| 1   | C3    | 117 | THR  | 2.7  |
| 1   | CT    | 126 | ARG  | 2.7  |
| 1   | CJ    | 151 | HIS  | 2.7  |
| 1   | AE    | 107 | ASP  | 2.7  |
| 1   | AO    | 152 | TRP  | 2.7  |
| 1   | AO    | 18  | VAL  | 2.7  |
| 1   | BY    | 92  | CYS  | 2.7  |
| 1   | AW    | 136 | TYR  | 2.7  |
| 1   | AF    | 153 | ALA  | 2.7  |
| 1   | AL    | 153 | ALA  | 2.7  |
| 1   | AM    | 5   | GLY  | 2.7  |
| 1   | CG    | 50  | ALA  | 2.7  |
| 1   | CY    | 83  | GLY  | 2.7  |
| 1   | CT    | 77  | LEU  | 2.7  |
| 1   | CZ    | 50  | ALA  | 2.7  |
| 1   | C3    | 32  | GLY  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AN    | 45  | ASN  | 2.7  |
| 1   | AV    | 10  | THR  | 2.7  |
| 1   | BG    | 44  | GLU  | 2.7  |
| 1   | BH    | 43  | GLU  | 2.7  |
| 1   | CE    | 151 | HIS  | 2.7  |
| 1   | AJ    | 101 | SER  | 2.7  |
| 1   | C3    | 59  | PRO  | 2.7  |
| 1   | BS    | 153 | ALA  | 2.7  |
| 1   | CF    | 15  | GLY  | 2.7  |
| 1   | CZ    | 100 | ALA  | 2.7  |
| 1   | AG    | 10  | THR  | 2.7  |
| 1   | AV    | 43  | GLU  | 2.7  |
| 1   | AV    | 86  | THR  | 2.7  |
| 1   | CL    | 23  | GLU  | 2.7  |
| 1   | AT    | 151 | HIS  | 2.7  |
| 1   | C4    | 87  | HIS  | 2.7  |
| 1   | AF    | 101 | SER  | 2.7  |
| 1   | AW    | 14  | VAL  | 2.7  |
| 1   | CR    | 14  | VAL  | 2.7  |
| 1   | CS    | 110 | VAL  | 2.7  |
| 1   | AI    | 35  | ASP  | 2.7  |
| 1   | A2    | 48  | ASP  | 2.7  |
| 1   | BB    | 152 | TRP  | 2.7  |
| 1   | AX    | 102 | LEU  | 2.7  |
| 1   | CR    | 109 | PRO  | 2.7  |
| 1   | AU    | 105 | GLN  | 2.7  |
| 1   | AF    | 127 | ALA  | 2.7  |
| 1   | AH    | 127 | ALA  | 2.7  |
| 1   | AK    | 146 | ALA  | 2.7  |
| 1   | A3    | 73  | ALA  | 2.7  |
| 1   | CS    | 142 | ALA  | 2.7  |
| 1   | AF    | 116 | THR  | 2.7  |
| 1   | AI    | 144 | GLU  | 2.7  |
| 1   | AM    | 92  | CYS  | 2.7  |
| 1   | BU    | 4   | GLU  | 2.7  |
| 1   | CS    | 86  | THR  | 2.7  |
| 1   | AK    | 28  | LYS  | 2.7  |
| 1   | CT    | 150 | LYS  | 2.7  |
| 1   | AC    | 6   | HIS  | 2.7  |
| 1   | BW    | 68  | SER  | 2.7  |
| 1   | CP    | 87  | HIS  | 2.7  |
| 1   | AN    | 8   | VAL  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AV    | 8   | VAL  | 2.7  |
| 1   | B4    | 34  | LEU  | 2.7  |
| 1   | C2    | 17  | VAL  | 2.7  |
| 1   | AC    | 35  | ASP  | 2.7  |
| 1   | AX    | 107 | ASP  | 2.7  |
| 1   | BR    | 35  | ASP  | 2.7  |
| 1   | AD    | 84  | ALA  | 2.7  |
| 1   | AW    | 96  | ALA  | 2.7  |
| 1   | CD    | 111 | ILE  | 2.7  |
| 1   | CR    | 135 | GLY  | 2.7  |
| 1   | AV    | 23  | GLU  | 2.7  |
| 1   | AQ    | 6   | HIS  | 2.6  |
| 1   | CS    | 17  | VAL  | 2.6  |
| 1   | C1    | 16  | VAL  | 2.6  |
| 1   | AC    | 69  | GLY  | 2.6  |
| 1   | AH    | 96  | ALA  | 2.6  |
| 1   | AK    | 69  | GLY  | 2.6  |
| 1   | BI    | 135 | GLY  | 2.6  |
| 1   | C1    | 9   | GLY  | 2.6  |
| 1   | CC    | 86  | THR  | 2.6  |
| 1   | C3    | 116 | THR  | 2.6  |
| 1   | CY    | 94  | GLU  | 2.6  |
| 1   | AR    | 102 | LEU  | 2.6  |
| 1   | AB    | 68  | SER  | 2.6  |
| 1   | CO    | 92  | CYS  | 2.6  |
| 1   | CQ    | 92  | CYS  | 2.6  |
| 1   | CJ    | 17  | VAL  | 2.6  |
| 1   | CQ    | 42  | VAL  | 2.6  |
| 1   | CZ    | 95  | VAL  | 2.6  |
| 1   | A1    | 69  | GLY  | 2.6  |
| 1   | BH    | 152 | TRP  | 2.6  |
| 1   | CK    | 15  | GLY  | 2.6  |
| 1   | CO    | 107 | ASP  | 2.6  |
| 1   | CQ    | 107 | ASP  | 2.6  |
| 1   | B3    | 4   | GLU  | 2.6  |
| 1   | CZ    | 65  | MET  | 2.6  |
| 1   | A2    | 34  | LEU  | 2.6  |
| 1   | CQ    | 133 | ASN  | 2.6  |
| 1   | AH    | 47  | ILE  | 2.6  |
| 1   | CT    | 13  | LYS  | 2.6  |
| 1   | CZ    | 134 | LYS  | 2.6  |
| 1   | AH    | 9   | GLY  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AJ    | 31  | GLY  | 2.6  |
| 1   | AZ    | 146 | ALA  | 2.6  |
| 1   | CV    | 78  | GLY  | 2.6  |
| 1   | CW    | 66  | ALA  | 2.6  |
| 1   | A3    | 35  | ASP  | 2.6  |
| 1   | BE    | 7   | LEU  | 2.6  |
| 1   | CA    | 116 | THR  | 2.6  |
| 1   | BG    | 107 | ASP  | 2.6  |
| 1   | A4    | 44  | GLU  | 2.6  |
| 1   | BP    | 4   | GLU  | 2.6  |
| 1   | CB    | 101 | SER  | 2.6  |
| 1   | AM    | 42  | VAL  | 2.6  |
| 1   | AL    | 13  | LYS  | 2.6  |
| 1   | CR    | 64  | LYS  | 2.6  |
| 1   | AA    | 73  | ALA  | 2.6  |
| 1   | AF    | 151 | HIS  | 2.6  |
| 1   | AJ    | 131 | ALA  | 2.6  |
| 1   | AL    | 6   | HIS  | 2.6  |
| 1   | AY    | 73  | ALA  | 2.6  |
| 1   | AD    | 41  | GLY  | 2.6  |
| 1   | AO    | 65  | MET  | 2.6  |
| 1   | CC    | 116 | THR  | 2.6  |
| 1   | CS    | 90  | TYR  | 2.6  |
| 1   | AI    | 107 | ASP  | 2.6  |
| 1   | AK    | 35  | ASP  | 2.6  |
| 1   | A4    | 43  | GLU  | 2.6  |
| 1   | BS    | 4   | GLU  | 2.6  |
| 1   | CL    | 4   | GLU  | 2.6  |
| 1   | CM    | 4   | GLU  | 2.6  |
| 1   | AI    | 22  | ASN  | 2.6  |
| 1   | CD    | 133 | ASN  | 2.6  |
| 1   | AL    | 99  | VAL  | 2.6  |
| 1   | CE    | 96  | ALA  | 2.6  |
| 1   | CF    | 65  | MET  | 2.6  |
| 1   | CF    | 153 | ALA  | 2.6  |
| 1   | CX    | 153 | ALA  | 2.6  |
| 1   | CZ    | 127 | ALA  | 2.6  |
| 1   | AG    | 147 | HIS  | 2.6  |
| 1   | AL    | 69  | GLY  | 2.6  |
| 1   | CS    | 19  | GLY  | 2.6  |
| 1   | CS    | 78  | GLY  | 2.6  |
| 1   | AJ    | 88  | TYR  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CF    | 116 | THR  | 2.6  |
| 1   | AO    | 23  | GLU  | 2.6  |
| 1   | CC    | 23  | GLU  | 2.6  |
| 1   | CO    | 4   | GLU  | 2.6  |
| 1   | CZ    | 57  | GLU  | 2.6  |
| 1   | C4    | 23  | GLU  | 2.6  |
| 1   | BS    | 107 | ASP  | 2.6  |
| 1   | A1    | 133 | ASN  | 2.6  |
| 1   | CT    | 18  | VAL  | 2.6  |
| 1   | C2    | 74  | VAL  | 2.6  |
| 1   | C4    | 13  | LYS  | 2.6  |
| 1   | BV    | 145 | MET  | 2.6  |
| 1   | AK    | 31  | GLY  | 2.6  |
| 1   | BW    | 69  | GLY  | 2.6  |
| 1   | C1    | 41  | GLY  | 2.6  |
| 1   | C4    | 5   | GLY  | 2.6  |
| 1   | C4    | 32  | GLY  | 2.6  |
| 1   | CJ    | 6   | HIS  | 2.5  |
| 1   | CS    | 71  | TYR  | 2.5  |
| 1   | C1    | 152 | TRP  | 2.5  |
| 1   | AY    | 4   | GLU  | 2.5  |
| 1   | A2    | 43  | GLU  | 2.5  |
| 1   | BG    | 43  | GLU  | 2.5  |
| 1   | CT    | 144 | GLU  | 2.5  |
| 1   | AW    | 110 | VAL  | 2.5  |
| 1   | CQ    | 110 | VAL  | 2.5  |
| 1   | CZ    | 8   | VAL  | 2.5  |
| 1   | AB    | 100 | ALA  | 2.5  |
| 1   | AG    | 131 | ALA  | 2.5  |
| 1   | AH    | 73  | ALA  | 2.5  |
| 1   | BJ    | 55  | ALA  | 2.5  |
| 1   | CA    | 66  | ALA  | 2.5  |
| 1   | CI    | 153 | ALA  | 2.5  |
| 1   | CW    | 55  | ALA  | 2.5  |
| 1   | BD    | 128 | GLY  | 2.5  |
| 1   | C1    | 132 | GLY  | 2.5  |
| 1   | CO    | 26  | THR  | 2.5  |
| 1   | CT    | 129 | THR  | 2.5  |
| 1   | BT    | 20  | ARG  | 2.5  |
| 1   | CD    | 23  | GLU  | 2.5  |
| 1   | CQ    | 23  | GLU  | 2.5  |
| 1   | CZ    | 94  | GLU  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AP    | 29  | LEU  | 2.5  |
| 1   | AV    | 34  | LEU  | 2.5  |
| 1   | CF    | 7   | LEU  | 2.5  |
| 1   | CZ    | 77  | LEU  | 2.5  |
| 1   | AH    | 45  | ASN  | 2.5  |
| 1   | AJ    | 67  | ASN  | 2.5  |
| 1   | BC    | 107 | ASP  | 2.5  |
| 1   | AK    | 66  | ALA  | 2.5  |
| 1   | A3    | 153 | ALA  | 2.5  |
| 1   | C1    | 127 | ALA  | 2.5  |
| 1   | AO    | 64  | LYS  | 2.5  |
| 1   | A3    | 130 | LYS  | 2.5  |
| 1   | CZ    | 25  | ILE  | 2.5  |
| 1   | C4    | 150 | LYS  | 2.5  |
| 1   | AH    | 129 | THR  | 2.5  |
| 1   | BH    | 151 | HIS  | 2.5  |
| 1   | AX    | 101 | SER  | 2.5  |
| 1   | CJ    | 149 | SER  | 2.5  |
| 1   | AG    | 99  | VAL  | 2.5  |
| 1   | A1    | 99  | VAL  | 2.5  |
| 1   | CX    | 17  | VAL  | 2.5  |
| 1   | CX    | 18  | VAL  | 2.5  |
| 1   | C4    | 60  | LEU  | 2.5  |
| 1   | AG    | 56  | PHE  | 2.5  |
| 1   | AU    | 35  | ASP  | 2.5  |
| 1   | CA    | 107 | ASP  | 2.5  |
| 1   | CF    | 48  | ASP  | 2.5  |
| 1   | C2    | 33  | ALA  | 2.5  |
| 1   | AG    | 9   | GLY  | 2.5  |
| 1   | AJ    | 5   | GLY  | 2.5  |
| 1   | B2    | 47  | ILE  | 2.5  |
| 1   | CS    | 75  | ILE  | 2.5  |
| 1   | CT    | 58  | ILE  | 2.5  |
| 1   | C3    | 113 | GLY  | 2.5  |
| 1   | AF    | 147 | HIS  | 2.5  |
| 1   | AJ    | 6   | HIS  | 2.5  |
| 1   | AQ    | 101 | SER  | 2.5  |
| 1   | A1    | 102 | LEU  | 2.5  |
| 1   | BW    | 151 | HIS  | 2.5  |
| 1   | CS    | 29  | LEU  | 2.5  |
| 1   | CS    | 60  | LEU  | 2.5  |
| 1   | CT    | 151 | HIS  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CZ    | 102 | LEU  | 2.5  |
| 1   | C2    | 102 | LEU  | 2.5  |
| 1   | AI    | 17  | VAL  | 2.5  |
| 1   | AI    | 18  | VAL  | 2.5  |
| 1   | AX    | 52  | VAL  | 2.5  |
| 1   | AC    | 44  | GLU  | 2.5  |
| 1   | AG    | 43  | GLU  | 2.5  |
| 1   | AM    | 44  | GLU  | 2.5  |
| 1   | CM    | 23  | GLU  | 2.5  |
| 1   | CP    | 145 | MET  | 2.5  |
| 1   | C2    | 152 | TRP  | 2.5  |
| 1   | C4    | 94  | GLU  | 2.5  |
| 1   | AH    | 141 | ALA  | 2.5  |
| 1   | AW    | 72  | ASP  | 2.5  |
| 1   | A2    | 35  | ASP  | 2.5  |
| 1   | BN    | 55  | ALA  | 2.5  |
| 1   | BW    | 46  | ASP  | 2.5  |
| 1   | B2    | 96  | ALA  | 2.5  |
| 1   | CK    | 134 | LYS  | 2.5  |
| 1   | CS    | 143 | ILE  | 2.5  |
| 1   | CZ    | 35  | ASP  | 2.5  |
| 1   | CZ    | 143 | ILE  | 2.5  |
| 1   | C4    | 73  | ALA  | 2.5  |
| 1   | AA    | 128 | GLY  | 2.5  |
| 1   | BC    | 5   | GLY  | 2.5  |
| 1   | AB    | 60  | LEU  | 2.5  |
| 1   | AH    | 20  | ARG  | 2.5  |
| 1   | A2    | 86  | THR  | 2.5  |
| 1   | CC    | 12  | LEU  | 2.5  |
| 1   | CR    | 86  | THR  | 2.5  |
| 1   | C2    | 106 | THR  | 2.5  |
| 1   | AS    | 68  | SER  | 2.5  |
| 1   | CQ    | 95  | VAL  | 2.5  |
| 1   | CS    | 8   | VAL  | 2.5  |
| 1   | AU    | 23  | GLU  | 2.5  |
| 1   | A2    | 44  | GLU  | 2.5  |
| 1   | BU    | 43  | GLU  | 2.5  |
| 1   | CZ    | 51  | TRP  | 2.5  |
| 1   | AI    | 133 | ASN  | 2.5  |
| 1   | BZ    | 45  | ASN  | 2.5  |
| 1   | CE    | 150 | LYS  | 2.5  |
| 1   | CR    | 63  | LYS  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AL    | 47  | ILE  | 2.5  |
| 1   | AH    | 105 | GLN  | 2.5  |
| 1   | AV    | 50  | ALA  | 2.5  |
| 1   | AW    | 105 | GLN  | 2.5  |
| 1   | BI    | 66  | ALA  | 2.5  |
| 1   | AV    | 72  | ASP  | 2.5  |
| 1   | CB    | 9   | GLY  | 2.5  |
| 1   | CE    | 128 | GLY  | 2.5  |
| 1   | AH    | 86  | THR  | 2.5  |
| 1   | AI    | 117 | THR  | 2.5  |
| 1   | AX    | 26  | THR  | 2.5  |
| 1   | AX    | 86  | THR  | 2.5  |
| 1   | CT    | 117 | THR  | 2.5  |
| 1   | AJ    | 52  | VAL  | 2.5  |
| 1   | AR    | 110 | VAL  | 2.5  |
| 1   | CA    | 6   | HIS  | 2.4  |
| 1   | CX    | 6   | HIS  | 2.4  |
| 1   | A1    | 13  | LYS  | 2.4  |
| 1   | BG    | 4   | GLU  | 2.4  |
| 1   | AL    | 143 | ILE  | 2.4  |
| 1   | CG    | 51  | TRP  | 2.4  |
| 1   | AQ    | 133 | ASN  | 2.4  |
| 1   | CX    | 131 | ALA  | 2.4  |
| 1   | AY    | 109 | PRO  | 2.4  |
| 1   | CP    | 37  | LEU  | 2.4  |
| 1   | CS    | 59  | PRO  | 2.4  |
| 1   | AX    | 83  | GLY  | 2.4  |
| 1   | CS    | 36  | GLY  | 2.4  |
| 1   | AC    | 107 | ASP  | 2.4  |
| 1   | AO    | 85  | THR  | 2.4  |
| 1   | CJ    | 116 | THR  | 2.4  |
| 1   | CR    | 145 | MET  | 2.4  |
| 1   | C2    | 138 | SER  | 2.4  |
| 1   | A1    | 2   | VAL  | 2.4  |
| 1   | AC    | 71  | TYR  | 2.4  |
| 1   | CY    | 88  | TYR  | 2.4  |
| 1   | AN    | 44  | GLU  | 2.4  |
| 1   | AV    | 147 | HIS  | 2.4  |
| 1   | CK    | 143 | ILE  | 2.4  |
| 1   | CL    | 25  | ILE  | 2.4  |
| 1   | CS    | 144 | GLU  | 2.4  |
| 1   | AM    | 96  | ALA  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A2    | 127 | ALA  | 2.4  |
| 1   | CL    | 133 | ASN  | 2.4  |
| 1   | CS    | 141 | ALA  | 2.4  |
| 1   | CR    | 65  | MET  | 2.4  |
| 1   | C4    | 9   | GLY  | 2.4  |
| 1   | AC    | 101 | SER  | 2.4  |
| 1   | CB    | 107 | ASP  | 2.4  |
| 1   | CS    | 72  | ASP  | 2.4  |
| 1   | AO    | 8   | VAL  | 2.4  |
| 1   | CB    | 8   | VAL  | 2.4  |
| 1   | CT    | 80  | VAL  | 2.4  |
| 1   | AA    | 3   | PHE  | 2.4  |
| 1   | AH    | 136 | TYR  | 2.4  |
| 1   | AG    | 151 | HIS  | 2.4  |
| 1   | AR    | 23  | GLU  | 2.4  |
| 1   | AU    | 102 | LEU  | 2.4  |
| 1   | AX    | 23  | GLU  | 2.4  |
| 1   | A2    | 23  | GLU  | 2.4  |
| 1   | B1    | 23  | GLU  | 2.4  |
| 1   | AJ    | 100 | ALA  | 2.4  |
| 1   | AH    | 133 | ASN  | 2.4  |
| 1   | BB    | 133 | ASN  | 2.4  |
| 1   | AF    | 53  | PRO  | 2.4  |
| 1   | AK    | 19  | GLY  | 2.4  |
| 1   | BJ    | 5   | GLY  | 2.4  |
| 1   | CB    | 19  | GLY  | 2.4  |
| 1   | CW    | 86  | THR  | 2.4  |
| 1   | AH    | 18  | VAL  | 2.4  |
| 1   | CF    | 17  | VAL  | 2.4  |
| 1   | CZ    | 91  | VAL  | 2.4  |
| 1   | AM    | 107 | ASP  | 2.4  |
| 1   | C3    | 61  | ILE  | 2.4  |
| 1   | AF    | 104 | LEU  | 2.4  |
| 1   | AZ    | 90  | TYR  | 2.4  |
| 1   | CO    | 94  | GLU  | 2.4  |
| 1   | BB    | 153 | ALA  | 2.4  |
| 1   | BK    | 73  | ALA  | 2.4  |
| 1   | B1    | 127 | ALA  | 2.4  |
| 1   | B3    | 66  | ALA  | 2.4  |
| 1   | CC    | 142 | ALA  | 2.4  |
| 1   | CR    | 55  | ALA  | 2.4  |
| 1   | CR    | 96  | ALA  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A2    | 45  | ASN  | 2.4  |
| 1   | CG    | 59  | PRO  | 2.4  |
| 1   | CR    | 19  | GLY  | 2.4  |
| 1   | CR    | 128 | GLY  | 2.4  |
| 1   | CS    | 103 | SER  | 2.4  |
| 1   | AA    | 86  | THR  | 2.4  |
| 1   | BM    | 14  | VAL  | 2.4  |
| 1   | CS    | 26  | THR  | 2.4  |
| 1   | CW    | 117 | THR  | 2.4  |
| 1   | AA    | 143 | ILE  | 2.4  |
| 1   | AQ    | 102 | LEU  | 2.4  |
| 1   | CB    | 77  | LEU  | 2.4  |
| 1   | CP    | 115 | LEU  | 2.4  |
| 1   | CS    | 104 | LEU  | 2.4  |
| 1   | AB    | 43  | GLU  | 2.4  |
| 1   | CN    | 4   | GLU  | 2.4  |
| 1   | AQ    | 151 | HIS  | 2.4  |
| 1   | AX    | 147 | HIS  | 2.4  |
| 1   | BJ    | 40  | HIS  | 2.4  |
| 1   | BO    | 6   | HIS  | 2.4  |
| 1   | BU    | 66  | ALA  | 2.4  |
| 1   | BZ    | 145 | MET  | 2.4  |
| 1   | B1    | 62  | ALA  | 2.4  |
| 1   | AM    | 41  | GLY  | 2.4  |
| 1   | CS    | 67  | ASN  | 2.4  |
| 1   | C4    | 59  | PRO  | 2.4  |
| 1   | AG    | 8   | VAL  | 2.4  |
| 1   | AO    | 42  | VAL  | 2.4  |
| 1   | AT    | 14  | VAL  | 2.4  |
| 1   | BZ    | 8   | VAL  | 2.4  |
| 1   | CX    | 14  | VAL  | 2.4  |
| 1   | BF    | 35  | ASP  | 2.4  |
| 1   | C3    | 89  | ASP  | 2.4  |
| 1   | AM    | 33  | ALA  | 2.4  |
| 1   | AQ    | 84  | ALA  | 2.4  |
| 1   | AW    | 127 | ALA  | 2.4  |
| 1   | A1    | 43  | GLU  | 2.4  |
| 1   | A4    | 146 | ALA  | 2.4  |
| 1   | CP    | 84  | ALA  | 2.4  |
| 1   | CZ    | 144 | GLU  | 2.4  |
| 1   | C2    | 84  | ALA  | 2.4  |
| 1   | CC    | 6   | HIS  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AB    | 3   | PHE  | 2.3  |
| 1   | AZ    | 112 | PHE  | 2.3  |
| 1   | BW    | 67  | ASN  | 2.3  |
| 1   | BY    | 128 | GLY  | 2.3  |
| 1   | B1    | 27  | SER  | 2.3  |
| 1   | CR    | 12  | LEU  | 2.3  |
| 1   | CT    | 115 | LEU  | 2.3  |
| 1   | AD    | 106 | THR  | 2.3  |
| 1   | BW    | 110 | VAL  | 2.3  |
| 1   | CP    | 49  | VAL  | 2.3  |
| 1   | C2    | 110 | VAL  | 2.3  |
| 1   | CZ    | 90  | TYR  | 2.3  |
| 1   | AO    | 107 | ASP  | 2.3  |
| 1   | BO    | 150 | LYS  | 2.3  |
| 1   | BQ    | 107 | ASP  | 2.3  |
| 1   | AF    | 123 | ALA  | 2.3  |
| 1   | AK    | 57  | GLU  | 2.3  |
| 1   | AK    | 94  | GLU  | 2.3  |
| 1   | AR    | 57  | GLU  | 2.3  |
| 1   | AS    | 23  | GLU  | 2.3  |
| 1   | AW    | 43  | GLU  | 2.3  |
| 1   | BU    | 73  | ALA  | 2.3  |
| 1   | CA    | 131 | ALA  | 2.3  |
| 1   | CZ    | 139 | ALA  | 2.3  |
| 1   | AN    | 87  | HIS  | 2.3  |
| 1   | B2    | 151 | HIS  | 2.3  |
| 1   | CO    | 151 | HIS  | 2.3  |
| 1   | BU    | 69  | GLY  | 2.3  |
| 1   | CC    | 149 | SER  | 2.3  |
| 1   | CP    | 81  | ILE  | 2.3  |
| 1   | C2    | 59  | PRO  | 2.3  |
| 1   | C2    | 77  | LEU  | 2.3  |
| 1   | C3    | 75  | ILE  | 2.3  |
| 1   | C4    | 53  | PRO  | 2.3  |
| 1   | AA    | 133 | ASN  | 2.3  |
| 1   | AG    | 133 | ASN  | 2.3  |
| 1   | AK    | 92  | CYS  | 2.3  |
| 1   | AR    | 119 | THR  | 2.3  |
| 1   | CP    | 116 | THR  | 2.3  |
| 1   | CR    | 140 | VAL  | 2.3  |
| 1   | CT    | 79  | THR  | 2.3  |
| 1   | AK    | 145 | MET  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CD    | 71  | TYR  | 2.3  |
| 1   | CE    | 90  | TYR  | 2.3  |
| 1   | C3    | 88  | TYR  | 2.3  |
| 1   | AG    | 66  | ALA  | 2.3  |
| 1   | AI    | 96  | ALA  | 2.3  |
| 1   | CT    | 4   | GLU  | 2.3  |
| 1   | CW    | 144 | GLU  | 2.3  |
| 1   | AH    | 108 | ILE  | 2.3  |
| 1   | BH    | 3   | PHE  | 2.3  |
| 1   | CQ    | 47  | ILE  | 2.3  |
| 1   | BC    | 68  | SER  | 2.3  |
| 1   | CQ    | 151 | HIS  | 2.3  |
| 1   | CZ    | 19  | GLY  | 2.3  |
| 1   | C4    | 36  | GLY  | 2.3  |
| 1   | C4    | 78  | GLY  | 2.3  |
| 1   | AK    | 14  | VAL  | 2.3  |
| 1   | BU    | 14  | VAL  | 2.3  |
| 1   | CS    | 80  | VAL  | 2.3  |
| 1   | C3    | 93  | ASN  | 2.3  |
| 1   | AF    | 129 | THR  | 2.3  |
| 1   | AX    | 129 | THR  | 2.3  |
| 1   | A1    | 10  | THR  | 2.3  |
| 1   | CL    | 152 | TRP  | 2.3  |
| 1   | CQ    | 117 | THR  | 2.3  |
| 1   | CU    | 86  | THR  | 2.3  |
| 1   | AA    | 90  | TYR  | 2.3  |
| 1   | AI    | 84  | ALA  | 2.3  |
| 1   | AK    | 84  | ALA  | 2.3  |
| 1   | AY    | 102 | LEU  | 2.3  |
| 1   | CB    | 127 | ALA  | 2.3  |
| 1   | CD    | 33  | ALA  | 2.3  |
| 1   | CZ    | 7   | LEU  | 2.3  |
| 1   | C4    | 141 | ALA  | 2.3  |
| 1   | BV    | 43  | GLU  | 2.3  |
| 1   | C1    | 57  | GLU  | 2.3  |
| 1   | C1    | 107 | ASP  | 2.3  |
| 1   | CT    | 101 | SER  | 2.3  |
| 1   | CS    | 83  | GLY  | 2.3  |
| 1   | CX    | 9   | GLY  | 2.3  |
| 1   | AH    | 80  | VAL  | 2.3  |
| 1   | AR    | 14  | VAL  | 2.3  |
| 1   | BM    | 8   | VAL  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CW    | 6   | HIS  | 2.3  |
| 1   | C1    | 114 | VAL  | 2.3  |
| 1   | A3    | 133 | ASN  | 2.3  |
| 1   | CS    | 133 | ASN  | 2.3  |
| 1   | AQ    | 152 | TRP  | 2.3  |
| 1   | AH    | 29  | LEU  | 2.3  |
| 1   | CS    | 92  | CYS  | 2.3  |
| 1   | AH    | 62  | ALA  | 2.3  |
| 1   | AO    | 108 | ILE  | 2.3  |
| 1   | AZ    | 3   | PHE  | 2.3  |
| 1   | BD    | 62  | ALA  | 2.3  |
| 1   | CQ    | 66  | ALA  | 2.3  |
| 1   | CS    | 50  | ALA  | 2.3  |
| 1   | CV    | 25  | ILE  | 2.3  |
| 1   | CY    | 90  | TYR  | 2.3  |
| 1   | C4    | 120 | ILE  | 2.3  |
| 1   | AJ    | 23  | GLU  | 2.3  |
| 1   | AU    | 4   | GLU  | 2.3  |
| 1   | BL    | 4   | GLU  | 2.3  |
| 1   | CR    | 144 | GLU  | 2.3  |
| 1   | A1    | 103 | SER  | 2.3  |
| 1   | AJ    | 32  | GLY  | 2.3  |
| 1   | AK    | 110 | VAL  | 2.3  |
| 1   | AW    | 9   | GLY  | 2.3  |
| 1   | BU    | 48  | ASP  | 2.3  |
| 1   | CB    | 83  | GLY  | 2.3  |
| 1   | C4    | 107 | ASP  | 2.3  |
| 1   | AX    | 8   | VAL  | 2.3  |
| 1   | AW    | 87  | HIS  | 2.3  |
| 1   | AZ    | 38  | LYS  | 2.3  |
| 1   | A4    | 6   | HIS  | 2.3  |
| 1   | BH    | 64  | LYS  | 2.3  |
| 1   | CA    | 65  | MET  | 2.3  |
| 1   | CQ    | 20  | ARG  | 2.3  |
| 1   | C4    | 10  | THR  | 2.3  |
| 1   | AA    | 102 | LEU  | 2.3  |
| 1   | AC    | 102 | LEU  | 2.3  |
| 1   | CR    | 60  | LEU  | 2.3  |
| 1   | AJ    | 120 | ILE  | 2.3  |
| 1   | CT    | 143 | ILE  | 2.3  |
| 1   | BU    | 136 | TYR  | 2.3  |
| 1   | CT    | 127 | ALA  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AI    | 94  | GLU  | 2.3  |
| 1   | AM    | 68  | SER  | 2.3  |
| 1   | BQ    | 4   | GLU  | 2.3  |
| 1   | CC    | 144 | GLU  | 2.3  |
| 1   | AB    | 9   | GLY  | 2.3  |
| 1   | AM    | 70  | LYS  | 2.3  |
| 1   | AV    | 5   | GLY  | 2.3  |
| 1   | AV    | 70  | LYS  | 2.3  |
| 1   | AX    | 41  | GLY  | 2.3  |
| 1   | CR    | 59  | PRO  | 2.3  |
| 1   | C3    | 15  | GLY  | 2.3  |
| 1   | AH    | 65  | MET  | 2.3  |
| 1   | CC    | 106 | THR  | 2.2  |
| 1   | CY    | 116 | THR  | 2.2  |
| 1   | AH    | 87  | HIS  | 2.2  |
| 1   | BW    | 40  | HIS  | 2.2  |
| 1   | CR    | 77  | LEU  | 2.2  |
| 1   | AL    | 3   | PHE  | 2.2  |
| 1   | CT    | 61  | ILE  | 2.2  |
| 1   | AA    | 127 | ALA  | 2.2  |
| 1   | AG    | 62  | ALA  | 2.2  |
| 1   | CE    | 73  | ALA  | 2.2  |
| 1   | CT    | 27  | SER  | 2.2  |
| 1   | AB    | 44  | GLU  | 2.2  |
| 1   | AF    | 43  | GLU  | 2.2  |
| 1   | AR    | 94  | GLU  | 2.2  |
| 1   | AT    | 92  | CYS  | 2.2  |
| 1   | AU    | 57  | GLU  | 2.2  |
| 1   | CR    | 23  | GLU  | 2.2  |
| 1   | C1    | 44  | GLU  | 2.2  |
| 1   | AN    | 17  | VAL  | 2.2  |
| 1   | AV    | 54  | GLY  | 2.2  |
| 1   | A2    | 135 | GLY  | 2.2  |
| 1   | CV    | 132 | GLY  | 2.2  |
| 1   | CX    | 128 | GLY  | 2.2  |
| 1   | CC    | 102 | LEU  | 2.2  |
| 1   | AC    | 45  | ASN  | 2.2  |
| 1   | AV    | 111 | ILE  | 2.2  |
| 1   | AW    | 3   | PHE  | 2.2  |
| 1   | BR    | 61  | ILE  | 2.2  |
| 1   | CZ    | 111 | ILE  | 2.2  |
| 1   | AM    | 73  | ALA  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AX    | 84  | ALA  | 2.2  |
| 1   | CT    | 62  | ALA  | 2.2  |
| 1   | CT    | 146 | ALA  | 2.2  |
| 1   | CZ    | 142 | ALA  | 2.2  |
| 1   | CT    | 145 | MET  | 2.2  |
| 1   | AZ    | 44  | GLU  | 2.2  |
| 1   | BX    | 137 | GLU  | 2.2  |
| 1   | CS    | 23  | GLU  | 2.2  |
| 1   | AS    | 102 | LEU  | 2.2  |
| 1   | A4    | 148 | LEU  | 2.2  |
| 1   | BL    | 9   | GLY  | 2.2  |
| 1   | C4    | 52  | VAL  | 2.2  |
| 1   | AE    | 10  | THR  | 2.2  |
| 1   | AH    | 3   | PHE  | 2.2  |
| 1   | AI    | 72  | ASP  | 2.2  |
| 1   | AO    | 45  | ASN  | 2.2  |
| 1   | BD    | 45  | ASN  | 2.2  |
| 1   | CE    | 107 | ASP  | 2.2  |
| 1   | CM    | 35  | ASP  | 2.2  |
| 1   | CO    | 67  | ASN  | 2.2  |
| 1   | CP    | 48  | ASP  | 2.2  |
| 1   | CP    | 108 | ILE  | 2.2  |
| 1   | CW    | 124 | ILE  | 2.2  |
| 1   | BF    | 112 | PHE  | 2.2  |
| 1   | CZ    | 107 | ASP  | 2.2  |
| 1   | A2    | 151 | HIS  | 2.2  |
| 1   | CA    | 151 | HIS  | 2.2  |
| 1   | CR    | 151 | HIS  | 2.2  |
| 1   | AE    | 55  | ALA  | 2.2  |
| 1   | A1    | 123 | ALA  | 2.2  |
| 1   | CG    | 139 | ALA  | 2.2  |
| 1   | CR    | 13  | LYS  | 2.2  |
| 1   | C1    | 64  | LYS  | 2.2  |
| 1   | C1    | 100 | ALA  | 2.2  |
| 1   | AD    | 145 | MET  | 2.2  |
| 1   | AX    | 90  | TYR  | 2.2  |
| 1   | BH    | 65  | MET  | 2.2  |
| 1   | CC    | 145 | MET  | 2.2  |
| 1   | AF    | 7   | LEU  | 2.2  |
| 1   | CF    | 29  | LEU  | 2.2  |
| 1   | C1    | 42  | VAL  | 2.2  |
| 1   | C3    | 30  | LEU  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AC    | 4   | GLU  | 2.2  |
| 1   | AL    | 32  | GLY  | 2.2  |
| 1   | AT    | 53  | PRO  | 2.2  |
| 1   | AV    | 69  | GLY  | 2.2  |
| 1   | AW    | 137 | GLU  | 2.2  |
| 1   | CS    | 98  | GLY  | 2.2  |
| 1   | CT    | 121 | GLU  | 2.2  |
| 1   | CU    | 4   | GLU  | 2.2  |
| 1   | C2    | 109 | PRO  | 2.2  |
| 1   | AR    | 108 | ILE  | 2.2  |
| 1   | AW    | 111 | ILE  | 2.2  |
| 1   | CW    | 119 | THR  | 2.2  |
| 1   | AJ    | 134 | LYS  | 2.2  |
| 1   | AO    | 89  | ASP  | 2.2  |
| 1   | BJ    | 150 | LYS  | 2.2  |
| 1   | BP    | 107 | ASP  | 2.2  |
| 1   | B2    | 35  | ASP  | 2.2  |
| 1   | CF    | 107 | ASP  | 2.2  |
| 1   | CU    | 107 | ASP  | 2.2  |
| 1   | BT    | 40  | HIS  | 2.2  |
| 1   | AO    | 153 | ALA  | 2.2  |
| 1   | CR    | 152 | TRP  | 2.2  |
| 1   | BF    | 65  | MET  | 2.2  |
| 1   | BM    | 102 | LEU  | 2.2  |
| 1   | CC    | 8   | VAL  | 2.2  |
| 1   | C4    | 140 | VAL  | 2.2  |
| 1   | AL    | 36  | GLY  | 2.2  |
| 1   | CQ    | 59  | PRO  | 2.2  |
| 1   | CS    | 69  | GLY  | 2.2  |
| 1   | CX    | 23  | GLU  | 2.2  |
| 1   | C2    | 83  | GLY  | 2.2  |
| 1   | C3    | 144 | GLU  | 2.2  |
| 1   | AP    | 119 | THR  | 2.2  |
| 1   | AU    | 3   | PHE  | 2.2  |
| 1   | CD    | 85  | THR  | 2.2  |
| 1   | CI    | 3   | PHE  | 2.2  |
| 1   | CK    | 3   | PHE  | 2.2  |
| 1   | AU    | 67  | ASN  | 2.2  |
| 1   | AK    | 107 | ASP  | 2.2  |
| 1   | AY    | 84  | ALA  | 2.2  |
| 1   | A1    | 107 | ASP  | 2.2  |
| 1   | BG    | 127 | ALA  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BI    | 35  | ASP  | 2.2  |
| 1   | B4    | 127 | ALA  | 2.2  |
| 1   | CB    | 72  | ASP  | 2.2  |
| 1   | CP    | 92  | CYS  | 2.2  |
| 1   | CW    | 127 | ALA  | 2.2  |
| 1   | C3    | 62  | ALA  | 2.2  |
| 1   | AH    | 102 | LEU  | 2.2  |
| 1   | AU    | 101 | SER  | 2.2  |
| 1   | AV    | 105 | GLN  | 2.2  |
| 1   | B1    | 152 | TRP  | 2.2  |
| 1   | CC    | 29  | LEU  | 2.2  |
| 1   | C1    | 77  | LEU  | 2.2  |
| 1   | AB    | 99  | VAL  | 2.2  |
| 1   | AH    | 8   | VAL  | 2.2  |
| 1   | AM    | 14  | VAL  | 2.2  |
| 1   | C4    | 17  | VAL  | 2.2  |
| 1   | CF    | 57  | GLU  | 2.2  |
| 1   | CF    | 69  | GLY  | 2.2  |
| 1   | CP    | 132 | GLY  | 2.2  |
| 1   | CQ    | 111 | ILE  | 2.2  |
| 1   | AC    | 3   | PHE  | 2.2  |
| 1   | BO    | 4   | GLU  | 2.2  |
| 1   | CW    | 5   | GLY  | 2.2  |
| 1   | AP    | 134 | LYS  | 2.2  |
| 1   | AY    | 119 | THR  | 2.2  |
| 1   | CK    | 86  | THR  | 2.2  |
| 1   | C1    | 106 | THR  | 2.2  |
| 1   | BU    | 65  | MET  | 2.2  |
| 1   | AW    | 66  | ALA  | 2.1  |
| 1   | BC    | 66  | ALA  | 2.1  |
| 1   | BP    | 100 | ALA  | 2.1  |
| 1   | CB    | 153 | ALA  | 2.1  |
| 1   | CN    | 153 | ALA  | 2.1  |
| 1   | CV    | 102 | LEU  | 2.2  |
| 1   | C3    | 66  | ALA  | 2.1  |
| 1   | AL    | 103 | SER  | 2.1  |
| 1   | AP    | 147 | HIS  | 2.1  |
| 1   | CL    | 151 | HIS  | 2.1  |
| 1   | CT    | 92  | CYS  | 2.1  |
| 1   | C4    | 46  | ASP  | 2.1  |
| 1   | AD    | 8   | VAL  | 2.1  |
| 1   | AK    | 52  | VAL  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BL    | 47  | ILE  | 2.1  |
| 1   | CS    | 16  | VAL  | 2.1  |
| 1   | CS    | 58  | ILE  | 2.1  |
| 1   | CT    | 110 | VAL  | 2.1  |
| 1   | AR    | 3   | PHE  | 2.1  |
| 1   | AH    | 94  | GLU  | 2.1  |
| 1   | AK    | 144 | GLU  | 2.1  |
| 1   | AM    | 59  | PRO  | 2.1  |
| 1   | CB    | 128 | GLY  | 2.1  |
| 1   | CC    | 59  | PRO  | 2.1  |
| 1   | CI    | 5   | GLY  | 2.1  |
| 1   | C4    | 132 | GLY  | 2.1  |
| 1   | AV    | 44  | GLU  | 2.1  |
| 1   | AY    | 94  | GLU  | 2.1  |
| 1   | A3    | 125 | GLU  | 2.1  |
| 1   | BH    | 4   | GLU  | 2.1  |
| 1   | AI    | 10  | THR  | 2.1  |
| 1   | AL    | 26  | THR  | 2.1  |
| 1   | AK    | 34  | LEU  | 2.1  |
| 1   | AV    | 145 | MET  | 2.1  |
| 1   | AG    | 55  | ALA  | 2.1  |
| 1   | AS    | 66  | ALA  | 2.1  |
| 1   | A3    | 50  | ALA  | 2.1  |
| 1   | BA    | 153 | ALA  | 2.1  |
| 1   | BQ    | 73  | ALA  | 2.1  |
| 1   | CS    | 84  | ALA  | 2.1  |
| 1   | CS    | 96  | ALA  | 2.1  |
| 1   | AD    | 107 | ASP  | 2.1  |
| 1   | AJ    | 46  | ASP  | 2.1  |
| 1   | A2    | 6   | HIS  | 2.1  |
| 1   | CA    | 91  | VAL  | 2.1  |
| 1   | CD    | 47  | ILE  | 2.1  |
| 1   | CK    | 35  | ASP  | 2.1  |
| 1   | CN    | 72  | ASP  | 2.1  |
| 1   | AZ    | 42  | VAL  | 2.1  |
| 1   | CF    | 91  | VAL  | 2.1  |
| 1   | CS    | 47  | ILE  | 2.1  |
| 1   | CW    | 51  | TRP  | 2.1  |
| 1   | AH    | 38  | LYS  | 2.1  |
| 1   | AO    | 3   | PHE  | 2.1  |
| 1   | BB    | 78  | GLY  | 2.1  |
| 1   | BR    | 113 | GLY  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CG    | 9   | GLY  | 2.1  |
| 1   | CJ    | 135 | GLY  | 2.1  |
| 1   | CP    | 15  | GLY  | 2.1  |
| 1   | CT    | 128 | GLY  | 2.1  |
| 1   | C4    | 11  | GLY  | 2.1  |
| 1   | AA    | 23  | GLU  | 2.1  |
| 1   | AX    | 125 | GLU  | 2.1  |
| 1   | BS    | 144 | GLU  | 2.1  |
| 1   | CH    | 23  | GLU  | 2.1  |
| 1   | BD    | 129 | THR  | 2.1  |
| 1   | BP    | 10  | THR  | 2.1  |
| 1   | CB    | 86  | THR  | 2.1  |
| 1   | CF    | 129 | THR  | 2.1  |
| 1   | C1    | 116 | THR  | 2.1  |
| 1   | CG    | 34  | LEU  | 2.1  |
| 1   | CU    | 145 | MET  | 2.1  |
| 1   | C3    | 12  | LEU  | 2.1  |
| 1   | AP    | 127 | ALA  | 2.1  |
| 1   | AX    | 39  | ARG  | 2.1  |
| 1   | CR    | 133 | ASN  | 2.1  |
| 1   | CZ    | 33  | ALA  | 2.1  |
| 1   | AA    | 101 | SER  | 2.1  |
| 1   | AS    | 101 | SER  | 2.1  |
| 1   | AR    | 105 | GLN  | 2.1  |
| 1   | AV    | 143 | ILE  | 2.1  |
| 1   | CQ    | 143 | ILE  | 2.1  |
| 1   | AF    | 8   | VAL  | 2.1  |
| 1   | AL    | 42  | VAL  | 2.1  |
| 1   | CC    | 40  | HIS  | 2.1  |
| 1   | CD    | 6   | HIS  | 2.1  |
| 1   | CG    | 42  | VAL  | 2.1  |
| 1   | C3    | 74  | VAL  | 2.1  |
| 1   | AH    | 48  | ASP  | 2.1  |
| 1   | CG    | 107 | ASP  | 2.1  |
| 1   | CR    | 72  | ASP  | 2.1  |
| 1   | AK    | 90  | TYR  | 2.1  |
| 1   | AT    | 51  | TRP  | 2.1  |
| 1   | AU    | 152 | TRP  | 2.1  |
| 1   | CC    | 51  | TRP  | 2.1  |
| 1   | AT    | 41  | GLY  | 2.1  |
| 1   | B4    | 5   | GLY  | 2.1  |
| 1   | CB    | 69  | GLY  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CL    | 36  | GLY  | 2.1  |
| 1   | CQ    | 132 | GLY  | 2.1  |
| 1   | CZ    | 92  | CYS  | 2.1  |
| 1   | C2    | 69  | GLY  | 2.1  |
| 1   | AK    | 109 | PRO  | 2.1  |
| 1   | BU    | 109 | PRO  | 2.1  |
| 1   | CR    | 53  | PRO  | 2.1  |
| 1   | AL    | 102 | LEU  | 2.1  |
| 1   | AP    | 7   | LEU  | 2.1  |
| 1   | AT    | 102 | LEU  | 2.1  |
| 1   | AX    | 4   | GLU  | 2.1  |
| 1   | BA    | 43  | GLU  | 2.1  |
| 1   | CP    | 94  | GLU  | 2.1  |
| 1   | AT    | 79  | THR  | 2.1  |
| 1   | AW    | 10  | THR  | 2.1  |
| 1   | BF    | 86  | THR  | 2.1  |
| 1   | CP    | 86  | THR  | 2.1  |
| 1   | C3    | 86  | THR  | 2.1  |
| 1   | AI    | 39  | ARG  | 2.1  |
| 1   | AE    | 50  | ALA  | 2.1  |
| 1   | AG    | 146 | ALA  | 2.1  |
| 1   | CP    | 73  | ALA  | 2.1  |
| 1   | CR    | 127 | ALA  | 2.1  |
| 1   | C4    | 50  | ALA  | 2.1  |
| 1   | AH    | 61  | ILE  | 2.1  |
| 1   | AL    | 133 | ASN  | 2.1  |
| 1   | AU    | 120 | ILE  | 2.1  |
| 1   | BV    | 45  | ASN  | 2.1  |
| 1   | AE    | 150 | LYS  | 2.1  |
| 1   | AR    | 17  | VAL  | 2.1  |
| 1   | AR    | 21  | PHE  | 2.1  |
| 1   | CS    | 2   | VAL  | 2.1  |
| 1   | C2    | 18  | VAL  | 2.1  |
| 1   | C3    | 3   | PHE  | 2.1  |
| 1   | AV    | 151 | HIS  | 2.1  |
| 1   | AA    | 104 | LEU  | 2.1  |
| 1   | AA    | 136 | TYR  | 2.1  |
| 1   | AV    | 128 | GLY  | 2.1  |
| 1   | AY    | 5   | GLY  | 2.1  |
| 1   | BR    | 152 | TRP  | 2.1  |
| 1   | CG    | 15  | GLY  | 2.1  |
| 1   | CM    | 34  | LEU  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CS    | 41  | GLY  | 2.1  |
| 1   | C2    | 60  | LEU  | 2.1  |
| 1   | AF    | 109 | PRO  | 2.1  |
| 1   | AU    | 65  | MET  | 2.1  |
| 1   | CF    | 145 | MET  | 2.1  |
| 1   | CZ    | 109 | PRO  | 2.1  |
| 1   | AG    | 118 | GLU  | 2.1  |
| 1   | AH    | 144 | GLU  | 2.1  |
| 1   | AY    | 137 | GLU  | 2.1  |
| 1   | A2    | 144 | GLU  | 2.1  |
| 1   | BG    | 23  | GLU  | 2.1  |
| 1   | C1    | 43  | GLU  | 2.1  |
| 1   | AB    | 153 | ALA  | 2.1  |
| 1   | AW    | 62  | ALA  | 2.1  |
| 1   | AC    | 149 | SER  | 2.1  |
| 1   | AE    | 64  | LYS  | 2.1  |
| 1   | A4    | 64  | LYS  | 2.1  |
| 1   | CJ    | 127 | ALA  | 2.1  |
| 1   | CK    | 62  | ALA  | 2.1  |
| 1   | CR    | 123 | ALA  | 2.1  |
| 1   | CU    | 73  | ALA  | 2.1  |
| 1   | AD    | 45  | ASN  | 2.1  |
| 1   | AO    | 67  | ASN  | 2.1  |
| 1   | AR    | 45  | ASN  | 2.1  |
| 1   | AV    | 133 | ASN  | 2.1  |
| 1   | CP    | 122 | GLN  | 2.1  |
| 1   | AJ    | 49  | VAL  | 2.1  |
| 1   | AU    | 42  | VAL  | 2.1  |
| 1   | BR    | 74  | VAL  | 2.1  |
| 1   | CP    | 17  | VAL  | 2.1  |
| 1   | CR    | 42  | VAL  | 2.1  |
| 1   | CS    | 140 | VAL  | 2.1  |
| 1   | AI    | 102 | LEU  | 2.1  |
| 1   | CD    | 30  | LEU  | 2.1  |
| 1   | CD    | 115 | LEU  | 2.1  |
| 1   | C4    | 148 | LEU  | 2.1  |
| 1   | B4    | 40  | HIS  | 2.1  |
| 1   | AG    | 132 | GLY  | 2.1  |
| 1   | AV    | 31  | GLY  | 2.1  |
| 1   | A2    | 107 | ASP  | 2.1  |
| 1   | BB    | 69  | GLY  | 2.1  |
| 1   | BE    | 128 | GLY  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CD    | 83  | GLY  | 2.1  |
| 1   | CF    | 128 | GLY  | 2.1  |
| 1   | CT    | 32  | GLY  | 2.1  |
| 1   | CV    | 9   | GLY  | 2.1  |
| 1   | AD    | 85  | THR  | 2.1  |
| 1   | AW    | 26  | THR  | 2.1  |
| 1   | A2    | 57  | GLU  | 2.1  |
| 1   | CC    | 79  | THR  | 2.1  |
| 1   | CD    | 117 | THR  | 2.1  |
| 1   | CR    | 117 | THR  | 2.1  |
| 1   | AE    | 134 | LYS  | 2.1  |
| 1   | CR    | 108 | ILE  | 2.1  |
| 1   | CS    | 28  | LYS  | 2.1  |
| 1   | AG    | 68  | SER  | 2.1  |
| 1   | BN    | 141 | ALA  | 2.1  |
| 1   | CD    | 123 | ALA  | 2.1  |
| 1   | CF    | 27  | SER  | 2.1  |
| 1   | CW    | 33  | ALA  | 2.1  |
| 1   | C2    | 149 | SER  | 2.1  |
| 1   | C3    | 153 | ALA  | 2.1  |
| 1   | BV    | 3   | PHE  | 2.1  |
| 1   | CQ    | 148 | LEU  | 2.1  |
| 1   | AE    | 5   | GLY  | 2.0  |
| 1   | AF    | 19  | GLY  | 2.0  |
| 1   | AF    | 54  | GLY  | 2.0  |
| 1   | AJ    | 132 | GLY  | 2.0  |
| 1   | AL    | 147 | HIS  | 2.0  |
| 1   | AZ    | 69  | GLY  | 2.0  |
| 1   | BB    | 32  | GLY  | 2.0  |
| 1   | BR    | 69  | GLY  | 2.0  |
| 1   | CG    | 6   | HIS  | 2.0  |
| 1   | C1    | 98  | GLY  | 2.0  |
| 1   | AZ    | 152 | TRP  | 2.0  |
| 1   | AE    | 129 | THR  | 2.0  |
| 1   | BK    | 107 | ASP  | 2.0  |
| 1   | BQ    | 72  | ASP  | 2.0  |
| 1   | CQ    | 51  | TRP  | 2.0  |
| 1   | BQ    | 129 | THR  | 2.0  |
| 1   | AK    | 58  | ILE  | 2.0  |
| 1   | CI    | 4   | GLU  | 2.0  |
| 1   | CQ    | 130 | LYS  | 2.0  |
| 1   | CR    | 94  | GLU  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CS    | 118 | GLU  | 2.0  |
| 1   | CZ    | 47  | ILE  | 2.0  |
| 1   | CZ    | 64  | LYS  | 2.0  |
| 1   | A2    | 66  | ALA  | 2.0  |
| 1   | A3    | 146 | ALA  | 2.0  |
| 1   | BZ    | 27  | SER  | 2.0  |
| 1   | CB    | 96  | ALA  | 2.0  |
| 1   | C2    | 73  | ALA  | 2.0  |
| 1   | C4    | 96  | ALA  | 2.0  |
| 1   | AL    | 34  | LEU  | 2.0  |
| 1   | B4    | 29  | LEU  | 2.0  |
| 1   | CS    | 37  | LEU  | 2.0  |
| 1   | C1    | 30  | LEU  | 2.0  |
| 1   | AG    | 91  | VAL  | 2.0  |
| 1   | AI    | 140 | VAL  | 2.0  |
| 1   | BP    | 8   | VAL  | 2.0  |
| 1   | CQ    | 14  | VAL  | 2.0  |
| 1   | C1    | 14  | VAL  | 2.0  |
| 1   | CG    | 65  | MET  | 2.0  |
| 1   | CQ    | 65  | MET  | 2.0  |
| 1   | CW    | 65  | MET  | 2.0  |
| 1   | A4    | 128 | GLY  | 2.0  |
| 1   | AI    | 25  | ILE  | 2.0  |
| 1   | BZ    | 47  | ILE  | 2.0  |
| 1   | C1    | 20  | ARG  | 2.0  |
| 1   | AY    | 86  | THR  | 2.0  |
| 1   | C2    | 111 | ILE  | 2.0  |
| 1   | AD    | 144 | GLU  | 2.0  |
| 1   | AI    | 57  | GLU  | 2.0  |
| 1   | AK    | 4   | GLU  | 2.0  |
| 1   | BL    | 107 | ASP  | 2.0  |
| 1   | BU    | 46  | ASP  | 2.0  |
| 1   | C1    | 46  | ASP  | 2.0  |
| 1   | AB    | 50  | ALA  | 2.0  |
| 1   | AC    | 34  | LEU  | 2.0  |
| 1   | AH    | 33  | ALA  | 2.0  |
| 1   | AH    | 142 | ALA  | 2.0  |
| 1   | AQ    | 127 | ALA  | 2.0  |
| 1   | CD    | 142 | ALA  | 2.0  |
| 1   | CJ    | 60  | LEU  | 2.0  |
| 1   | CL    | 153 | ALA  | 2.0  |
| 1   | C3    | 102 | LEU  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AI    | 8   | VAL  | 2.0  |
| 1   | AL    | 17  | VAL  | 2.0  |
| 1   | AL    | 49  | VAL  | 2.0  |
| 1   | CP    | 91  | VAL  | 2.0  |
| 1   | CW    | 52  | VAL  | 2.0  |
| 1   | C3    | 114 | VAL  | 2.0  |
| 1   | C2    | 65  | MET  | 2.0  |
| 1   | AD    | 133 | ASN  | 2.0  |
| 1   | AJ    | 133 | ASN  | 2.0  |
| 1   | AS    | 67  | ASN  | 2.0  |
| 1   | CD    | 45  | ASN  | 2.0  |
| 1   | CQ    | 22  | ASN  | 2.0  |
| 1   | AI    | 9   | GLY  | 2.0  |
| 1   | BE    | 28  | LYS  | 2.0  |
| 1   | CT    | 113 | GLY  | 2.0  |
| 1   | C1    | 78  | GLY  | 2.0  |
| 1   | AC    | 90  | TYR  | 2.0  |
| 1   | AI    | 108 | ILE  | 2.0  |
| 1   | AO    | 53  | PRO  | 2.0  |
| 1   | AX    | 109 | PRO  | 2.0  |
| 1   | CA    | 47  | ILE  | 2.0  |
| 1   | CX    | 71  | TYR  | 2.0  |
| 1   | AM    | 86  | THR  | 2.0  |
| 1   | AP    | 86  | THR  | 2.0  |
| 1   | BV    | 6   | HIS  | 2.0  |
| 1   | CM    | 116 | THR  | 2.0  |
| 1   | AL    | 51  | TRP  | 2.0  |
| 1   | AH    | 89  | ASP  | 2.0  |
| 1   | AH    | 104 | LEU  | 2.0  |
| 1   | AK    | 48  | ASP  | 2.0  |
| 1   | AM    | 35  | ASP  | 2.0  |
| 1   | AM    | 102 | LEU  | 2.0  |
| 1   | AN    | 94  | GLU  | 2.0  |
| 1   | A4    | 60  | LEU  | 2.0  |
| 1   | A4    | 137 | GLU  | 2.0  |
| 1   | BG    | 152 | TRP  | 2.0  |
| 1   | BN    | 4   | GLU  | 2.0  |
| 1   | CS    | 3   | PHE  | 2.0  |
| 1   | C4    | 34  | LEU  | 2.0  |
| 1   | C4    | 125 | GLU  | 2.0  |
| 1   | AM    | 50  | ALA  | 2.0  |
| 1   | AN    | 100 | ALA  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BH    | 153 | ALA  | 2.0  |
| 1   | BL    | 50  | ALA  | 2.0  |
| 1   | CD    | 153 | ALA  | 2.0  |
| 1   | CJ    | 146 | ALA  | 2.0  |
| 1   | CP    | 66  | ALA  | 2.0  |
| 1   | C2    | 66  | ALA  | 2.0  |
| 1   | C2    | 142 | ALA  | 2.0  |
| 1   | C3    | 55  | ALA  | 2.0  |
| 1   | AG    | 17  | VAL  | 2.0  |
| 1   | CS    | 95  | VAL  | 2.0  |
| 1   | CT    | 8   | VAL  | 2.0  |
| 1   | CW    | 74  | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | CT    | 4201 | 5/5   | 0.40 | 0.23 | 23,28,53,142                | 0     |
| 2   | PO4  | CC    | 1001 | 5/5   | 0.53 | 0.17 | 34,46,111,116               | 0     |
| 2   | PO4  | CG    | 1201 | 5/5   | 0.57 | 0.15 | 74,78,104,213               | 0     |
| 2   | PO4  | CB    | 1001 | 5/5   | 0.59 | 0.20 | 74,78,104,213               | 0     |
| 2   | PO4  | CD    | 1001 | 5/5   | 0.65 | 0.22 | 58,65,106,138               | 0     |
| 2   | PO4  | CW    | 2201 | 5/5   | 0.65 | 0.13 | 34,46,111,116               | 0     |
| 2   | PO4  | C1    | 1201 | 5/5   | 0.68 | 0.13 | 74,78,104,213               | 0     |
| 2   | PO4  | CH    | 2201 | 5/5   | 0.69 | 0.12 | 34,46,111,116               | 0     |
| 2   | PO4  | CF    | 201  | 5/5   | 0.72 | 0.14 | 80,81,83,167                | 0     |
| 2   | PO4  | CP    | 201  | 5/5   | 0.73 | 0.13 | 80,81,83,167                | 0     |
| 2   | PO4  | CE    | 1001 | 5/5   | 0.76 | 0.15 | 23,28,53,142                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | BG    | 1001 | 5/5   | 0.76 | 0.12 | 74,78,104,213               | 0     |
| 2   | PO4  | C2    | 2201 | 5/5   | 0.76 | 0.15 | 34,46,111,116               | 0     |
| 2   | PO4  | CX    | 3201 | 5/5   | 0.77 | 0.11 | 58,65,106,138               | 0     |
| 2   | PO4  | CZ    | 201  | 5/5   | 0.77 | 0.15 | 80,81,83,167                | 0     |
| 2   | PO4  | CQ    | 1201 | 5/5   | 0.78 | 0.18 | 74,78,104,213               | 0     |
| 2   | PO4  | CR    | 2201 | 5/5   | 0.78 | 0.18 | 34,46,111,116               | 0     |
| 2   | PO4  | C4    | 4201 | 5/5   | 0.78 | 0.17 | 23,28,53,142                | 0     |
| 2   | PO4  | BS    | 1001 | 5/5   | 0.79 | 0.13 | 58,65,106,138               | 0     |
| 2   | PO4  | CY    | 4201 | 5/5   | 0.79 | 0.14 | 23,28,53,142                | 0     |
| 2   | PO4  | BV    | 1001 | 5/5   | 0.79 | 0.11 | 74,78,104,213               | 0     |
| 2   | PO4  | B2    | 1001 | 5/5   | 0.80 | 0.13 | 34,46,111,116               | 0     |
| 2   | PO4  | B3    | 1001 | 5/5   | 0.80 | 0.10 | 58,65,106,138               | 0     |
| 2   | PO4  | BL    | 1001 | 5/5   | 0.81 | 0.11 | 74,78,104,213               | 0     |
| 2   | PO4  | AI    | 1001 | 5/5   | 0.82 | 0.13 | 58,65,106,138               | 0     |
| 2   | PO4  | CA    | 1001 | 5/5   | 0.82 | 0.14 | 80,81,83,167                | 0     |
| 2   | PO4  | AX    | 1001 | 5/5   | 0.83 | 0.16 | 58,65,106,138               | 0     |
| 2   | PO4  | BM    | 1001 | 5/5   | 0.83 | 0.10 | 34,46,111,116               | 0     |
| 2   | PO4  | BX    | 1001 | 5/5   | 0.83 | 0.09 | 58,65,106,138               | 0     |
| 2   | PO4  | BR    | 1001 | 5/5   | 0.83 | 0.08 | 34,46,111,116               | 0     |
| 2   | PO4  | CN    | 3201 | 5/5   | 0.84 | 0.09 | 58,65,106,138               | 0     |
| 2   | PO4  | BO    | 1001 | 5/5   | 0.84 | 0.09 | 23,28,53,142                | 0     |
| 2   | PO4  | BF    | 1001 | 5/5   | 0.84 | 0.11 | 80,81,83,167                | 0     |
| 2   | PO4  | BC    | 1001 | 5/5   | 0.84 | 0.10 | 34,46,111,116               | 0     |
| 2   | PO4  | C3    | 3201 | 5/5   | 0.85 | 0.10 | 58,65,106,138               | 0     |
| 2   | PO4  | CS    | 3201 | 5/5   | 0.85 | 0.18 | 58,65,106,138               | 0     |
| 2   | PO4  | AN    | 1001 | 5/5   | 0.86 | 0.12 | 58,65,106,138               | 0     |
| 2   | PO4  | BE    | 1001 | 5/5   | 0.86 | 0.11 | 23,28,53,142                | 0     |
| 2   | PO4  | AW    | 201  | 5/5   | 0.86 | 0.12 | 34,46,111,116               | 0     |
| 2   | PO4  | AC    | 1001 | 5/5   | 0.86 | 0.10 | 34,46,111,116               | 0     |
| 2   | PO4  | BA    | 1001 | 5/5   | 0.86 | 0.12 | 80,81,83,167                | 0     |
| 2   | PO4  | BY    | 1001 | 5/5   | 0.87 | 0.09 | 23,28,53,142                | 0     |
| 2   | PO4  | BB    | 1001 | 5/5   | 0.87 | 0.09 | 74,78,104,213               | 0     |
| 2   | PO4  | BU    | 1001 | 5/5   | 0.87 | 0.10 | 80,81,83,167                | 0     |
| 2   | PO4  | BH    | 1001 | 5/5   | 0.87 | 0.12 | 34,46,111,116               | 0     |
| 2   | PO4  | AP    | 1001 | 5/5   | 0.87 | 0.10 | 80,81,83,167                | 0     |
| 2   | PO4  | BJ    | 1001 | 5/5   | 0.88 | 0.09 | 23,28,53,142                | 0     |
| 2   | PO4  | CL    | 1201 | 5/5   | 0.88 | 0.11 | 74,78,104,213               | 0     |
| 2   | PO4  | AF    | 1001 | 5/5   | 0.88 | 0.11 | 80,81,83,167                | 0     |
| 2   | PO4  | BP    | 1001 | 5/5   | 0.88 | 0.08 | 80,81,83,167                | 0     |
| 2   | PO4  | BT    | 1001 | 5/5   | 0.89 | 0.08 | 23,28,53,142                | 0     |
| 2   | PO4  | BK    | 1001 | 5/5   | 0.89 | 0.11 | 80,81,83,167                | 0     |
| 2   | PO4  | BD    | 1001 | 5/5   | 0.89 | 0.08 | 58,65,106,138               | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | BW    | 1001 | 5/5   | 0.89 | 0.09 | 34,46,111,116               | 0     |
| 2   | PO4  | AH    | 1001 | 5/5   | 0.89 | 0.08 | 34,46,111,116               | 0     |
| 2   | PO4  | AL    | 1001 | 5/5   | 0.89 | 0.15 | 74,78,104,213               | 0     |
| 2   | PO4  | CJ    | 4201 | 5/5   | 0.89 | 0.13 | 23,28,53,142                | 0     |
| 2   | PO4  | AQ    | 1001 | 5/5   | 0.89 | 0.09 | 74,78,104,213               | 0     |
| 2   | PO4  | BQ    | 1001 | 5/5   | 0.89 | 0.10 | 74,78,104,213               | 0     |
| 2   | PO4  | AU    | 1001 | 5/5   | 0.89 | 0.15 | 80,81,83,167                | 0     |
| 2   | PO4  | AV    | 1001 | 5/5   | 0.89 | 0.10 | 74,78,104,213               | 0     |
| 2   | PO4  | A2    | 1001 | 5/5   | 0.90 | 0.09 | 34,46,111,116               | 0     |
| 2   | PO4  | BZ    | 1001 | 5/5   | 0.90 | 0.09 | 80,81,83,167                | 0     |
| 2   | PO4  | BN    | 1001 | 5/5   | 0.90 | 0.06 | 58,65,106,138               | 0     |
| 2   | PO4  | AB    | 1001 | 5/5   | 0.90 | 0.10 | 74,78,104,213               | 0     |
| 2   | PO4  | CK    | 201  | 5/5   | 0.90 | 0.08 | 80,81,83,167                | 0     |
| 2   | PO4  | B4    | 1001 | 5/5   | 0.90 | 0.07 | 23,28,53,142                | 0     |
| 2   | PO4  | CM    | 2201 | 5/5   | 0.90 | 0.10 | 34,46,111,116               | 0     |
| 2   | PO4  | AS    | 1001 | 5/5   | 0.91 | 0.12 | 58,65,106,138               | 0     |
| 2   | PO4  | CI    | 3201 | 5/5   | 0.91 | 0.08 | 58,65,106,138               | 0     |
| 2   | PO4  | AT    | 1001 | 5/5   | 0.91 | 0.08 | 23,28,53,142                | 0     |
| 2   | PO4  | AA    | 1001 | 5/5   | 0.91 | 0.10 | 80,81,83,167                | 0     |
| 2   | PO4  | AZ    | 1001 | 5/5   | 0.91 | 0.12 | 80,81,83,167                | 0     |
| 2   | PO4  | BI    | 1001 | 5/5   | 0.92 | 0.08 | 58,65,106,138               | 0     |
| 2   | PO4  | AG    | 1001 | 5/5   | 0.92 | 0.09 | 74,78,104,213               | 0     |
| 2   | PO4  | AE    | 1001 | 5/5   | 0.92 | 0.07 | 23,28,53,142                | 0     |
| 2   | PO4  | A1    | 1001 | 5/5   | 0.92 | 0.08 | 74,78,104,213               | 0     |
| 2   | PO4  | AD    | 1001 | 5/5   | 0.92 | 0.07 | 58,65,106,138               | 0     |
| 2   | PO4  | CV    | 1201 | 5/5   | 0.92 | 0.08 | 74,78,104,213               | 0     |
| 2   | PO4  | CO    | 4201 | 5/5   | 0.92 | 0.07 | 23,28,53,142                | 0     |
| 2   | PO4  | A3    | 1001 | 5/5   | 0.93 | 0.08 | 58,65,106,138               | 0     |
| 2   | PO4  | A4    | 1001 | 5/5   | 0.93 | 0.06 | 23,28,53,142                | 0     |
| 2   | PO4  | AY    | 1001 | 5/5   | 0.93 | 0.08 | 23,28,53,142                | 0     |
| 2   | PO4  | AR    | 1001 | 5/5   | 0.93 | 0.05 | 34,46,111,116               | 0     |
| 2   | PO4  | AJ    | 1001 | 5/5   | 0.94 | 0.11 | 23,28,53,142                | 0     |
| 2   | PO4  | AO    | 1001 | 5/5   | 0.94 | 0.07 | 23,28,53,142                | 0     |
| 2   | PO4  | AM    | 1001 | 5/5   | 0.94 | 0.06 | 34,46,111,116               | 0     |
| 2   | PO4  | CU    | 201  | 5/5   | 0.95 | 0.09 | 80,81,83,167                | 0     |
| 2   | PO4  | AK    | 1001 | 5/5   | 0.95 | 0.12 | 80,81,83,167                | 0     |
| 2   | PO4  | B1    | 1001 | 5/5   | 0.96 | 0.06 | 74,78,104,213               | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.